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Accurate calculations of the ground and excited state energies of the hydrogen molecule

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PREFACE

This thesis presents a computational approach to various states of hydrogen molecule isotopologues, aiming at providing high accuracy with well-controlled uncertainties.

Chapter I outlines the basic concepts used throughout the thesis. Chapter II summarizes the employed methodology, which is rooted in the variational principle, with the use of Exponential, and Gaussian, Explicitly Correlated bases. Chapter III presents the results for molecular hydrogen obtained through variational calculations in Kołos-Wolniewicz basis, including Σ, Π, Δ, and Φ symmetries with pointwise accuracy no worse than 10^{-4} cm^{-1}. Chapter IV presents how the recently established method of Nonadiabatic Perturbation Theory (NAPT), which allows for the systematic inclusion of finite-nuclear mass effects on the molecular spectra in a perturbative manner, can be applied to an arbitrary two-electron diatomic system. Then, the implementation details of the adiabatic and nonadiabatic corrections in the Kołos-Wolniewicz basis are discussed and the capabilities of the method are illustrated with a few examples. Chapter V gives a brief introduction to Nonrelativistic Quantum Electrodynamics (NRQED), emphasizing how effective Hamiltonians operating on Schrödinger wave functions are constructed. The discussion is followed by a summary of previously obtained relativistic corrections and a presentation of the results for pure heteronuclear contribution to the relativistic recoil effects. Next, we present the calculation of Born-Oppenheimer QED corrections in Explicitly Correlated Gaussian basis, which removes the numerical uncertainty of those effects from the total uncertainty budget. Chapter VI addresses some of the numerical details concerning performed calculations. An extensive set of tabulated numerical data (103 Born-Oppenheimer potentials of H_2) is presented as an Appendix.

This thesis includes results published in four articles listed below. It is augmented with many results, which did not make it into the above articles or are yet to be published.

[A1] M. Siłkowski and K. Pachucki, J. Chem. Phys. **152**, 174308 (2020).

[A2] M. Siłkowski, M. Zientkiewicz and K. Pachucki, Adv. Quant. Chem. **83**, 255 (2021).

[A3] M. Siłkowski and K. Pachucki, Mol. Phys., e2062471 (2022).

[A4] M. Siłkowski, J. Komasa, M. Puchalski and K. Pachucki, Phys. Rev. A **107**, 032807 (2023).

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ABSTRACT

The hydrogen molecule is a fascinating system, located at the intersection of simplicity hydrogen atom, an exactly solvable quantum mechanical (QM) problem, for which many subtle effects beyond QM, due to finite nuclear mass and quantum electrodynamics has been deeply studied, and large chemical molecules with additional rich structure due to rotational and vibrational degrees of freedom.

Although here we study just this one particular physical system, main results of the thesis address three substantially different aspects.

Firstly, armed with the recently developed efficient method of evaluating molecular integrals in the two-center two-electron exponential basis we pursue the decades long controversy concerning the functional form of the long-range asymptotics of the exchange energy in the two lowest states $X^1\Sigma_g^+$ and $b^3\Sigma_u^+$, which is an exponentially small effect due to Pauli exclusion principle.

Secondly, the most recent spectroscopic measurements of rovibrational transitions in HD molecule are determined with an unprecedented sub-ppb accuracy. Those are at least an order of magnitude more accurate than the current best theoretical predictions, yet the theoretical values are systematically by $1.4 - 1.9\sigma$ too small. It is currently unclear, what is the source of this discrepancy and whether the deficiency of theoretical model can be attributed to unaccounted-for, purely heteronuclear effects. To address this issue, we evaluate the leading order QED correction to the rovibrational spectra of hydrogen molecule isotopologues in its electronic ground state. Our new results do not resolve the discrepancy, but remove the uncertainty due to QED effects from the uncertainty budget of theoretical predictions and hint toward the significance of the finite nuclear mass QED effects on the order of a few MHz.

Thirdly, we address the scarcity of accurate theoretical predictions for excited states of hydrogen molecule. Even though experimental results concerning those states are plentiful, theoretical knowledge about excited states is limited to roughly about a two dozen of potential energy curves for Σ^+ symmetry and about a few less for the Π symmetry. Crucially, the accuracy of previous calculations is uncertain and those obtained concurrently by other methods are by far insufficient in view of meaningful confrontation with the modern experimental data. For symmetries corresponding to even larger angular momentum projections (Λ) our knowledge was virtually limited to two lowest $^{1,3}\Delta_g$ states.

With our computational method we demonstrate that trial basis sets of Kołos-Wolniewicz type still find a niche in high-accuracy variational calculations of excited states of a diatomic two-electron molecules and as a result we deliver a set of nearly one hundred highly-accurate Born-Oppenheimer potentials for Σ, Π, Δ, and Φ symmetry, typically with a relative accuracy better than 1 ppb. The successfulness of our method originates from a concentrated effort, summarized in a series of works lead by Prof. K. Pachucki (Supervisor of this thesis), towards efficient and versatile approach to evaluation of molecular integrals in exponential basis of two-electron diatomics.

Our results find an immediate application to the MQDT-assisted Rydberg spectroscopy of f electrons and lastly they shall provide a valuable benchmark for other computational methods.

With these results we reconcile with all the previous *ab initio* calculations of Born-Oppenheimer potentials of H_2 by elucidating the lack of accuracy of the former calculations. Numerical uncertainty of Born-Oppenheimer potentials has been alleviated from a level of a few to the millionth parts of cm^{-1}. Resultantly, we pave the way towards evaluation of higher-order corrections to the energy levels, as their absence currently hinders the comparison with state-of-the-art spectroscopic results.

ABSTRAKT

Temat rozprawy doktorskiej w języku polskim:

Precyzyjne obliczenia energii wiązania stanu podstawowego oraz stanów wzbudzonych molekuły wodoru

Cząsteczka wodoru jest fascynującym układem, znajdującym się na przecięciu prostoty atomu wodoru, ściśle rozwiązywalnego problemu mechaniki kwantowej, na którym dogłębnie zbadano wiele subtelnych efektów wynikających ze skończonej masy jądra atomowego, relatywistyki oraz elektrodynamiki kwantowej, a bogatą strukturą cząsteczek spowodowaną rotacyjnymi i wibracyjnymi stopniami swobody.

Rozprawa ta koncentruje na tym jednym układzie, ale jej główne wyniki dotyczą zasadniczo trzech różnych aspektów. Po pierwsze, przy pomocy niedawno opracowanej efektywnej metody obliczania dwucentrowych dwuelektronowych całek molekularnych w bazie wykładniczej, rozwiązany zostaje trwający od dziesięcioleci spór dotyczący wykładniczo małego efektu wynikającego z zasady wykluczenia Pauliego, dotyczący asymptotycznej postaci dalekozasięgowej energii wymiany pomiędzy dwoma najniższymi stanami cząsteczki wodoru.

Po drugie, pomiary spektroskopowe przejść rotacyjno-wibracyjnych w cząsteczce HD w ostatnich latach osiągają bezprecedensową dokładność, lepszą niż jedna część na miliard. Pomiary te są co najmniej o rząd wielkości dokładniejsze od najdokładniejszych przewidywań teoretycznych, a mimo to wartości teoretyczne są systematycznie za małe o $1.4-1.9\sigma$. Obecnie nie jest jasne, co jest źródłem tej rozbieżności i czy braki modelu teoretycznego można powiązać z nieuwzględnionymi, czysto heterojądrowymi efektami. W ramach rozprawy dokonano obliczeń poprawek wynikających z elektrodynamiki kwantowej do widm rotacyjno-wibracyjnych izotopologów cząsteczek wodoru w elektronowym stanie podstawowym. Okazało się jednak, że nowe wyniki nie rozwiązują rozbieżności, usuwają jednak one niepewność wynikającą z efektów QED z budżetu niepewności przewidywań teoretycznych i wskazują na istotność efektów QED związanych ze skończoną masą jądra atomowego na poziomie kilku MHz.

Po trzecie, rozprawa ta uzupełnia niedostatek dokładnych przewidywań teoretycznych dla stanów wzbudzonych. Poza kilkoma wyjątkami, wiedza na temat stanów wzbudzonych jest ograniczona do około kilkunastu potencjałów Borna-Oppenheimera dla symetrii Σ^+ i nieco mniej dla symetrii Π. Co istotne, dokładność poprzednich obliczeń nie jest znana, a te uzyskane innymi metodami w ostatnich latach są o zdecydowanie zbyt niskiej dokładności, aby mogły być konstruktywnie porównane ze współczesnymi danymi eksperymentalnymi. Dla symetrii odpowiadających jeszcze większym rzutom momentu pędu (Λ) wiedza jest praktycznie ograniczona do dwóch najniższych stanów o symetrii $^{1,3}\Delta_g$.

Przy pomocy metody obliczeniowej zaprezentowanej w rozprawie pokazano, że funkcje próbne Kołosa-Wolniewicza nadal znajdują niszę w obliczeniach wariacyjnych stanów wzbudzonych dwuatomowych cząsteczek dwuelektronowych. W rezultacie otrzymano ponad sto wysoce dokładnych potencjałów Borna-Oppenheimera dla symetrii Σ, Π, Δ oraz Φ, osiągając zazwyczaj dokładność względną lepszą niż jedna część na bilion. Skuteczność zaprezentowanej metody bazuje na serii prac prowadzonych przez prof. K. Pachuckiego (promotora niniejszej rozprawy), w których rozwinięto metodę wydajnego obliczania całek molekularnych w bazie wykładniczej. Uzyskane wyniki natychmiastowo znalazły zastosowanie w spektroskopii stanów rydbergowskich, a także będą stanowić cenny punkt odniesienia dla każdej innej metody obliczeniowej. W wyniku przedstawionych obliczeń, niepewność numeryczna potencjałów Borna-Oppenheimera została zmniejszona z poziomu kilku, do milionowych części cm^{-1}. W rezultacie utorowana została droga do obliczeń poprawek wyższego rzędu do poziomów energetycznych, ponieważ ich brak uniemożliwia obecnie konfrontację z najnowocześniejszymi wynikami spektroskopowymi.

CONTENTS

CHAPTER I

MOLECULAR HYDROGEN THEORY

1 Introduction

The hydrogen molecule is one of the most intensively studied two-electron system. Its rotational and vibrational energy levels in the ground electronic state are known with the relative accuracy reaching 10^{-10}. Theoretical description reaching such a precision requires inclusion of nonadiabatic effects, relativistic and quantum electrodynamic corrections up to the order of $\alpha^6\, m$, where $\alpha \sim 1/137$ is the fine-structure constant and m is the electron mass.

Theoretical predictions for the hydrogen molecule agree very well the recent high-precision measurements [1–3], including those of the dissociation energy, which reach the accuracy of 10^{-4} cm^{-1} [4–6]. Similar if not better experimental accuracy is achieved for the transitions to the excited electronic states, but theoretical predictions are far less accurate there.

Due to very recent advancements Although recent campaign imporving the accuracy of ... seems to bring this discrepancy close to 1σ, the evidence in recent measurements of transitions involving vibrationally excited states[7–13], including the sub-ppb accurate 1-0 R(0) [8] reveals consistent $\sim 2\sigma$ shift of theoretical values.

Due to the possiblity to drive weak dipole-allowed vibrational transitions the majority of the accurate measured rovibrational transitions are in the HD isotopologue. Such dipole-transition are strongly forbidden in the homonuclear isotopologues (due to ortho/para selection rules) such as H_2 and D_2 and much weaker quadrupole transitions [14] have to be involved or strong electric dipole-inducing field has to be applied [15]. Most recent measurements also point out the discrepancies (with respect to theory) in the D_2 transitions: $S_1(0)$ 0.5 MHz (1.4σ) [15] [1] $S_3(0)$ 2.2 MHz (2.6σ) and $S_4(0)$ 3.4 MHz (3.4σ), both re-

[1] Although the Authors of Ref. [15] cite 94,925,100.0(4) MHz as the theoretical value as obtained with H2SPECTRE, which leads to $\sim 1.25\sigma$ discrepancy in $S_1(0)$ overtone transition in D_2, I believe that the value

Figure I.1: recent exptheo

ported in Refs. [14, 16]. Curiously, the theoretical predictions systematically fall below the experimentally determined values, same as in HD. In this isotopologue the finite nuclear mass corrections are suppressed with respect to HD by a factor of $\mu_{\rm HD}/\mu_{\rm D_2} \approx 3/2$, however the physics of those effects might be quite different due to the lack of gerade/ungerade symmetry in HD. Resultantly, one should not expect the near ideal linear scaling of the leading-order finite nuclear mass effects with the reduced mass.

Unlike measurements, which have to be suited individually for each of the isotopologue and tackle the technical difficulties associated with the radioactivity in case of tritiated samples, the ab-initio caluclations virtually do not differ among the 6 isotopologues. In case of NAPT, some effects can be left in a form parametrized by the reduced nuclear mass, so that the mass input is required only at the very last stage of the calculations.

The agreement between theoretical calculations and state-of-the-art spectroscopy is in general very good (within 1σ interval), however recently a few notable cases of $\sim 2\sigma$ discrepancy were observed after the measurements reaching order of magnitude better accuracy than the theoretical predictions. Although one of them is in slight disagreement with the other three (with < 100 kHz uncertainty), all of those measured values are systematically higher from the theoretical prediction by 1.4-1.9σ. of transitions such as HD R(1) line in the overtone band (1-0) or

Are not only observed in the heteronuclear isotopologues, but also in the D_2, in particular the recent measurement of , which is 20 times as accurate as the theoretical prediction shows a 1.4σ discrepancy. For even higher principal quantum numbers and higher values of Λ there exists a set of data obtained using full-CI [18**? ?** –20], as well as with Free-Complement local-Schrödinger equationmethod of Nakatsuji [**? ?**]. The purpose of former was however to investigate the evolution of electronic density with internuclear distance R and explain qualitative features of PECs as its accuracy is no better than thousands of cm^{-1}. The latter results, although obtained through novel method are not of competitive accuracy, which gets dramatically worse at higher principal quantum numbers. Resultantly, with our recent works [A2] and [A3] and with yet to published results we, at least partially, answer the demand set by many experimental campaigns by providing ultra-accurate Born-Oppenheimer potentials (with pointwise accuracy no worse than 10^{-4} cm^{-1}) and auxiliary expectation values, as well as provide a computational method, which allows for a universal approach to variational calculations of highly excited states of two-electron diatomic systems.

obtained by the Authors of Ref. [15] is mistakenly higher by 50kHz due to premature rounding (probably to four or five digits) of the value as obtained in units of cm^{-1}. This can not be an issue of the precision of the conversion factor, because it is the speed of light and since 1983 it is defined in the SI units to be *exactly* 299 792 458 m/s, thus 1 cm^{-1} $= 29979.2458$ MHz. Nevertheless that shift is still two orders of magnitude smaller than the uncertainty assigned due to unknown finite nuclear mass QED effects.

2 Molecular Hamiltonian

As a starting point of treatment of the structure and energy spectrum of the hydrogen molecule, we start with the Hamiltonian formulation. The nonrelativistic Hamiltonian (in atomic units, $\hbar = c = e = m_e = 1$) for an n-electron diatomic molecule in the space-fixed coordinate system reads,

$$H = -\frac{1}{2M_A}\boldsymbol{\nabla}_A^2 - \frac{1}{2M_B}\boldsymbol{\nabla}_B^2 - \frac{1}{2}\sum_{i=1}^{n}\boldsymbol{\nabla}_i^2 + V, \tag{I.1}$$

where the subscripts A and B pertain to two nuclei and i labels the electrons. Without external fields [2] the potential operator V is simply a function of the interparticle distances and particles' charges. Consequently, one can easily separate the center of mass motion. Curiously enough, the choice of coordinates for the internal degrees of freedom is not unique. From the continuum of such coordinates systems, two sets appear to be most practical. The first one, fixed in the midpoint between two nuclei ($t = 1/2$, geometrical center)

$$\mathbf{R} \equiv \mathbf{R}_a - \mathbf{R}_b \quad \text{and} \quad \mathbf{r}_i \equiv \mathbf{r'}_i - \frac{1}{2}\left(\mathbf{R}_A + \mathbf{R}_B\right) \tag{I.2}$$

and the second one, with the origin fixed in the center of mass of the nuclei,

$$\mathbf{R} \equiv \mathbf{R}_a - \mathbf{R}_b \quad \text{and} \quad \mathbf{r}_i \equiv \mathbf{r'}_i - \frac{M_A\mathbf{R}_A + M_B\mathbf{R}_B}{M_A + M_B} \tag{I.3}$$

The transformation of the kinetic energy operator to the center of mass frame will not be repeated here as it can be found in many textbooks, the result is,

$$T \equiv -\frac{1}{2(M_A + M_B + n)}\boldsymbol{\nabla}_{XYZ}^2 - \frac{1}{2\mu_n}\boldsymbol{\nabla}_R^2 - \frac{1}{2}\sum_{i=1}^{n}\boldsymbol{\nabla}_i^2 - \frac{1}{8\mu}\left(\sum_{i=1}^{n}\boldsymbol{\nabla}_i\right)^2 + \frac{1}{2\lambda}\boldsymbol{\nabla}_R\sum_{i=1}n\boldsymbol{\nabla}_i, \tag{I.4}$$

where $\mu_n^{-1} \equiv 1/M_A + 1/M_B$ is the reduced nuclear mass and $\lambda \equiv 1/M_A - 1/M_B$ is the mass-asymmetry parameter. The expecation value of the latter term, proportional to λ can be nonvanishing only in the heteronuclear case. This can be justified simply by the definition of λ, but the expectation value of $\boldsymbol{\nabla}_R\boldsymbol{\nabla}_{\text{el}}$ also vanishes whenever the total wavefunction has the inversion symmetry with respect to the geometrical center.

The second to last term is called the mass polarization term (or specific mass shift) and is known already from the theory of few-electron atoms. The presence of this term is a chief result of the many-body separation of the motion of the center of mass (see for instance

[2]The interaction with external electromagnetic field would most conveniently be introduced at the level of Lagrangian of the system by the minimal coupling (covariant derivative) to the vector potential or by considering more general coupling by introducing so called form factors. The problem of inseparability of the internal degrees of freedom from the center of mass motion in external fields leads to interesting and nontrivial effects, especially in the context of description of bound system of particles, we refer the Reader to Refs. [21–23]

section 13.2.3 of Ref. [17]). Namely, with three of more masses, after the motion of the total center of mass is separated, one cannot separate exactly the motion as described by the internal degrees of freedom any further. Thus, such a term can be interpreted as as a mutual correlation between the motion of electrons.

With the choice of the internal coordinates fixed at the center of mass, the heteronuclear term $\boldsymbol{\nabla}_R \cdot \sum_{i=1}^{n} \boldsymbol{\nabla}_i$ is absent and the kinetic energy operator reads,

$$T_{\mathrm{CM}} \equiv -\frac{1}{2(M_A+M_B+n)}\boldsymbol{\nabla}^2_{XYZ} - \frac{1}{2\mu_n}\boldsymbol{\nabla}^2_R - \frac{1}{2}\sum_{i=1}^{n}\boldsymbol{\nabla}^2_i - \frac{1}{2(M_A+M_B)}\left(\sum_{i=1}^{n}\boldsymbol{\nabla}_i\right)^2, \tag{I.5}$$

but the electronic coordinates $\mathbf{r}_i$ are now dependent on nuclear masses, which complicates the formulas for the matrix elements, especially those involving $\boldsymbol{\nabla}_i$.

3 Born-Oppenheimer approximation

The key idea behind the Born-Oppenheimer (BO) approximation exploits the very different timescales of electrons and nuclei dynamics, which is a result of significant difference between their masses – more than 3 orders of magnitude,

$$\Psi_{\mathrm{total}} = \phi_{\mathrm{el}}\phi_{\mathrm{nucl}}. \tag{I.6}$$

The nuclear wavefunction is further factored into,

$$\phi_{\mathrm{nucl}} = \phi_{\mathrm{vibr}}\phi_{\mathrm{rot}}\phi_{\mathrm{ns}}, \tag{I.7}$$

where ϕ_{vibr} is the vibrational wavefunction, ϕ_{ns} is the spin function and in the case of a diatomic molecule the rotational wavefunction ψ_{rot} can be conveniently represented by the solution of the symmetric top (rotor). This is possible because the rotational dynamics of two-nuclei dressed by the effective potential coming from electrons can be formulated as a one-body problem with the reduced mass. Such an adiabatic factorization into vibrational and rotational wavefunction does entail that the effects of vibronic couplings are ommited and thus one considers a series of rovibrational levels belonging to exactly one electronic potential given by the BO PES. This approximation is often too crude, however performs extremely well whenever given potential energy surface is well separated on the energy scale from others, such as the case of ground electronic state of hydrogen molecule.

The effect of rotation on the vibrational motion emerges as the centrifugal potential,

$$V_{\mathrm{rot}} = \frac{1}{2\mu_n}\frac{N(N+1)}{R^2}, \tag{I.8}$$

so that the underlying equation for the vibrational wavefunction is, $\phi_{\text{vibr}} = \chi_\nu(R)/R$,

$$\left[-\frac{1}{2\mu_n}\frac{d^2}{dR^2} + V_{\text{el}} + V_{\text{rot}}\right]\chi_\nu^{(N)} = E_{\nu,N}\chi_\nu^{(N)} \tag{I.9}$$

In practice, the eigenproblem for the nuclear wavefunction, Eq. (I.9) is then pretty much always solved numerically and $E_{\nu,J}$ is the energy of the molecular level labeled by its vibrational and rotational numbers, (ν, J).

4 Beyond Born-Oppenheimer approximation

4.1 Coupled equations

The total molecular wavefunction can be expanded in a basis of electronic funcitons. (we follow the notation of Quadrelli, Dressler and Wolniewicz[**?**]).

$$\mathbf{\Psi}(\mathbf{r}, R) = \frac{1}{R}\sum_i \Psi_i(\mathbf{r}; R) f_i(R) \tag{I.10}$$

$$H' = -\frac{1}{2\mu_n}\left[\boldsymbol{\nabla}_R^2 + \frac{1}{4}\left(\boldsymbol{\nabla}_1 + \boldsymbol{\nabla}_2\right)^2\right] - \frac{1}{2\lambda}\boldsymbol{\nabla}_R\left(\boldsymbol{\nabla}_1 + \boldsymbol{\nabla}_2\right) \tag{I.11}$$

which after integration of electronic and rotational degrees of freedom leads to a set of coupled equations

$$\left\{-\frac{1}{2\mu_n}\left[\frac{d^2}{dR^2} - \frac{J(J+1)}{2R^2} + \mathbf{A}(R) + \mathbf{B}(R)\frac{d}{dR}\right] + \mathbf{U}(R) - E\right\}\mathbf{f}(R) = 0, \tag{I.12}$$

with

$$A_{ij}^{\Lambda+1,\Lambda}(R) = \frac{1}{R^2}\langle\Psi_i|\, L^+ \,|\Psi_j\rangle \left[J(J+1) - \Lambda(\Lambda+1)\right]^{1/2} \tag{I.13}$$

and

$$A_{ij}(R) = \langle\Psi_i|\, \frac{d^2}{dR^2} - \frac{L^+L^- - \Lambda(\Lambda+1)}{R^2} + \frac{1}{4}\left(\boldsymbol{\nabla}_1 + \boldsymbol{\nabla}_2\right)^2 |\Psi_j\rangle\,, \tag{I.14}$$

$$B_{ij}(R) = \langle\Psi_i|\, \frac{d}{dR}\, |\Psi_j\rangle \tag{I.15}$$

$$L_{ij}(R) = \langle\Lambda+1|\, L^+ \,|\Lambda\rangle \tag{I.16}$$

The operator L^+ raises angular momentum and couples states for which $\Delta\Lambda = \pm 1$. With the knowledge of coupling elements $A_{ij}(R)$, $B_{ij}(R)$ and $L_{ij}(R)$ one can consider Eq. (I.12) as a set of coupled equations. Ab-initio caluclations of such elements are addressed later in the thesis.

4.2 Finite nuclear mass effects

The isotopologues of the hydrogen molecule are one of the most suitable systems for studying the effect of the finite nuclear mass on the molecular transitions and dynamics. Due to the nuclei being the lightest – a proton or its isotopic variants, the effect of rovibronic interactions on the energy levels is in general the largest among all neutral molecules. Quite in general, the departure of the theoretical predictions based on the Born-Oppenheimer approximation from the experimental results is the largest whenever the contribution from the H' is significant. The reason behind the large contribution from the H' can be, however, multifold.

Two of the rotational coordinates can be trivially decoupled from the Schrödinger equationof diatomic molecule, by representing the angular momentum in the basis, in which the total angular momentum squared operator, $\mathbf{J}^2$, $\mathbf{J}_{z'}$, and $\underline{\mathrm{n}}\mathbf{J}$ are diagonal. Those operators are referred to the space-fixed coordinates (x', y', z'). Clearly, in diatomics, the latter operator is just equal to L_z the z-th component of the electronic angular momentum. Moreover, since L_z does not commute with the "nonadiabatic correction" part of the full Hamiltonian, with this representation of the angular momentum the molecular Hamiltonian cannot be simultaneously diagonal, which introduces the coupling between the equations describing different nuclear levels. Namely, on the level of adiabatic approximation, an adiabatic representation, in which nuclear movement can be introduced, which ensures uncoupling of the nuclear wavefunctions. This cannot be ensured once corrections beyond the diagonal adiabatic correction are introduced, because one cannot simultaneously impose $\langle\phi'|\,\mathbf{T}_N\,|\phi\rangle = 0$ on top of the condition defining the adiabatic basis (diagonal H_{el}).

CHAPTER II

VARIATIONAL SOLUTION OF THE SCHRÖDINGER EQUATION

This Chapter outlines the key concepts behind basis functions used in the context of variational calculations reported further in the thesis.

1 Kato's cusp condition

The *cusp* condition is the cornerstone of all the *explicitly* correlated methods [26, 27] – methods which build the interparticle (interelectron) dependence explicitly in to the functional form of the basis functions. This condition can be formulated and understood through a simple analysis of Schrödinger equation in the asymptotic region of small r_{ij}, where $r_{ij} = |\mathbf{r}_j - \mathbf{r}_i|$. The derivation crucially assumes that only i-th and j-th particles coalesce, $r_{ij} < \rho$ and all the other are far apart from both of those and from each other, $r_{ik}, \dots, r_{nk} \gg \rho$, $i, k = 3, n$. A very convenient step, facilitating the analysis, involves transforming to the frame of center of mass of particles i and j. Then, the kinetic energy transforms to,

$$-\frac{\nabla^2_{R_{ij}}}{2(m_i + m_j)} - \frac{\nabla^2_{r_{ij}}}{2\mu_{ij}} - \sum_{k=3}^{n} \frac{\nabla^2_k}{2m_k}, \tag{II.1}$$

where $\mathbf{R}_{ij} = \frac{\mathbf{r}_i m_i + \mathbf{r}_j m_j}{m_i + m_j}$, $\mathbf{r}_{ij} = \mathbf{r}_j - \mathbf{r}_i$ and $\mu_{ij} = \frac{m_i\, m_j}{m_i + m_j}$ is the reduced mass. Evidently, the lowest order term in ρ is the Coulombic interaction between i-th and j-th particle, therefore it has to be balanced by the kinetic energy term,

$$\left[\frac{\nabla^2_{r_{ij}}}{2\mu_{ij}} + \frac{z_i z_j}{r_{ij}} + O(\rho^0)\right]\Psi = 0 \tag{II.2}$$

The most general bounded solution (with $r = r_{ij}$, $\gamma = z_i z_j \mu_{ij}$) for $r < \rho$ can be written as [28]

$$\Psi = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} r^l f_{lm}(r) Y_{lm}(\theta, \phi), \tag{II.3}$$

and evaluating the action of kinetic energy term we have (separately for each f_{lm}, due to linear independence of Y_{lm},

$$\left[\frac{\partial^2}{\partial r^2} + 2\frac{l+1}{r}\frac{\partial}{\partial r} - \frac{2\gamma}{r} + O(\rho^0) \right] f_{lm}(r) = 0. \tag{II.4}$$

Because this differential equation is regular singular at $r = 0$ it must have the form of a Taylor series,

$$f_{lm}(r) = \sum_{k=0}^{\infty} f_{lm}^{(k)} r^k, \tag{II.5}$$

with nonvanishing $f_{lm}^{(0)}$. Finally, by plugging the series ansatz back into the Eq. (II.4) we have

$$(l+1) f_{lm}^{(1)} = \gamma f_{lm}^{(0)}, \tag{II.6}$$

for all l, m. In particular for singlet electron pair, the wave function satisfies,

$$\lim_{r \to 0} \frac{\partial \Psi(r=0)}{\partial r} = \gamma \Psi(r=0), \tag{II.7}$$

and called the Kato's *cusp* condition.

This first-order cusp condition is of much significance in the construction of wavefunction ansätze because it is a local and universal constraint, relating the first radial derivative at the Coulombic singularity with the value of the wave function itself. In contrast, higher-order cusp conditions relate higher-order derivatives with quantities in all of the coordinate space and are thus strongly system dependent[28–30], making them of less practical value to due to lack of universality.

2 Explicitly Correlated Exponential basis

Typical functional forms of orbital bases are smooth in the vicinity of (nucleus-electron) coalescence points. Therefore, a practical approach is to build the cusp condition into the basis a multiplicative manner. The variational calculations reported in this thesis are obtained with the use of explicitly correlated exponential functions [36] of the form,

$$\Psi_\Sigma = \sum_{\{n\}} c_{\{n\}} \left(1 \pm P_{AB}\right) \left(1 \pm P_{12}\right) \Phi_{\{n\}}, \tag{II.8}$$

where P_{AB} permutes the nuclei A and B, P_{12} interchanges the two electrons and appropriate $\pm$ signs are chosen to fulfil the symmetry criteria for *gerade*/*ungerade* and *singlet*/*triplet* states. Linear coefficients $c_{\{n\}}$ form an eigenvector, which is a solution of a secular equation. Trial wavefunctions $\Phi_{\{n\}}$ are given by,

$$\Phi_{\{n\}} \quad = \quad e^{-y\,\eta_1 - x\,\eta_2 - u\,\xi_1 - w\,\xi_2} r_{12}^{n_0}\,\eta_1^{n_1}\,\eta_2^{n_2}\,\xi_1^{n_3}\,\xi_2^{n_4}, \tag{II.9}$$

where η_i and ξ_i are proportional to confocal elliptic coordinates and are given by

$$\begin{aligned} \eta_i &= r_{iA} - r_{iB}, \\ \xi_i &= r_{iA} + r_{iB}. \end{aligned} \tag{II.10}$$

The real parameters y, x, u and w are the only one subject to variational minimization. By $\{n\}$ we denote an ordered set of interparticle coordinate exponents, $(n_0, n_1, n_2, n_3, n_4)$ which are conventionally restricted by a shell parameter Ω,

$$\sum_{j=0}^{4} n_j \leq \Omega. \tag{II.11}$$

If a symmetry restriction is imposed, the set of allowed $\{n\}$ is constrained even more.

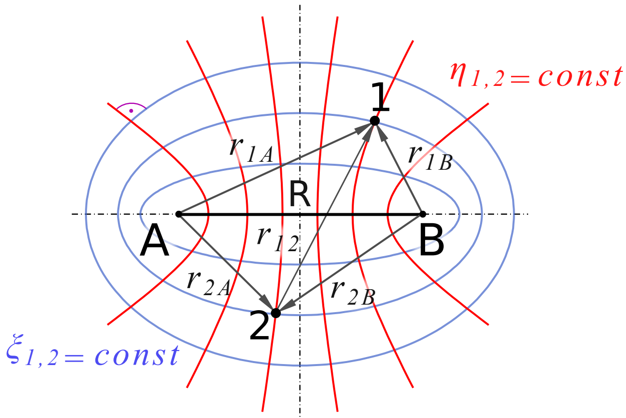


Figure II.1: Graphical representation of interparticle coordinates and confocal elliptic coordinate system.

The Kolos-Wolniewicz (KW) basis was introduced by W. Kołos and C. C. J. Roothan in the milestone companion papers of 1960 devoted to variational calculation of ground state[31, 32] and B state, its use was later mastered in a series of works by Wolniewicz and coworkers [48, 170**? ? ?**]. The initial success of Kołos-Wolniewicz basis relied on years of extensive work on molecular integrals with Slater functions by many Authors [33–35], with particular emphasis on the suitability of those methods to implement on the early computers.

An extreme case of basis set, where each element is characterized by an individual set of parameters are Explicitly Correlated Gaussians [62] or Korobov's three-body basis[**?**]. KW basis it represents the wavefunction with a polynomial, thus by construction appealing to the radial nodes encountered in excited states.

Another representation of the exponential basis can be used [? ?],

$$\Phi_{\{n\}} \quad = \quad e^{-y\,\eta_1 - x\,\eta_2 - u\,\xi_1 - w\,\xi_2} r_{12}^{n_0}\, r_{1A}^{n_1}\, r_{1B}^{n_2}\, r_{2A}^{n_3}\, r_{2B}^{n_4}, \tag{II.12}$$

which are clearly very closely related to each other through relations given by Eq. (II.10). Analogously to the Hylleraas basis, a trial wavefunction is uniquely characterized by the set of $\{n\}$ and nonlinear parameters, which are common to all trial functions within a given sector.

In the calculation of helium energy states, a major improvement in both the convergence rate and final accuracy of the nonrelativistic energy resulted from "doubling" the basis set. Doubling of the basis set is closely related to "double zeta" prescriptions, omnipresent in quantum-chemical calculations. Although many-electron systems admit a very wide range of length scales, introducing just another set of parameters associated with tailor to another length scale proves to already be very beneficial for the convergence properties of the basis. Therefore in this work we also use two sectors, each with its own nonlinear parameters, and with no additional symmetry restrictions. With Ω determining the total size of the first sector, the second sector's principal number is chosen as $\Omega - 2$, a heurestic optimum for most cases. In previous works [38, 39] concerning ground $X\,^1\Sigma_g^+$ or $b\,^3\Sigma_u^+$ states the James-Coolidge ($x = y = 0$) or generalized Heitler-London ($x = -y, u = w$) was utilized. The reasoning behind the more general basis used in this work stems from a fairly universal trend of wavefunctions being composed predominantly of $(1s, n'l)$ configurations with high values of n' and l [18, 19, 40, 41], where in the language of atomic orbitals, one electron is highly excited. This implies substantial asymmetry, $x \neq y$ and $u \neq w$, and demands a more flexible basis to accurately represent the wavefunction. In addition, the contribution of ionic configuration $(1s', 1s')$ grows more significant not only for singlet [18, 19, 42] but also for triplet symmetry [40], and there are states in the $^1\Sigma^+$ manifolds where it is essential [43] for significantly broad ranges of internuclear distances.

Justification for introducing a second sector into the basis set follows from the presence of distinct scales of motion, namely, around the nuclei and another for larger distances [44, 45]. The impact of the second sector on the convergence was thoroughly studies in calculation of helium [45]. Many previous calculations utilize specific structure of the basis, tailored for a single state or symmetry, often with *a priori* knowledge about the chemical bond character or atomic orbitals approximation. Here, we emphasize the universality of our approach – nonlinear parameters for both sectors are thoroughly optimized in an unrestricted Kolos-Wolniewicz basis [43, 46] separately for each state and every internuclear distance. This basis is capable of accurately representing ionic and covalent structure with correct long-range asymptotics and short-range vicinities of interparticle cusps, as well as complicated radial nodes, which are expected in highly excited states.

By construction these functions depend on two-electron coordinates and account for the electronic correlation via explicit dependence on the coordinate r_{12}. We emphasize that a construction of the basis according to Eq. (II.11) allows for a very compact parametrization of the basis, because it is completely specified by just four nonlinear parameters and an integer value of Ω. To recapitulate, the trial wavefunction is represented as

$$\Psi_{\Sigma^+} = \sum_{\{n\}} c_{\{n\}} \hat{S}^{\pm}_{AB} \hat{S}^{\pm}_{12} \Phi_{\{n\}}, \tag{II.13}$$

where $\hat{S}^{\pm}_{AB} = 1 \pm P_{AB}$ and P_{AB} permutes the nuclei A and B, $\hat{S}^{\pm}_{12} = 1 \pm P_{12}$ and P_{12} interchange the two electrons, and appropriate $\pm$ signs are chosen to fulfil the symmetry criteria for *gerade*/*ungerade* and *singlet*/*triplet* states. By solving the secular equation one obtains linear coefficients $c_{\{n\}}$. Such a form of wavefunction expansion is commonly referred to as the Kołos-Wolniewicz basis [37]. This nomenclature originated from the series of pioneering works of Kołos, Wolniewicz, and co-workers. It was introduced as a flexible generalization of the James-Coolidge basis aiming to represent the electron density asymmetry between the two nuclei, ubiquitous in excited states of H_2.

In previous calculations [37, 47–49] involving tens or hundreds of KW functions in the basis, the set of $\{n\}$ was carefully optimized by incremental selection of configurations that give the most significant contribution to the energy. Here we resort to a much simpler rule, given by Eq. (II.11), and introduce double basis functions with common values of nonlinear parameters. For convenience we introduce a shorthand notation for our basis $S(\Omega_A, \Omega_B)$, where S denotes a shorthand symmetry of the basis: either JC for generalized James-Coolidge ($x = y = 0, u \neq w$) [50] or KW for a general Kolos-Wolniewicz basis with no additional restrictions. Values of Ω_A and Ω_B define the size of sectors, which are the basis subsets carrying common independent nonlinear parameters and are constructed according to the Ω constraint, Eq. (II.11).

Construction of the basis by Eq. (II.11) for all the states considered in this work entails a universal and practical approach. It is expected, however, that more sophisticated selection of basis functions, in particular a subdivision into three Ω, each restricting the maximal value of exponents of η_i, ξ_i, and r_{12} individually, as investigated by Sims [51] in James-Coolidge basis or utilized in our approach to long-range exchange splitting [52], will lead to more compact wave function expansions. Although this does not seem to be a limiting factor and accurate enough energies are obtained with just a single Ω parameter per sector, it might be necessery for more complicated quantities such as radial couplings, which are very sensitive to energies of a pair of adiabatic eigenstates.

2.1 Master Integral

In the 1987, the work by D.M. Fromm and R.N. Hill presenting an analytic evaluation of three-electron (four body) exponential integral came as a surprise to atomic physics community. It addressed the problem of analytical evaluation of the class of integrals,

$$I(u_1, u_2, u_3, u_{12}, u_{23}, u_{13}) = \int \mathrm{d}^3 r_1 \mathrm{d}^3 r_2 \mathrm{d}^3 r_3 \frac{e^{-u_1 r_1 - u_2 r_2 - u_3 r_3 - u_{12} r_{12} - u_{23} r_{23} - u_{13} r_{13}}}{r_1\, r_2\, r_3\, r_{12}\, r_{23}\, r_{13}}, \tag{II.14}$$

and associated integrals with powers of interparticle coordinates $r_1, r_2, r_3, r_{12}, r_{23}, r_{13}$ raised by a natural number. The main result of the paper was to show that such integrals are expressible in terms of dilogarithms and its derivatives with respect to nonlinear parameters, $u_1, u_2, u_3, u_{12}, u_{23}, u_{13}$. Although the result was indeed a great breakthrough, giving insight into analytic properties, the practicality of this result was unclear, because the formulas were given in terms of contour integrals in the complex plane, requiring complicated branch tracking. This also made them cumbersome to implement in the computer programs. Refinements of the complicated form of the solutions were later done by Remiddi and Harris.

This generic four-body exponential integrals are the starting point towards:

- two-center two-electron (H_2, HeH^+),
- one-center three-electron integrals (Lithium),
- singly-linked four-electron Hylleraas basis (Beryllium),
- nonadiabatic generalized James-Coolidge (four-body problem) (H_2).

In the context of this thesis we are interested in the first case.

In the momentum space those integrals are given by,

$$G(m_1, m_2, m_3; m_4, m_5, m_6) \equiv \frac{1}{8\pi^6} \int \mathrm{d}^3 k_1 \mathrm{d}^3 k_2 \mathrm{d}^3 k_3 \tag{II.15}$$
$$(k_1^2 + u_1^2)^{-m_1} \, (k_2^2 + u_2^2)^{-m_2} \, (k_3^2 + u_3^2)^{-m_3} \, (k_{32}^2 + w_1^2)^{-m_4} \, (k_{13}^2 + w_2^2)^{-m_5} \, (k_{21}^2 + w_3^2)^{-m_6}$$

Fromm and Hill pursued the evaluation of this integral by its direct integration in the momentum space, while carefully keeping track of branch cuts for given nonlinear parameter combinations.

Master Integral through differential equation

In a series of papers by K. Pachucki (the supervisor of this Thesis), a completely new approach to evaluation of such integrals was pursued. It was found already by Fromm and Hill (though not directly utilized by them), that the four-body integral, satisfies the following differential equation with respect to one of the nonlinear parameters,

$$\sqrt{\sigma} \frac{\partial}{\partial w_1} (\sqrt{\sigma} g) + P\left(w_1, u_1; w_2, u_2; w_3, u_3\right) = 0, \tag{II.16}$$

with σ being the polynomial in nonlinear parameters, which has the symmetry of S_4 group (4 element permutation group),

$$\begin{aligned}\sigma = {} & u_1^2 u_2^2 w_3^2 + u_2^2 u_3^2 w_1^2 + u_1^2 u_3^2 w_2^2 + w_1^2 w_2^2 w_3^2 + u_1^2 w_1^2 \left(u_1^2 + w_1^2 - u_2^2 - u_3^2 - w_2^2 - w_3^2\right) \\ & + u_2^2 w_2^2 \left(u_2^2 + w_2^2 - u_1^2 - u_3^2 - w_1^2 - w_3^2\right) + u_3^2 w_3^2 \left(u_3^2 + w_3^2 - u_2^2 - u_1^2 - w_1^2 - w_2^2\right),\end{aligned} \tag{II.17}$$

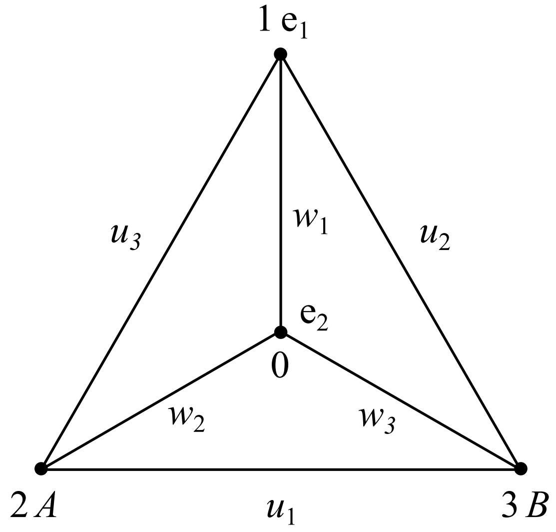


Figure II.2: Tetrahedral topology of the generic four-body integral. The vertices correspond to the particle positions in the coordinate space. The inverse Laplace transform with respect to the parameter u_1 of the generic four-body integral specializes it to the two-center two-electron case. Adapted from Ref. [53].

and the inhomogeneous term

$$
\begin{aligned}
&P\left(w_1,u_1;w_2,u_2;w_3,u_3\right)\\
&=u_1w_1\left[\left(u_1+w_2\right)^2-u_3^2\right]\tilde{\Gamma}\left(u_2+w_1,u_3,u_1+w_2\right)\\
&\quad+u_1w_1\left[\left(u_1+u_3\right)^2-w_2^2\right]\tilde{\Gamma}\left(w_1+w_3,w_2,u_1+u_3\right)\\
&\quad-\left[u_1^2w_1^2+u_2^2w_2^2-u_3^2w_3^2+w_1w_2\left(u_1^2+u_2^2-w_3^2\right)\right]\tilde{\Gamma}\left(u_1+u_2,w_3,w_1+w_2\right)\\
&\quad-\left[u_1^2w_1^2-u_2^2w_2^2+u_3^2w_3^2+w_1w_3\left(u_1^2+u_3^2-w_2^2\right)\right]\tilde{\Gamma}\left(u_1+u_3,w_2,w_1+w_3\right)\\
&\quad+\left[u_2\left(u_2+w_1\right)\left(u_1^2+u_3^2-w_2^2\right)-u_3^2\left(u_1^2+u_2^2-w_3^2\right)\right]\tilde{\Gamma}\left(u_1+w_2,u_3,u_2+w_1\right)\\
&\quad+\left[u_3\left(u_3+w_1\right)\left(u_1^2+u_2^2-w_3^2\right)-u_2^2\left(u_1^2+u_3^2-w_2^2\right)\right]\tilde{\Gamma}\left(u_1+w_3,u_2,u_3+w_1\right)\\
&\quad-w_1\left[w_2\left(u_1^2-u_2^2+w_3^2\right)+w_3\left(u_1^2+w_2^2-u_3^2\right)\right]\tilde{\Gamma}\left(u_2+u_3,w_1,w_2+w_3\right)\\
&\quad-w_1\left[u_2\left(u_1^2-w_2^2+u_3^2\right)+u_3\left(u_1^2+u_2^2-w_3^2\right)\right]\tilde{\Gamma}\left(w_2+w_3,w_1,u_2+u_3\right),
\end{aligned}
\tag{II.18}
$$

is expressed in terms of

$$\tilde{\Gamma}(\alpha,\beta,\gamma)\equiv\Gamma(0,0,-1;\alpha,\beta,\gamma), \tag{II.19}$$

where

$$\Gamma(n_1,n_2,n_3;\alpha,\beta,\gamma)\equiv\int\frac{d^3r_1}{4\pi}\,\frac{d^3r_2}{4\pi}\,r_1^{n_1-1}\,r_2^{n_2-1}\,r_{12}^{n_3-1}\,e^{-\alpha r_1-\beta r_2-\gamma r_{12}} \tag{II.20}$$

is the general two-electron (three-body) integral.

The analytic formula,

$$\tilde{\Gamma}(\alpha,\beta,\gamma) = \frac{\ln(\beta+\gamma) - \ln(\alpha+\gamma)}{(\beta-\alpha)(\alpha+\beta)}, \tag{II.21}$$

can be easily obtained by direct integration of the well-known two-electron master integral,

$$\Gamma(0,0,0;\alpha,\beta,\gamma) = \frac{1}{(\alpha+\beta)(\alpha+\gamma)(\alpha+\beta)}, \tag{II.22}$$

over the auxiliary parameter $\tilde{\gamma}$,

$$\tilde{\Gamma}(\alpha,\beta,\gamma) = -\int_0^\infty d\tilde{\gamma}\, \Gamma(0,0,0;\alpha,\beta,\gamma+\tilde{\gamma}). \tag{II.23}$$

The differential equation can be viewed as an immensely strong constraint on the analytical form of the solution, and with the proper allows to attack the problem from another angle. To relate it to the coordinate space, in particular to the two-electron two-center integrals, the connection[1] to the generic integral (**??**) is established by the inverse Laplace transform with respect to parameter u_1, see Fig. II.2,

$$f(r) = \frac{1}{2\pi i}\int_{-i\infty+\epsilon}^{i\infty+\epsilon} dt\, e^{u_1 r}\; g(u_1) \tag{II.24}$$

With analogous connection for the inhomogeneous term,

$$F(r) = \frac{1}{2\pi i}\int_{-i\infty+\epsilon}^{i\infty+\epsilon} dt\, e^{u_1 r}\; P\left(w_1,u_1;w_2,u_2;w_3,u_3\right) \tag{II.25}$$

[1]This connection is crucial from the point of view of relation of the generic four-body integral to the two-center two-electron molecular case

$$
\begin{aligned}
F(r) \;=\;& w_1\left(\frac{1}{r^2}+\frac{2\,w_1+u+w+x-y}{r}\right)e^{-r\,(u+w+w_1+x-y)} \\
&+w_1\left(\frac{1}{r^2}+\frac{2\,w_1+u+w-x+y}{r}\right)e^{-r\,(u+w+w_1-x+y)} \\
&-w_1\left(\frac{1}{r^2}+\frac{u+w-x-y}{r}\right)e^{-r\,(u+w-x-y)} \\
&-w_1\left(\frac{1}{r^2}+\frac{u+w+x+y}{r}\right)e^{-r\,(u+w+x+y)} \\
&+\left[\frac{w_1^2}{2}\,(u-w+x-y)+2\,u\,w\,(y-x)+2\,x\,y\,(w-u)\right]F_1 \\
&+\left[\frac{w_1^2}{2}\,(u-w-x+y)+2\,u\,w\,(x-y)+2\,x\,y\,(w-u)\right]F_2 \\
&+\left[\frac{w_1^2}{2}\,(u+w+x+y)+2\,u\,w\,(x+y)+2\,x\,y\,(u+w)\right]F_3 \\
&+\left[\frac{w_1^2}{2}\,(u+w-x-y)-2\,u\,w\,(x+y)+2\,x\,y\,(u+w)\right]F_4\,, \qquad \text{(II.26)}
\end{aligned}
$$

where

$$
\begin{aligned}
F_1 \;=\;& \mathrm{Ei}[-r\,(w_1+2\,u)]\,\exp[r\,(u-w+x-y)]-\mathrm{Ei}[-r\,(w_1+2\,w)]\,\exp[-r\,(u-w+x-y)]\,, \\
F_2 \;=\;& \mathrm{Ei}[-r\,(w_1+2\,u)]\,\exp[r\,(u-w-x+y)]-\mathrm{Ei}[-r\,(w_1+2\,w)]\,\exp[-r\,(u-w-x+y)]\,, \\
F_3 \;=\;& \mathrm{Ei}[-2\,r\,(u+w)]\,\exp[r\,(u+w+x+y)]+\Bigg\{\mathrm{Ei}[2\,r\,(x+y)]-\mathrm{Ei}[-r\,(w_1-2\,x)] \\
&-\mathrm{Ei}[-r\,(w_1-2\,y)]-\ln\left[\frac{(w_1+2\,u)\,(w_1+2\,w)\,(x+y)}{(u+w)\,(w_1-2\,x)\,(w_1-2\,y)}\right]\Bigg\}\,\exp[-r\,(u+w+x+y)]\,, \\
F_4 \;=\;& \mathrm{Ei}[-2\,r\,(u+w)]\,\exp[r\,(u+w-x-y)]+\Bigg\{\mathrm{Ei}[-2\,r\,(x+y)]-\mathrm{Ei}[-r\,(w_1+2\,x)] \\
&-\mathrm{Ei}[-r\,(w_1+2\,y)]-\ln\left[\frac{(w_1+2\,u)\,(w_1+2\,w)\,(x+y)}{(u+w)\,(w_1+2\,x)\,(w_1+2\,y)}\right]\Bigg\}\,\exp[-r\,(u+w-x-y)]\,,
\end{aligned}
\qquad \text{(II.27)}
$$

and Ei is the exponential integral function, we obtain the coordinate space version of the differential equation [54, 55],

$$
\left[\sigma_4\,\frac{d^2}{d\,r^2}\,r\,\frac{d^2}{d\,r^2}+\sigma_2\,\frac{d}{d\,r}\,r\,\frac{d}{d\,r}+\sigma_0\,r\right]f(r)=F(r), \qquad \text{(II.28)}
$$

where

$$\begin{aligned}
\sigma_0 &= w_1^2\,(u+w-x-y)\,(u-w+x-y)\,(u-w-x+y)\,(u+w+x+y) \\
&\quad +16\,(w\,x-u\,y)\,(u\,x-w\,y)\,(u\,w-x\,y) \\
&= \sigma_{00}+w_1^2\,\sigma_{02}\,, \\
\sigma_2 &= w_1^4-2\,w_1^2\,(u^2+w^2+x^2+y^2)+16\,u\,w\,x\,y \\
&= \sigma_{20}+w_1^2\,\sigma_{22}+w_1^4\,, \\
\sigma_4 &= w_1^2\,.
\end{aligned} \tag{II.29}$$

The function $f(r)$ is the solution of this differential equation, with r being the internuclear distance. The function $f(r)$ satisfying Eq. III.44 is called the master integral. It is not known in a closed analytical form, but it can be expressed in terms of a one-dimensional integral representation, see Refs. [55**?**] for details.

Series expansion

generated by the reduction formulas was found to be rather impractical, due to the multitude of special cases (special parameter) which require dedicated special treatment, rather than the use of generic recursion formulas. This problem was circumvented by introducing Taylor-like ansatz for $f(r)$,

$$f(r)=\sum_{n=1}^{\infty}\left[f^{(1)}(n)\,(\ln(r)+\gamma_{\rm E})+f^{(2)}(n)\right]r^n\,, \tag{II.30}$$

where $\gamma_{\rm E}$ is the Euler-Mascheroni constant. Since all the other integrals, $f(r,n_0,n_1,n_2,n_3,n_4)$, are connected to the master by the differentiation over nonlinear parameter, it is evident from the ansatz that those derivatives act only on the $f_n^{(1)}$ and $f_n^{(2)}$ coefficients, thus ansatz given by Eq. (II.30) is valid for any $f(r,n_0,n_1,n_2,n_3,n_4)$ integral.

Set of recurrences for the Taylor coefficients of the master integral (at $w_1=0$) are relatively simple,

$$f_{k+1}^{(1)}=\frac{F_k^{(1)}-\sigma_{00}f_{k-1}^{(1)}}{\sigma_{20}(k+1)^2}, \tag{II.31}$$

$$f_{k+1}^{(2)}=\frac{F_k^{(2)}-\sigma_{00}f_{k-1}^{(2)}}{\sigma_{20}(k+1)^2}-\frac{2}{k+1}f_{k+1}^{(1)}, \tag{II.32}$$

$$\tag{II.33}$$

and much more lengthy for arbitrary, n-th coefficients of the series.

2.2 Integrals with exponential correlation

As shown in the beginning of this Chapter, the form of two-center exponential basis usually assumes $w_1 = 0$. Resultantly, during the derivation of the f-integrals $w_1 \neq 0$ is kept only during intermediate steps, which vastly simplifies the evaluation of f-integrals.

Evaluation of f-integrals with non-zero w_1, thus with exponential correlation, $e^{-w_1 r_{12}}$ was previously considered in Refs. [54–56]. In Ref. [55] the scheme of evaluating f-integrals with arbitrary w_1 was presented in the context of methodology outlined in present Chapter. With the ability to evaluate such integrals, one can extended the basis set to include the exponential factor, $e^{-w_1 r_{12}}$. Although, in the actual calculations addressed throughout this Thesis, we have not observed the necessity to include the exponential correlation, as the polynomial dependence on r_{12} is by far sufficient in typical molecular calculations, we conjecture that the inclusion of such factor might become of significance in systems where short-range correlations are essential with respect to total binding energy. In particular, in weakly-bound four body matter-antimatter systems, such as H$\bar{\text{H}}$.

In previous calculations of H-$\bar{\text{H}}$ interaction curve it was recognized that the CI-type trial wave functions perform very poorly. In fact, the problem of variational calculations of H-$\bar{\text{H}}$ interaction in the Born-Oppenheimer setting was addressed by W. Kołos, D. L. Morgan, D. M. Schrader, and L. Wolniewicz a few decades ago with the methodology of exponential basis, although with relatively small basis sets. Nevertheless, the explicit correlation built into the basis was "only" a relatively low-order polynomial in r_{12}, whereas the trial wavefunction with $w_1 \neq 0$ would be able to perfectly represent the structure of the "virtual" positronium, which is described by the hydrogen-like wavefunction, $e^{-r_{12}/2}$.

Another applications, where the basis set with exponential correlation ($w_1 \neq 0$) might prove to be useful are the calculations of relativistic and QED corrections in two-electron diatomic molecules. This is justified by the singular nature of the operators comprising effective Hamiltonians for those corrections, which are very sensitive to the electronic density in the vicinity of Coulombic singularities, including the electron-electron coalescence. How impactful would the use of exponential correlation be in this context is not clear. In the further Chapters of the Thesis, we present that the appropriate scheme utilizing ECG basis enables obtaining leading-order QED corrections in H_2 with a very satisfactory accuracy. This in a way diminishes the impact and lowers the priority of developing a computational method in the exponential basis. Nevertheless, is seems plausible to assume that the correct short-range asymptotic behaviour of exponential basis would constitute an ideal tool for evaluating singular operators, which probe the wavefunction in the vicinity of Coulombic singularities and such operators are ubiquitous in all the corrections to both the energy and molecular properties beyond the nonrelativistic, adiabatic level. We emphasize though, that if the leading-order QED corrections are to be evaluated directly, even more difficult class of integrals involving -2 and even -3 power of interparticle distances has to be worked out, somewhat analogously to the singular and extended Hylleraas integrals in lithium.

2.3 Integrals with polynomial correlation

The integrals with $w_1 = 0$ are given by differentiation with respect to the corresponding nonlinear parameter, with $r = r_{AB}$,

$$f(r, n_0, n_1, n_2, n_3, n_4) = \frac{(-1)^{n_0+n_1+n_2+n_3+n_4}}{n_0!\, n_1!\, n_2!\, n_3!\, n_4!} \frac{\partial^{n_0}}{\partial w_1^{n_0}}\bigg|_{w_1=0} \frac{\partial^{n_1}}{\partial y^{n_1}} \frac{\partial^{n_2}}{\partial x^{n_2}} \frac{\partial^{n_3}}{\partial u^{n_3}} \frac{\partial^{n_4}}{\partial w^{n_4}} f(r)\,, \tag{II.34}$$

of $f(r)$, called the master integral. Therefore is still required at the intermediate steps, but the final formulas simplify considerably. The order of the differential equation satisfied by the master integral (III.44) is now lowered to two,

$$\left[\sigma_{20}\, \frac{d}{d\,r}\, r\, \frac{d}{d\,r} + \sigma_{00}\, r\right] f(r) = F(r)|_{w_1=0}\,, \tag{II.35}$$

where

$$\sigma_{00} = \sigma_0|_{w_1=0} = 16\,(w\,x - u\,y)\,(u\,x - w\,y)\,(u\,w - x\,y), \tag{II.36}$$

$$\sigma_{20} = \sigma_2|_{w_1=0} = 16\,u\,w\,x\,y. \tag{II.37}$$

The apparent simplicity of this $w_1 = 0$ case is deceiving because the inhomogeneous term $F(r)|_{w_1=0}$ is still quite complicated, an involves exponential functions, exponential integral functions Ei, and the natural logarithm, with nonlinear parameters as their arguments, see Eq. (7) of Ref. [36] for explicit expression.

Nevertheless, the general solution is now relatively simple and it can be written in terms of one-dimensional integrals over solutions of the homogeneous equation,

$$f(r) = -\frac{1}{\sigma_{20}} \left[I_0(pr) \int_r^\infty dr' F(r') K_0(pr') + K_0(pr') \int_0^r dr' F(r') I_0(pr')\right], \tag{II.38}$$

where $p^2 = \sigma_{00}/\sigma_{20}$ and I_0, K_0 are modified Bessel functions. The set of recurrences and are not extensive with the size of the shell parameter. The formulation however is not, which make use of arbitrary precision inevitable. Especially, the expansion of the inhomogeneous terms has to be of high accuracy because those enter the recursions at every step. Moreover in most cases a huge cancellation between logarithmic and nonlogarithmic part of the series can be observed, hinting at an opportunity for a better suited ansatz.

The slow convergence of the series can be connected to the distance in the complex plane to the four overlaping branch cuts, which are known to start at [55],

$$
\begin{aligned}
-t_1 &= u + y + w + x, \\
-t_2 &= u - y + w - x, \\
-t_3 &= u + y + w - x + w_1, \\
-t_4 &= u - y + w + x + w_1,
\end{aligned}
\tag{II.39}
$$

and closeness of $r = 0$, which is the point around expansion is performed, to the singularity or the branch cut might yield slow convergence of the series [57].

The recurrences (or rather reduction formulas) are quite complicated, but are obtained in an exact, closed form. In contrary to Neumann expansion or resolution of the r_{12}^{-1} kernel it does not involve infinite sums, thus completely avoid, often problematic, issues of analysing the infuence of the truncation of such sums on the completeness and convergence.

Small x, y parameters

In molecular applications, in particular with a few nonlinear parameter scales present in the basis, it may happen that the values of paramters x and y are very small. For sufficiently small value of paramter x, the f-integral can be expanded in a Taylor series around $x = 0$,

$$
f_{n_0,n_1,n_2,n_3,n_4}(y,x,u,w,r) = \sum_{k=0}^{\infty} \frac{x^k}{k!} \left(\frac{\partial}{\partial y}\right)^k \Bigg|_{y=0} f_{n_0,n_1,n_2,n_3,n_4}(y,x,u,w,r)
\tag{II.40}
$$

The workaround is implemented, based on the observation that for any x,

$$
f_{n_0,n_1+1,n_2,n_3,n_4}(y,x,u,w,r) = \left(-\frac{\partial}{\partial x}\right) f_{n_0,n_1,n_2,n_3,n_4}(y,x,u,w,r) \tag{II.41}
$$

$$
f_{n_0,n_1,n_2,n_3,n_4}(y,x,u,w,r) = \sum_{k=0}^{\infty} \frac{(-1)^k x^k}{k!} f_{n_0,n_1,n_2+k,n_3,n_4}(y,0,u,w,r) \tag{II.42}
$$

Therefore, for the case of small x one can use a special, simpler, case of recursion formulas for $x = 0$ instead of general formulas. The final values of the initial integrals with $x \neq 0$ are then given by a sum of K integrals with $x = 0$ and consecutively incremented index n_2. Clearly, in practice the Taylor series has to be truncated and be denote the number of terms used in the numerical summation as K. For evaluating the sum of the series one could apply convergence acceleation techniques instead of performing summation directly. aof integrals above the standard shell.

3 Explicitly Correlated Gaussian (ECG) basis

In general, Explicitly Correlated Gaussian function can be represented as,

$$\Psi_k(\mathbf{r}_1,\ldots,\mathbf{r}_n) = \exp\left[-\sum_{i=1,\ldots,n} a_{i,k}|\mathbf{r}_i - \mathbf{C}_{i,k}|^2 - \frac{1}{2}\sum_{i=1,\ldots,n-1}\sum_{j=i+1,\ldots,n} b_{ij,k}|\mathbf{r}_i - \mathbf{r}_j|^2\right] \tag{II.43}$$

with $\mathbf{C}_{i,k}$ being in principle, an arbitrary chosen vectors. The total wavefunction is then constructed as an appropriately symmetrized linear combination,

$$|\Psi_0\rangle = \mathcal{A}\sum_i c_i |\Psi_i(\{\alpha\}_i)\rangle, \tag{II.44}$$

where c_i are the linear parameters obtained as the solution of the secular equation and $\{\alpha\}_i$ is the set of nonlinear parameters pertaining to the i-th basis element. The product theorem is the cornerstone behind the popularity of Gaussian-type orbitals (GTOs) in quantum-chemical calculations.

An invesitgation reported in a series of works by J. Komasa and J. Rychlewski reveled that with careful optimization of nonlinear parameters, much higher accuracy of nonrelativistic energy than previously expected is achieveable with ECG basis. This observation was especially valueable in view of universality of the basis, allowing for effortless transferability of methodology to more complex systems (towards four-electron systems and further) although with the need of thorough optimization one one has to look for compromises by using geminals (GTG) and in the optimization strategy itself [58].

From now on, we focus on the two-center two-electron case[59].

$$\begin{aligned}\phi &= \sum_i c_i\phi_i(\vec{r}_1,\vec{r}_2),\\ \phi_i &= (1\pm\mathcal{P}_{A\leftrightarrow B})(1\pm\mathcal{P}_{1\leftrightarrow 2})\\ &\quad\times e^{-a_{12}r_{12}^2 - a_{1A}r_{1A}^2 - a_{1B}r_{1B}^2 - a_{2A}r_{2A}^2 - a_{2B}r_{2B}^2}.\end{aligned} \tag{II.45}$$

Direct inclusion of the interelectronic distance r_{12} in the exponent of trial wavefunction renders it a two-particle, two-center geminal, *explicitly correlated* basis.

For more extensive treatment, especially concerning the derivation of molecular integrals with ECG functions, the Reader is reffered to the pioneering milestone works by Boys [60] and Singer [61]. For more recent review of the application of ECGs to the variational calculations of a few-electron atomic and molecular systems we refer to the book by J. Rychlewski and J. Komasa. [26] as well as a review article by Mitroy *et al.*[62].

3.1 Integrals

Regular ECG integrals

The primary virtue of the ECG basis is that all the requisite integrals for calculations of nonrelativistic energy and $f(t)$ can be evaluated very efficiently. All required matrix elements can be expressed in terms of linear combinations of the following ECG integrals:

$$I(n_1, n_2, n_3, n_4, n_5) \equiv \int \frac{d^3 r_1}{\pi^{3/2}} \int \frac{d^3 r_2}{\pi^{3/2}} r_{1A}^{n_1} r_{1B}^{n_2} r_{2A}^{n_3} r_{2B}^{n_4} r_{12}^{n_5} \times e^{-a_{1A} r_{1A}^2 - a_{1B} r_{1B}^2 - a_{2A} r_{2A}^2 - a_{2B} r_{2B}^2 - a_{12} r_{12}^2}, \tag{II.46}$$

with integer n_i and real parameters a. It is clear that differentiation of this integral with respect to the given nonlinear parameter a raises the appropriate index n_i by 2. Consequently, disjoint families of ECG integrals arise. The first family is termed *regular* ECG integrals and is defined by $\Omega_1 = 0, 2, 4, \ldots$ and non-negative even integers n_i, such that $\sum_i n_i \leq \Omega_1$. Among *regular* ECG integrals, the following integral, called the *master* integral, plays a pivotal role,

$$I(0,0,0,0,0) = X^{-3/2} \, e^{-R^2 \, Y/X}, \tag{II.47}$$

where[2]

$$\begin{aligned} X &= (a_{1A} + a_{1B} + a_{12})(a_{2A} + a_{2B} + a_{12}) - a_{12}^2, && \text{(II.48)} \\ Y &= (a_{1A} + a_{1B}) \, a_{2A} \, a_{2B} + (a_{2A} + a_{2B}) \, a_{1A} \, a_{1B} \\ &+ a_{12}(a_{1A} + a_{2A})(a_{1B} + a_{2B}), && \text{(II.49)} \end{aligned}$$

because all other *regular* ECG integrals can be generated by differentiation of the master integral, $I(0,0,0,0,0)$, over a-parameters.

Due to the simplicity of X and Y (polynomial dependence on a-parameters) their derivatives are very simple. In particular,

$$\begin{aligned} \partial_{a_{1A}} X &= a_{12} + a_{2A} + a_{2B}, \\ \partial_{a_{1B}} X &= a_{12} + a_{2A} + a_{2B}, \\ \partial_{a_{2A}} X &= a_{12} + a_{1A} + a_{1B}, \\ \partial_{a_{2B}} X &= a_{12} + a_{1A} + a_{1B}, \\ \partial_{a_{12}} X &= a_{1A} + a_{1B} + a_{2A} + a_{2B} \end{aligned} \tag{II.50}$$

Note that $\partial_{a_{1A}} X = \partial_{a_{1B}} X$.

[2] From the numerical point of view, to avoid potentially unfortunate cancellation during subtraction it is beneficial to rewrite X as, $X = (a_{1A} + a_{1B})(a_{2A} + a_{2B}) + a_{12}(a_{1A} + a_{1B} + a_{2A} + a_{2B})$

Coulomb ECG integrals

Another family, *Coulomb* ECG integrals, permits a single odd index $n_i \geq -1$, with $\sum_i n_i \leq \Omega_2$ ($\Omega_2 = -1, 1, 3, \ldots$), and analogously to *regular* ECG integrals, all *Coulomb* ECG integrals can be generated by differentiation over a-parameters of appropriate master integrals,

$$I(-1_i) = \frac{1}{X\sqrt{X_i}}\, e^{-R^2\, Y/X}\, F\left[R^2\left(\frac{Y_i}{X_i} - \frac{Y}{X}\right)\right], \tag{II.51}$$

where $I(-1_i)$ denotes I with $n_i = -1$ and other indices equal zero, $X_i \equiv \partial_{a_i} X$, $Y_i \equiv \partial_{a_i} Y$, and $F(x) \equiv \mathrm{erf}(x)/x$.

Extended ECG integrals

In contrast to atomic ECG integrals, the molecular ones have no known analytic form whenever two or more indices are odd. Nevertheless, such *extended* ECG integrals arise either as a consequence of the regularization of expectation values, as described in the next Subsection, or as matrix elements of the coefficients of high-momentum asymptotic expansion of $f(t)$. Another circumstance, where integrals with three odd-indices appear is the rECG basis, which is an ECG basis augmented with the linear electron-electron cusp. In practice this involves premultiplying standard ECG trial function by $(1 + \frac{r_{12}}{2}$. Such basis is not utilized in this Thesis and interested Reader is referenced to Refs. []. In the context of hydrogen molecule calculations, such basis is crucial for efficient evaluation of the relativistic $m\alpha^4$ corrections and some of the higher-order QED $m\alpha^6$ corrections. Fortunately, such *extended* integrals can be efficiently evaluated by means of numerical quadrature. When there is no logarithm in the integrand, the quadrature relies on the following Gaussian integral transform,

$$\frac{1}{r^n} = \frac{2}{\Gamma(n/2)} \int_0^\infty dt\, t^{n-1}\, e^{-r^2 t^2},\ n > 0, \tag{II.52}$$

where the condition on the exponent n clearly results from the integrability condition around 0.

Resultantly, the integral (II.46) can be represented as

$$I(n_1 - n, n_2, n_3, n_4, n_5) = \\ \frac{2}{\Gamma(n/2)} \int_0^\infty \mathrm{d}y\, y^{n-1}\, I(n_1, n_2, n_3, n_4, n_5)\Big|_{a_{1A} \to a_{1A} + y^2}. \tag{II.53}$$

With the help of the variable transformation $y = -1 + 1/x$, which reduces the integration domain of *extended* ECG integral to a compact domain, $y \in (0, 1)$.

A variant of m-point extended Gauss-Legendre quadrature. The adjective “extended” implies that it is exact for a set of $2m$ functions, which are not necessarily polynomials, as in the case of standard Gauss-Legendre quadrature. In particular, we are interested in a variant which is exact for a set of functions, $\phi_m(x) \in \{1, x, \ldots, x^{m-1}, \ln x, \ldots, x^{m-1}\ln x\}$. Namely, the relation,

$$\int_0^1 \mathrm{d}x\, \phi(x) = \sum_i^m w_i \phi(x_i), \tag{II.54}$$

is exact for this set of functions,

$$\int_0^1 dx\big[W_1(x) + \ln(x)W_2(x)\big] = \sum_i^m w_i\big[W_1(x_i) + \ln(x_i)W_2(x_i)\big]; \tag{II.55}$$

Such a quadrature is termed "extended Gaussian quadrature" (gausext) and is suited specifically for handling integrands with the logarithmic singularities on the domain endpoint. The problem of computation of abscissae (nodes), x_i, and weights, w_i, of the gausext quadrature is more involved than in the case of standard quadratures, mainly due to lack of knowledge of the analytic formulas.

Nevertheless, by utilizing the set of $2m$ equations defining the quadrature,

$$\begin{aligned}\int_0^1 \mathrm{d}x\, x^{k-1} &= \sum_{i=1}^m w_i x_i^{k-1}, \\ \int_0^1 \mathrm{d}x\, x^{k-1}\ln x &= \sum_{i=1}^m w_i x_i^{k-1}\ln x_i,\end{aligned} \tag{II.56}$$

x_i and w_i can be obtained as the solution of this nonlinear system. Even though this system is numerically ill-conditioned, it can be solved very efficiently by iterative means, see Ref. [63] for details.

Crucially though, Ref. [63] is supplemented with a simple Mathematica script designed specifially for the purpose of determining the abscissae and weights for desired number of nodes and precision. Resultantly, practitioners can consider the problem of determining x_i and w_i for gausext quadrature to be solved. Now we have to connect it to the integrals which are the subject of this Section,

$$\begin{aligned}&I(n_1 - n, n_2, n_3, n_4, n_5) = \\ &\frac{2}{\Gamma(n/2)}\sum_{i=1}^m w_i \frac{(1-x_i)^{n-1}}{x_i^{n+1}}\, I(n_1, n_2, n_3, n_4, n_5)\bigg|_{a_{1A}\to a_{1A}+y_i^2}.\end{aligned} \tag{II.57}$$

We emphasize, the $a_{1A} \to a_{1A} + y_i^2$ substitution in the integrand. It entails that the appropriate nonlinear parameter of the $I(n_1, n_2, n_3, n_4, n_5)$ integral is shifted along the integration domain by $y_i^2 = (-1+1/x_i)^2$. This entails that the computational complexity of such a scheme to evaluate *extended* ECG integrals is substantially higher than previously described families of *regular* or *Coulomb* ECG integrals, with the complexity proportional to the complexity of evaluating given *regular* or *Coulomb*, $I(n_1, n_2, n_3, n_4, n_5)$ integral, times m – the number of quadrature nodes.

In the case of integrals involving logarithms, we utilize the following integral transforms:

$$\frac{\ln r}{r} = -\frac{1}{\sqrt{\pi}} \int_0^\infty dt \, (2 \ln t + \gamma_E + \ln 4) \, e^{-r^2 t^2}, \tag{II.58}$$
$$\frac{\ln r}{r^2} = -\int_0^\infty dt \, t \, (2 \ln t + \gamma_E) \, e^{-r^2 t^2}, \tag{II.59}$$
$$\frac{\ln r}{r^3} = -\frac{2}{\sqrt{\pi}} \int_0^\infty dt \, t^2 \, (2 \ln t + \gamma_E - 2 + \ln 4) \, e^{-r^2 t^2}. \tag{II.60}$$

This approach, based on gausext, can be straightforwardly generalized to double quadrature over Coulomb ECG integral over two different nonlinear parameters, which allows us to calculate integrals with three odd indices.

Quite in general, we have,

$$I(n_1 - k, n_2 - l, n_3, n_4, n_5) = \frac{4}{\Gamma(k/2)\Gamma(l/2)} \sum_{i=1}^{m} \sum_{j=1}^{m} w_i \, w_j \, y_i^{k-1} \, y_j^{l-1} \, I(n_1, n_2, n_3, n_4, n_5) \Big|_{\substack{a_{1A} \to a_{1A} + y_i^2 \\ a_{2A} \to a_{2A} + y_j^2}}.$$

In an analogous manner, one could also include the transforms involving the logarithm, Eq. (II.58). Such integrals arise, for example, during evaluation of large-photon momentum asymptotic coefficient of $f(t)$, f_4.

3.2 Expectation Value Identities (EVI)

It is well-known that the ECG basis cannot reproduce the correct asymptotic behavior of the wavefunction around electron-electron and electron-nucleus coalescence points (cusp conditions) and resultantly yields slow convergence of expectation values of singular operators with a very local integral kernel. The problem is even worse in conventional orbital bases, which lack explicit interelectron correlation.

The incapability of the ECG basis to satisfy the first-order cusp condition, which detriments the convergence of expectation values of such operators can be circumvented by utilizing strong operator identities, which probe the wavefunction more globally, making expectation values much less sensitive to the local deficiencies of the wavefunction [64–67].

The idea behind utilizing such identities, can probably be best illustrated on the case of the Dirac Delta function, because the following identity is of central importance to Green's functions of Poisson equation (for instance in classical electrostatics) and is known to all physicists,

$$-\nabla_i^2 \left(\frac{1}{r_{ij}} \right) = -\nabla_j^2 \left(\frac{1}{r_{ij}} \right) = 4\pi\delta(\mathbf{r}_{ij}). \tag{II.61}$$

The expectation value of $\delta(\mathbf{r}_{ij})$ is replaced by the expectation value of left-hand side of this equation and differentiation is moved onto the external wavefunctions by applying integration by parts twice.

$$\left\langle \frac{1}{r_{ij}^3} \right\rangle_\varepsilon \equiv \lim_{\varepsilon \to 0} \left[\left\langle \frac{\Theta(r_{ij} - \varepsilon)}{r_{ij}^3} \right\rangle + (\gamma_E + \ln \varepsilon) \big\langle 4\pi\delta(\vec{r}_{ij}) \big\rangle \right]. \tag{II.62}$$

The symbol γ_E denotes the Euler-Mascheroni constant, and $\Theta(x)$ is the Heaviside step function. Additionally, Dirac Delta functions are ubiquitous in atomic and molecular calculations. This result might be found to be quite instructive, since it highligths that the finite part of a singular operator, defined by $\langle r_{ij}^{-3} \rangle_\varepsilon$ must necessarily involve a counter term to render its expectation value finite.

The finite part of expectation value of r_{ij}^{-4} is defined as,

$$\left\langle \frac{1}{r_{ij}^4} \right\rangle_\varepsilon \equiv \lim_{\varepsilon \to 0} \left[\left\langle \frac{\Theta(r_{ij} - \varepsilon)}{r_{ij}^4} \right\rangle - \frac{\langle 4\pi\delta(\vec{r}_{ij}) \rangle}{\varepsilon} + 2 \left\langle 4\pi\delta(\vec{r}_{ij}) \frac{\partial}{\partial r_{ij}} \right\rangle (\gamma_E + \ln \varepsilon) \right]. \tag{II.63}$$

We note that in the term

$$\left\langle 4\pi\delta(\vec{r}_{ij}) \frac{\partial}{\partial r_{ij}} \right\rangle, \tag{II.64}$$

the derivative acts on the external wavefunction only. If preferred, its action can be moved onto the Delta function in the distributional sense by integration by parts. In any case, the derivative of the Dirac delta function can be simplified with the use of the first-order cusp condition,

$$\frac{\partial \Psi(\vec{r}_{ij} = 0)}{\partial r_{ij}} = z_i z_j \frac{m_i m_j}{m_i + m_j} \Psi(\vec{r}_{ij} = 0). \tag{II.65}$$

Which one of those forms is more useful would depend on the way this term is implemented in practice. We stress, however, that we do not need to calculate this terms for the sake of $\langle r_{ij}^{-4} \rangle_\varepsilon$, because this term results from the arbitrary separation of scales and vanishes in the limit. Consequently, it is dropped during the calculations.

In general though, one has to be catious with the implicit use of the cusp condition whenever it is used in conjuction with the dimensional regularization procedure. Namely, if the singular operator is regulated this way, the cusp condition used to simplify such a matrix element should pertain to the d-dimensional form of the Coulomb interaction and, consequently, to the d-dimensional form of the cusp condition.

For later use in the context of QED corrections we introduce the following identities for

$\delta(\mathbf{r}_{ij})$, r_{ij}^{-3}, and r_{ij}^{-4},

$$\begin{aligned}
\langle 4\pi\delta^3(\vec{r}_{ij})\rangle &= 2\mu_{ij}\left[2V_{ij}^{(1)} - R_{ij}^{(1)}\right], \\
\left\langle \frac{1}{r_{ij}^3} \right\rangle_\varepsilon &= (1+\gamma_E)\,\langle 4\pi\delta^3(\vec{r}_{ij})\rangle + 2\mu_{ij}\left[2\tilde{V}_{ij}^{(1)} - \tilde{R}_{ij}^{(1)}\right], \\
\left\langle \frac{1}{r_{ij}^4} \right\rangle_\varepsilon &= \mu_{ij}\left[-2V_{ij}^{(2)} + R_{ij}^{(2)} \pm \langle 12\pi\delta^3(\vec{r}_{ij})\rangle\right].
\end{aligned} \tag{II.66}$$

In the above, $\mu_{ij} = \frac{m_a m_b}{m_a + m_b}$ is the reduced mass of pair of particles a and b, and in the last formula '$+$' should be taken for particles with the same, and '$-$' with opposite charges, respectively. Furthermore,

$$V_{ij}^{(n)} \equiv \left\langle \frac{1}{r_{ij}^n}(E-V) \right\rangle, \tag{II.67}$$

$$\tilde{V}_{ij}^{(n)} \equiv \left\langle \frac{\ln r_{ij}}{r_{ij}^n}(E-V) \right\rangle, \tag{II.68}$$

$$R_{ij}^{(n)} \equiv -\sum_{i=1,2}\left\langle \vec{\nabla}_i \frac{1}{r_{ij}^n} \vec{\nabla}_i \right\rangle, \tag{II.69}$$

$$\tilde{R}_{ij}^{(n)} \equiv -\sum_{i=1,2}\left\langle \vec{\nabla}_i \frac{\ln r_{ij}}{r_{ij}^n} \vec{\nabla}_i \right\rangle, \tag{II.70}$$

where r_{ij} pertains to either electron-electron or electron-nucleus coordinates. This regularization procedure is pivotal for achieving well-converged, high-accuracy expectation values of singular operators with ECG functions [68, 69].

4 ECG vs KW

Optimization of the nonlinear parameters is the vital part of variational calculations and it often dominates the total computational cost. Ever since important works by Boys and Singer, the ECG were considered inferior to Slater basis, especially in the context of a few electron systems. It was until in the mid-1990s Komasa, Cencek, and Rychlewski [70–73] has proven with demanding benchmark systems, such as beryllium atom and helium dimer, that with the extensive optimization of each individual parameter of the ECG they can reach microhartee level and in the case of H_2 can even be competitive[74, 75] with the Kolos-Wolniewicz basis, where the latter was (and is) regarded to be one of the best suited for the diatomic two-electron systems. An example of performance of an extremely well optimized ECG basis and its convergence at the equilibrium distance of H_2 is illustrated in Fig. II.3.

Therefore, broadly speaking, it is computationally cheap to obtain relatively highly accurate variational results with ECG basis (or its variant with enforced linear cusp – rECG), however if only the state in interest is highly excited (either electronically or rovibra-

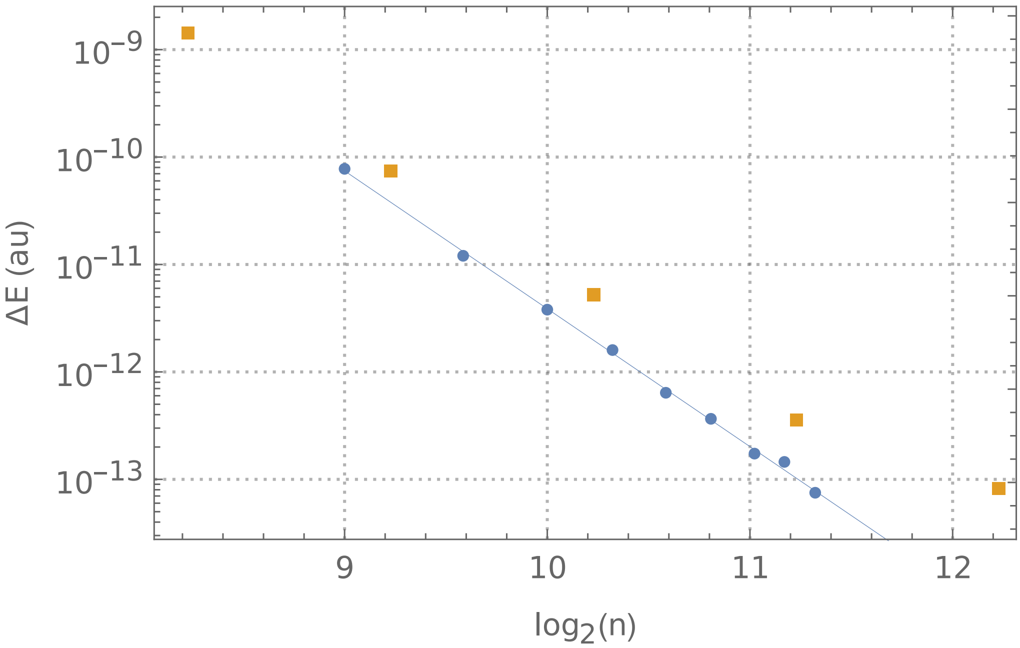


Figure II.3: Convergence of the BO energy error at the equilibrium distance of H_2, $R = 1.4011$ au (with respect to the most accurate value obtained with symmetric generalized James-Coolidge basis [38]) with the size (n) of ECG basis. Our data (blue circles) vs Cencek *et al.* [75] (orange squares). The thin line represents a linear regression fit attempt, showing that with extensive optimization of nonlinear parameters the convergence of ECG basis is exponential. With $n = 2580$ we beat the Cencek's result (Ref. [75]) obtained using $n = 4800$ basis elements, optimized in 128-bit precision arithmetics. Curiously, with extensive optimization of every nonlinear parameters even at much smaller basis sizes, such as $n = 512$, we were able to obtain the same lower bound than that of Ref. [75] with $n = 600$.

tionally in the case of fully nonadiabatic approach) or demanded relative accuracy is extremely high ($< 10^{-10}$) then KW basis usually performs better. In the context of electronically excited states, the natural ability of KW basis to represent multifold radial nodes in its wavefunction, associated with the presence of electronic configurations involving high electronic angular momenta is a decisive advantage. Methods based on ECG bases usually have to resort to extensions of the domain of its nonlinear parameters to the complex field and even then it is cumbersome to obtain highly accurate results.

The suitability of KW basis originates not only from its excellent ability to represent correct asymptotic behavior of total wavefunction near Coulombic coalescence points (short-range behavior) and on its tails, when one particle is distant (long-range behavior), but also from its extremely compact parametrization, typical to Hylleraas-like bases, which allows to easily obtain a large basis set close to an optimal one. The latter trait is in a very stark contrast to ECG bases in atomic and molecular applications, where thousands of parameters have to be optimized meticoulosly.

On the contrary, as will be shown in later Sections, when more complicated quantities are demanded, it is more practical to resort to ECG bases. Another undeniable advanatage of ECG bases is their versatility and universality, which are the reason why is similar, not explicitly correlated, variant of GTO based basis gained such a popularity in multi-electron quantum chemical calculations.

A reader familiar with atomic and molecular few-body variational calculations could notice, that the three-body basis introduced by Korobov [**?**] involves hundreds of nonlinear parameters, though parametrized by just a few in a pseudo-stochastic manner, yet its accuracy and convergence rate is usually superior to Hylleraas bases. It seems that with pseudo-stochastic approach to the choice of nonlinear parameters in the case of ECG one cannot obtain such an accuracy (or such a method is not yet known) and much more refined optimization of individual parameters is inevitable[3].

For states of Σ^+ symmetry, the overlap matrix is simply,

$$S_{kl} = I(0,0,0,0,0) \tag{II.71}$$

Kinetic energy matrix element[4]

$$\begin{aligned}
T_{kl} = &- 2b_{12}(2b_{12} + b_{1A} + b_{1B} + b_{2A} + b_{2B})\, I(0,0,0,0,2) \\
&+ 2[b_{12}(b_{1B} - b_{2B}) - b_{2B}(b_{2A} + b_{2B})]\, I(0,0,0,2,0) \\
&+ 2[b_{12}(b_{1A} - b_{2A}) - b_{2A}(b_{2A} + b_{2B})]\, I(0,0,2,0,0) \\
&- 2[b_{1B}(b_{1A} + b_{1B}) + b_{12}(b_{1B} - b_{2B})]\, I(0,2,0,0,0) \\
&- 2[b_{1A}(b_{1A} + b_{1B}) + b_{12}(b_{1A} - b_{2A})]\, I(2,0,0,0,0) \\
&+ [6b_{12} + 3b_{1A} + 3b_{1B} + 3b_{2A} + 3b_{2B} + 2b_{2A}b_{2B}\, R^2 + 2b_{1A}b_{1B}\, R^2] I(0,0,0,0,0).
\end{aligned} \tag{II.72}$$

$$\begin{aligned}
V_{kl} = &- Z_A\, I(-1,0,0,0,0) - Z_B\, I(0,-1,0,0,0) - Z_A\, I(0,0,-1,0,0) \\
&- Z_B\, I(0,0,0,-1,0) + I(0,0,0,0,-1) + \frac{Z_A\, Z_B}{R}\, I(0,0,0,0,0).
\end{aligned} \tag{II.73}$$

From those explicit formulas it is clear, that just regular ECG integrals with $\Omega = 2$ are sufficient for the kinetic energy and overlap, whereas master Coulomb integrals (with $\Omega_C = -1$) are the components of the potential matrix elements. Resultantly in the variational

In practice one is often interested in a broad range of internuclear distances, hence it is

[3] We conjecture, that this deficiency of stochastic ECG method, could probably (very coarsly) be understood with a loose analogy to Gaussian contractions, which are ubiquitious in quantum chemical calculations, where a few (or even tens) of GTOs form a linear combination, with weight chosen such that they approximate a single STO either in a geometrical sense or in terms of local energy density

[4] We note, that there is some freedom in the derivation of kinetic energy matrix element, one could implement it either as the action of both $\nabla_{\rm el}$ on the ket (as in the text) or act symmetrically, to the left on bra and to the right on ket. In practice, the difference between those variants in the well-conditioned ECG basis should be negligible, however we have noticed higher sensitivity to the way derivatives are implemented in the case of exponential basis (considered later in the text), especially in the scenarios on the verge of linear dependency.

beneficial to start on a very sparse grid in R. Ideally, to provide a somewhat deterministic[5] approach to the construction of the basis, one would start with well optimized basis at the dissociation limit ($R \to \infty$) and at united-atom limit ($R = 0$) limit and then use those bases as a starting point, for the optimization process along the R-grid, inwards and outwards, respectively. Unfortunately, it is nontrivial how to handle the process of splitting one-center basis into a two-center one. For the long-range however, one could follow the idea put forth by M. Puchalski [private communication] and start with the basis optimized for a properly symmetrized product of two monomers A and B. In the actual implementation this amounts to removing any interaction between the monomers, in case of H_2 the remaining interaction is simply,

$$V_{\text{mono}} = -\frac{Z_A}{r_{1A}} - \frac{Z_B}{r_{2B}}. \tag{II.74}$$

During the optimization the constraint,

$$a_{1B} = a_{2A} = a_{12} = 0, \tag{II.75}$$

is enforced in all the monomer basis elements. The variational energy limit of such a basis is clearly equal to twice the nonrelativistic binding energy of hydrogen atom, thus $E_{\text{mono}} = -1\ a.u.$ After such a basis is converged, the full interaction is enabled and it is used as a starting point for high-R. Another route is to include such a monomer basis without removing the constraint (II.75) and allow the rest of the basis to account for the monomer interaction.

In the context of nonadiabatic bases, naECG basis struggle to reach relative accuracy better than 10^{-10}. Typically this is not at all a decisive limitation in case of higher-order corrections, because much lower relative accuracy is sufficient. The dissocation energy of ground rovibrational state (D_0) of the hydrogen molecule isotopologues is a prominent example where an unprecedented relative numerical accuracy (10^{-15}) was achieved, which led to elimination from the total uncertainty budget the uncertainty originating from the finiteness of the nuclear mass on the nonrelativistic binding energy.

[5] It would not be truly deterministic because nonlinear parameters of new basis element(s) are drawn randomly.

CHAPTER III

ELECTRONIC STATES OF THE HYDROGEN MOLECULE

In this Chapter we follow the chronological order of research done during the PhD studies. We start with addressing the decades long controversy concerning the functional form of the asymptotic exchange energy in two lowest states of H_2. Then we follow with the application of Kolos-Wolniewicz basis to variational calculations of Born-Oppenheimer potentials of Σ^+, Π, Δ, and Φ symmetry ($\Lambda = 0, \ldots, 3$). Results presented here are in part the subject of works [A1], [A2], and [A3].

1 Long-range asymptotics of the exchange energy

The following Section is based on work [A1]. It addresses the decades-long controversy concerning the functional form of the leading order long-range asymptotics of the exchange energy in the ground state of hydrogen molecule[1].

1.1 Introduction

The calculations of molecular properties like rovibrational energies and various relativistic effects are routinely performed at small internuclear distances R. Numerical results with standard available quantum mechanical codes are not guaranteed to be accurate for large R, especially for exponentially small quantities. While the use of exponential functions with explicit electron correlations has become the natural choice for an approach with correct wave function asymptotics, no efficient method to perform corresponding integrals has been developed. Namely, the original calculations of Kołos and Roothaan [76] with exponential functions were an extension of earlier developments by Podolanski [77]

[1] Which was brought to our attention by Prof. B. Jeziorski

and Rüdenberg [78]. Their method was based on Neumann expansion of the $1/r_{12}$ term in spheroidal coordinates, which has a very slow numerical convergence. In spite of this, a few years later Kołos and Wolniewicz [79] were able to obtain for the time very accurate Born-Oppenheimer energies. This was a remarkable breakthrough in the field of precision molecular structure. Thus far, however, no accurate results for exchange energy have been obtained for large internuclear distances[2]. For this reason the discrepancies between conflicting analytic results have not yet been resolved.

From the point of view of instanton analysis for H_2^+, the electron is treated classically in the inverted potential. Thus along its classical trajectoriy they spend the majority of time in the vicinity of maxima, thus it seems that the classical action should be insensitive to the shape of the potential around the midplane. This holds true for the considerations about the exponential factor $\sim e^{-2R}$, but the R-dependent prefactor is actually sensitive to the details of the potential in the intermediate region because in the instanton picture it can be seen as arising from small fluctuations around the classical path.

We emphasize that all the approaches based on the instanton action pertain to single particle tunnelling. Precisely how, such an analysis can be extended to a multi-particle case is far from obvious and the literature is very scarce. All of this makes analysis of long-range asymptotics of the exchange much more complicated conceptually than in the single electron case of H_2^+ (which is already far from simple), because it involves the exchange of two-particles, hence depends on nontrivial electronic correlation while the internuclear separation is very large. It is conjectured that the exchange of two electrons must happen simultaneously[3] and interelecronic correlation is important in the process. In particular, an overly simplified picture of two independent electrons tunnelling in the potential of two nuclei, would just result in the leading term being twice the leading term of H_2^+, thus equal to $R^2 e^{-2R}$.

If one constructs the wave functions as a linear combination of nucleus-centered atomic orbitals (for example as Heitler-London orbital), their overlap vanishes exponentially $\sim e^{-R}$ when centered on different nuclei. The gerade and ungerade wave functions although very similar near the nuclei are very different in the vicinity of the inversion point, see Fig. III.1, and it is unclear, what this difference is as a function of R.

The hydrogen molecule is the most basic model of molecular bonding theory, therefore concerns raised here, can be considered as a model case for more complex phenomena of electron tunneling, by extension, to more complex molecules, where the tunnelling, especially simultaneous tunnelling of multiple electrons is a significant reaction channel. Indeed, there are some rare cases, where unlike most reactions, which can be described on the by either kinetic or thermodynamic control are dominated by the tunnelling rate. In the literature, reactions involving the tunneling of not only an electron, but whole H atom or even atoms as heavy as nitrogen. Such gain significance in cold chemistry, because in the temperatures of tens of kelvins all other reaction channels are frozen out.

[2] A notable exception are variational calculations by Kołos and Wolniewicz themselves [80]. From the context of the present work, it seems that both the accuracy and internuclear distances considered there were too low to support any of the analytic expansions

[3] Meaning that the contribution from ionic structres like H^+H^- and H^-H^+ is not important.

Before going into detail, let us introduce the notion of the exchange energy. The hydrogen molecule, assuming clamped nuclei, is described by the electronic wave function, which can be symmetric or antisymmetric with respect to the exchange of electrons and with respect to inversion through the geometrical center. For a large internuclear separation, the symmetry of the wave function does not matter, and one has two separate hydrogen atoms. It means that the difference between symmetric and antisymmetric state energies has to be exponentially small. Indeed, this splitting behaves as e^{-2R}, but the question remains concerning the prefactor. If we assume that the wave function is just a product of two properly symmetrized hydrogen orbitals, the so-called Heitler-London wave function [81], then the splitting is of the form given by Eq. (III.5), which is known to be invalid, even with regard to its sign [82]. It means that, even for large internuclear distances, one cannot assume that the electronic wave function is a symmetrized product of hydrogenic ones. Therefore, the asymptotics of the exchange energy and the functional form of the wave function that reproduces this asymptotic behavior is an interesting problem.

There are conflicting results among analytic calculations of the exchange energy for the leading term, and there are no conclusive results for subleading ones. The problem seems to be so difficult that no successful attempts to resolve these discrepancies have been reported so far. In this work, we develop a numerical approach to calculate the exchange energy at large internuclear distances with well controlled numerical accuracy. To achieve this, we employed a large basis of exponential functions of the generalized Heitler-London form with an arbitrary polynomial in all interparticle distances. We have previously developed an efficient recursive approach to calculate integrals with two-center exponential functions [36], and demonstrated its advantages by the most accurate calculation of Born-Oppenheimer (BO) energies for the hydrogen molecule. In this work, we use an efficient parallel version of linear algebra [83**?**] in an arbitrary precision arithmetic to fully control the precision of the exchange energy. For example, about 230-digit arithmetic is utilized at the largest internuclear separations of 57.5 au to obtain six significant digits of the exchange energy out of 50 digits for the total energy. To our knowledge, there is no better approach available that will give the exchange energy with full control of the numerical precision. In fact, the widely used Symmetry Adapted Perturbation Theory (SAPT) method [84], which aims to extract the exchange energy contribution in a perturbative manner, has pathologically slow convergence [85, 86] for large internuclear distances, and its results are far from accurate.

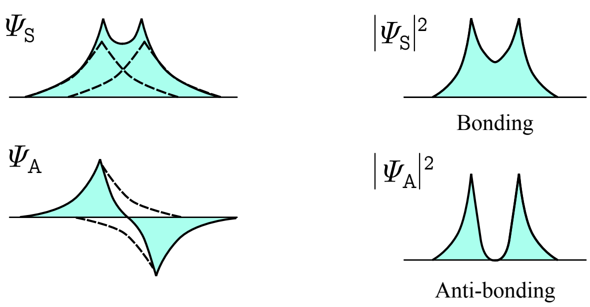


Figure III.1: gu

1.2 Formulation of the problem

Let us consider a stationary Schrödinger equation for two electrons with positions given by $\vec{r}_1$ and $\vec{r}_2$ in the H_2 molecule in the BO approximation with internuclear separation R,

$$H\Psi_g(\vec{r}_1, \vec{r}_2) = E_g(R)\Psi_g(\vec{r}_1, \vec{r}_2), \tag{III.1}$$

$$H\Psi_u(\vec{r}_1, \vec{r}_2) = E_u(R)\Psi_u(\vec{r}_1, \vec{r}_2), \tag{III.2}$$

where subscripts g and u denote *gerade* and *ungerade* symmetry under the inversion with respect to the geometrical center. They correspond to the ground electronic states with a total spin $S = 0$ and $S = 1$. H in the above equation is the nonrelativistic Hamiltonian of the hydrogen molecule with clamped nuclei,

$$H = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{1}{r_{1A}} - \frac{1}{r_{1B}} - \frac{1}{r_{2A}} - \frac{1}{r_{2B}} + \frac{1}{r_{12}} + \frac{1}{R}. \tag{III.3}$$

Within the BO approximation, one considers only the electronic part of the wave function of the system, and thus R serves as a parameter for electronic energies. The difference between these energies,

$$\Delta E = E_{\mathrm{u}} - E_{\mathrm{g}}, \tag{III.4}$$

is the *energy splitting*, and half of this splitting with the minus sign, $J = -\Delta E/2$, was the exchange energy according to the definition used in previous works. In this work, we always refer to ΔE and convert results of the previous works from J to ΔE. Consequently, we use the exchange energy as a synonym of the energy splitting.

The pioneering theory of Heitler and London [81] was one of the first attempts to explain chemical bonding [87] on the grounds of the freshly established foundations of quantum mechanics. Their method was based on approximation of the wave functions corresponding to the lowest energy states of H_2 with symmetrized and antisymmetrized products of the exact hydrogen atom solutions. This approach was pursued in the same year by Sugiura [88] who derived Born-Oppenheimer energies of the lowest gerade and ungerade states as a function of R. The asymptotic value for the energy splitting based on Sugiura [88] reads,

$$\begin{aligned}\Delta E_{\mathrm{HL}}(R) \quad &= \quad 2\left[\frac{28}{45} - \frac{2}{15}\left(\ln R + \gamma_E\right)\right] R^3 \exp(-2R) \\ &\quad + \mathcal{O}\left(R^2 \exp(-2R)\right),\end{aligned} \tag{III.5}$$

where $\gamma_E = 0.577\,215...$ is the Euler-Mascheroni constant.

The Heitler-London approach appeared plausible because it provided a reasonable mechanism of chemical bond formation and its comparison with the results of ab-initio numerical calculations [76] obtained later was satisfactory. Nevertheless, its long-range asymptotics is inherently flawed based on mathematical grounds. Analysis of Eq. (III.5) reveals that the asymptotic behavior of ΔE in Heitler-London theory becomes unacceptable, due to the logarithmic term being dominant as $R \to \infty$. As a consequence, for sufficiently large R ($\approx$ 60 au) the energy splitting becomes negative. The negative sign of $\Delta E_{\mathrm{HL}}(R)$ contradicts the well-established theorem on Sturm-Liouville operators with homogeneous boundary conditions stating that the lowest energy eigenstate should be nodeless in the coordinate space.

Many years later, it was recognized that the Heitler-London approach underestimates electron correlations [82], and the logarithmic term in Eq. (III.5) could be identified with a potential coming from the *exchange* charge distribution. This line of reasoning led to conjectures (see Refs. [89–91]) that the correct asymptotics might be in the same form as Heitler-London if only the logarithmic term is appropriately suppressed (e.g. via proper treatment of electron correlations). Indeed, Burrows *et al.* [91], on the grounds of algebraic perturbation theory [92], have derived their formula for the long-range asymptotics of the splitting

$$\Delta E_{\mathrm{BDC}}(R) = R^3 e^{-2R}\left(\gamma_{\mathrm{BDC}} + \mathcal{O}\left(\frac{1}{R}\right)\right), \tag{III.6}$$

with $\gamma_{\mathrm{BDC}} = 0.301\,672...$, a result similar to the Heitler-London result given by Eq. (III.5) aside from the unphysical logarithmic term.

A completely different line of reasoning was introduced by Gor'kov and Pitaevskii [93], followed only a few months later by a very similar method by Herring and Flicker [94]. They both used a kind of quasiclassical approximation for the wave function to derive its asymptotic form, and with the help of a surface integral summarized by Eq. (III.9), they obtained the exchange energy. A mistake in the numerical coefficient of the leading term in the former was indicated and corrected in the latter paper [94], and their final result is

$$\Delta E_{\mathrm{HF}} = \gamma_{\mathrm{HF}} R^{5/2} \exp(-2R) + \mathcal{O}\left(R^2 \exp(-2R)\right), \tag{III.7}$$

with the leading order coefficient

$$\gamma_{\mathrm{HF}} = 1.636\,572\,063\ldots \tag{III.8}$$

Accounting for the asymptotic wave function requires careful analysis of various regions of the 6-dimensional space (see for instance Ref. [94]). With the increasing internuclear distance the exact wave function approaches a symmetrized or antisymmetrized product of two isolated hydrogen atom solutions. Nonetheless, the exact way in which this limit is approached is of paramount importance for the asymptotics of exchange energy, as has been thoroughly discussed with the case of Heitler-London theory in Ref. [82]. In comparison to analytic approaches for H_2^+ [95–98], examination of asymptotic energy splitting in H_2 is substantially more challenging due to electron-electron correlation, and it is prone to mistakes, as made evident by the presence of conflicting results in the literature [90, 91, 93, 94], compare Eqs. (III.6) and (III.7).

1.3 Derivation of the leading asymptotics

To our knowledge, all of the analytic derivations presented in Refs. [89–94, 99, 100] ultimately rely on the Surface Integral Method (SIM), also referred to in the literature as the Smirnov [?] or Holstein-Herring [101] method. Here we follow the work of Gor'kov and Pitaevskii [93] to present the SIM and the derivation of the asymptotic exchange energy in Eq. (III.7). This derivation lacks mathematical rigor but nevertheless helped us to understand the crucial behavior of the asymptotic wave function. Moreover, their asymptotics is confirmed by our numerical calculations, which is only twice the uncertainty ($2\,\sigma$) away from their analytical value.

Let us assume that nuclei are on the z-axis with $z = a, -a$, $(R = 2\,a)$, and let Ω be half of the 6-dimensional space with $z_2 \geq z_1$, and Σ is a boundary of Ω, namely 5-dimensional space with $z_1 = z_2$. Consider the following integral

$$\begin{aligned}
&(E_g - E_u)\int_\Omega d^3r_1\, d^3r_2\, \Psi_g\, \Psi_u \\
&= \frac{1}{2}\int_\Omega d^3r_1\, d^3r_2\, \big[\Psi_g\,(\Delta_1 + \Delta_2)\,\Psi_u - \Psi_u\,(\Delta_1 + \Delta_2)\,\Psi_g\big] \\
&= \int_\Omega d^3r_1\, d^3r_2\, \vec\nabla_1\big[\Psi_g\,\vec\nabla_1\,\Psi_u - \Psi_u\,\vec\nabla_1\,\Psi_g\big] \\
&= \oint_\Sigma d\vec S\,\big[\Psi_g\,\vec\nabla_1\,\Psi_u - \Psi_u\,\vec\nabla_1\,\Psi_g\big]. \qquad \text{(III.9)}
\end{aligned}$$

which allows us to express the energy splitting in terms of a surface integral with Ψ_g and Ψ_u functions. Let us introduce a combination of these functions

$$\Psi_1 = \frac{1}{\sqrt{2}}(\Psi_g + \Psi_u), \qquad \text{(III.10)}$$

$$\Psi_2 = \frac{1}{\sqrt{2}}(\Psi_g - \Psi_u), \qquad \text{(III.11)}$$

with the respective phase chosen in a manner such that $\Psi_{1,2}$ are real and correspond to an electron localized at a specific nucleus, namely

$$\Psi_1 \approx \frac{1}{\pi}\, e^{-|\vec r_1 + \vec a| - |\vec r_2 - \vec a|}, \quad \text{for } \vec r_1 \to -\vec a;\ \vec r_2 \to \vec a \qquad \text{(III.12)}$$

$$\Psi_2 \approx \frac{1}{\pi}\, e^{-|\vec r_1 - \vec a| - |\vec r_2 + \vec a|}, \quad \text{for } \vec r_1 \to \vec a;\ \vec r_2 \to -\vec a \qquad \text{(III.13)}$$

and the $\Psi_{g/u}$ functions are normalized to 1. The left-hand side of Eq. (III.9) can be transformed to

$$\begin{aligned}
\int_\Omega d^3r_1\, d^3r_2\, \Psi_g \Psi_u &= \frac{1}{2}\int_\Omega d^3r_1\, d^3r_2 \big[\Psi_g^2 + \Psi_u^2 - (\Psi_g - \Psi_u)^2\big] \\
&= \frac{1}{2} - \int_\Omega d^3r_1\, d^3r_2\, \Psi_2^2 \qquad \text{(III.14)}
\end{aligned}$$

and the right hand side to

$$\begin{aligned}
&\oint_\Sigma d\vec{S}\,\big[\Psi_g\,\vec{\nabla}_1\,\Psi_u - \Psi_u\,\vec{\nabla}_1\,\Psi_g\big] \\
&= \oint_\Sigma d\vec{S}\,\big[\Psi_2\,\vec{\nabla}_1\,\Psi_1 - \Psi_1\,\vec{\nabla}_1\,\Psi_2\big]. \qquad \text{(III.15)}
\end{aligned}$$

As a result, one obtains

$$E_g - E_u = \frac{2\,\oint_\Sigma d\vec{S}\,\big[\Psi_2\,\vec{\nabla}_1\,\Psi_1 - \Psi_1\,\vec{\nabla}_1\,\Psi_2\big]}{1 - 2\,\int_\Omega dV\,\Psi_2^2}. \qquad \text{(III.16)}$$

The second term in the denominator is exponentially small, and thus can be safely neglected. By virtue of Eq. (III.16), the knowledge of the wave function and its derivative on Σ is sufficient to retrieve the energy splitting. The advantage of this method manifests itself especially in the regime of large internuclear distance, where exact wave functions of singlet and triplet states are close to the appropriately symmetrized and antisymmetrized products of the isolated hydrogen atom solutions.

Below we closely follow the procedure of Ref. [93] and correct several misprints there. Let us assume the following ansatz of the wave functions $\Psi_{1/2}$

$$\Psi_1(\vec{r}_1,\vec{r}_2) = \frac{\chi_1(\vec{r}_1,\vec{r}_2)}{\pi}\,e^{-|\vec{r}_1+\vec{a}|-|\vec{r}_2-\vec{a}|}, \qquad \text{(III.17)}$$

$$\Psi_2(\vec{r}_1,\vec{r}_2) = \frac{\chi_2(\vec{r}_1,\vec{r}_2)}{\pi}\,e^{-|\vec{r}_1-\vec{a}|-|\vec{r}_2+\vec{a}|}, \qquad \text{(III.18)}$$

where the functions $\chi_{1/2}$ change slowly in comparison to the exponential terms. Let us consider the region of $z_1 \approx a$, $z_2 \approx -a$ and $\rho_1, \rho_2 \sim \sqrt{a}$ where the exponentials become

$$\begin{aligned}
&e^{-|\vec{r}_1+\vec{a}|-|\vec{r}_2-\vec{a}|} \\
&\sim \exp\Big\{-2\,a - z_1 + z_2 - \frac{\rho_1^2}{2\,(a+z_1)} - \frac{\rho_2^2}{2\,(a-z_2)}\Big\}, \qquad \text{(III.19)}
\end{aligned}$$

and ρ_i is the perpendicular distance of i-th electron from the internuclear axis. From the Schrödinger equation one obtains for χ_1

$$\left[\frac{\partial}{\partial z_1} - \frac{\partial}{\partial z_2} + \frac{1}{2\,a} - \frac{1}{a-z_1} - \frac{1}{a+z_2} + \frac{1}{|\vec{r}_1-\vec{r}_2|}\right]\chi_1 = 0, \qquad \text{(III.20)}$$

where higher order $O(1/\sqrt{a})$ terms are neglected. Introducing $z_1 = (\xi+\eta)/2$ and $z_2 = (\xi-\eta)/2$, this equation takes the form

$$\left[\frac{\partial}{\partial \eta} - \frac{1}{2\,a-\xi-\eta} - \frac{1}{2\,a+\xi-\eta} + \frac{1}{2\,\sqrt{\eta^2+\rho_{12}^2}} + \frac{1}{4\,a}\right]\chi_1 = 0, \qquad \text{(III.21)}$$

and the general solution is

$$\chi_1 = C(\xi,\rho_{12})\, e^{-\frac{\eta}{4\,a}}\, \frac{\sqrt{\sqrt{\eta^2+\rho_{12}^2}-\eta}}{(2\,a-\xi-\eta)\,(2\,a+\xi-\eta)}, \tag{III.22}$$

up to the unknown function $C(\xi,\rho_{12})$. This function, which is not a rigorous argument, is determined from the condition that whenever $\vec{r}_1 \approx -\vec{a}$ or $\vec{r}_2 \approx \vec{a}$ the wave function Ψ_1 should be just exponential, and thus $\chi_1 = 1$ in this region. This argument can be justified because for $\vec{r}_1 \approx -\vec{a}$, the second electron interacts dominantly with its nucleus. From this condition one obtains

$$\begin{aligned}\Psi_1(\vec{r}_1,\vec{r}_2) = {} & \frac{2\,a\,(2\,a-|z_1+z_2|)}{\pi\,(a-z_1)(a+z_1)}\,\exp\!\left(-2\,a-z_1+z_2-\frac{\rho_1^2}{2\,(a+z_1)}-\frac{\rho_2^2}{2\,(a-z_2)}\right)\\ & \times\sqrt{\frac{\sqrt{(z_1-z_2)^2+\rho_{12}^2}+z_2-z_1}{\sqrt{(2\,a-|z_1+z_2|)^2+\rho_{12}^2}+2\,a-|z_1+z_2|}}\,\exp\!\left(-\frac{1}{2}+\frac{z_2-z_1+|z_1+z_2|}{4\,a}\right).\end{aligned} \tag{III.23}$$

The function Ψ_2 is obtained by the replacement $\vec{r}_1 \leftrightarrow \vec{r}_2$. The appearance of ρ_{12} in the wave functions Ψ_1 is in crucial distinction to the Heitler-London wave function and ensures the correct sign of the leading order asymptotics for all distances, as pointed out in Ref. [102]. Ψ_1, however, is not differentiable at $z_1 + z_2 = 0$ and this is one of the reasons we were not able to fully accept this derivation. A similar problem appears in a later derivation of Herring and Flicker [94] and this lack of analyticity at $z_1 + z_2 = 0$ was somehow ignored in all the previous works. One may even ask, why this nonanalytic wave function should give the right asymptotics, and here we show that, indeed, $\gamma\, R^{5/2}\, e^{-2\,R}$ behavior is in agreement with our numerical calculations, although γ is 2σ away.

Let us now return to Eq. (III.16) to obtain the energy splitting from the above Ψ_i. Because $\chi_{1/2}$ is slowly changing in comparison to dominant exponentials, their derivative can be neglected, and the splitting becomes

$$E_g - E_u = -8\int_0^a dz\, d^2\rho_1 d^2\rho_2\; \Psi_2\,\Psi_1\Big|_{z_1=z_2=z}, \tag{III.24}$$

where

$$\Psi_2\,\Psi_1\Big|_{z_1=z_2=z>0} = \frac{(2a)^2\,\rho_{12}\,e^{-4a-1}}{\pi^2(a-z)(a+z)^2}\,e^{\frac{z}{a}+\frac{a(\rho_1^2+\rho_2^2)}{z^2-a^2}}, \tag{III.25}$$

where only the leading terms in the limit of a large a are retained. Integrals over $\vec{\rho}_1$, $\vec{\rho}_2$ yield

$$\int \mathrm{d}^2\rho_1\mathrm{d}^2\rho_2\;\rho_{12}e^{-\alpha(\rho_1^2+\rho_2^2)} = \pi^2\sqrt{\frac{\pi}{2}}\alpha^{-5/2}. \tag{III.26}$$

As a result one is left with the one-dimensional z-integral

$$E_g - E_u = -32e^{-4a-1}\sqrt{\frac{\pi}{2a}}\int_0^a dz\, e^{z/a}(a-z)^{3/2}(a+z)^{1/2}, \tag{III.27}$$

which after change of a variable $q = 1 - z/a$ yields

$$E_g - E_u = -16\sqrt{2\pi}a^{5/2}e^{-4a}\int_0^1 dq\, e^{-q}q^{3/2}(2-q)^{1/2}. \tag{III.28}$$

After noting that $a = \frac{R}{2}$, this result

$$\gamma = 4\sqrt{\pi}\int_0^1 dq\, e^{-q}\, q^{3/2}\,(2-q)^{1/2} \tag{III.29}$$

coincides with Eq. (19) of Ref. [94] and this integration yields $\gamma = \gamma_{\mathrm{HF}}$. The numerical value $\gamma = \gamma_{\mathrm{HF}}$ from Eq. (III.8) will be verified in the next subsections by direct numerical calculations of the exchange energy.

1.4 Variational approach

Our numerical approach to this problem is variational with the use of generalized Heitler-London type trial basis. Due to symmetry of both singlet and triplet state, one type of exponent is used in the wave function, because the ionic structures like H^+H^-, which correspond to a different choice of the exponent $e^{-r_{1A}-r_{1B}}$, are subdominant in our problem, as was already discussed in Ref. [82], and thus they can be omitted. Because of this a single nonlinear parameter $y = -x = u = w = \alpha$, ($\alpha \approx 1/2$) describing the basis is sufficient, as it resembles a properly symmetrized product of two hydrogen atom ground state orbitals, except for the polynomial dependence on the interparticle coordinates.

In the simplest implementation of the variational approach one solves the Schrödinger equation by representing the wave function as a linear combination of some basis functions and finds linear coefficients with nonlinear parameters fixed. Because we are interested in the large-R asymptotics of the exchange energy, the only viable option is to employ the exponential basis. This ensures the short-range *cusp conditions* [103] and correct long-range asymptotic behavior of the trial wave function. Consequently, the basis of trial functions is chosen in the following form corresponding to separated Heitler-London orbitals, but generalized by allowing an arbitrary polynomial in elliptic coordinates.

$$\begin{aligned}\phi \;=\; & \sum_{\{n_i\}} c_{\{n_i\}}(1 \pm P_{AB})\,(1 \pm P_{12})\, e^{-r_{1A}-r_{2B}} \\ & \times r_{12}^{n_1}\,\eta_1^{n_2}\,\eta_2^{n_3}\,\xi_1^{n_4}\,\xi_2^{n_5},\end{aligned} \tag{III.30}$$

where

$$\eta_i = r_{iA} - r_{iB},\; \xi_i = r_{iA} + r_{iB}, \tag{III.31}$$

and where P_{AB} and P_{12} represent operators enforcing symmetry with respect to the permutation $r_A \leftrightarrow r_B$ and $r_1 \leftrightarrow r_2$.

It is tempting to assume that the sum over non-negative integer indices n_i is chosen such that for the so-called shell number Ω

$$\sum_{i=1}^{5} n_i \leq \Omega, \tag{III.32}$$

because it gives a good numerical convergence for the total binding energy. However, the main problem here is the very low numerical convergence of the exchange energy [**?**] at large internuclear distances R with the increasing size of the basis as given by Ω. It was the main reason that previous numerical attempts were not very successful.

We notice that for $R \to \infty$, the main contribution to the numerator of the surface integral in Eq. (III.16) comes from the integration over the neighborhood of the internuclear axis. We thus anticipate that the crucial behavior of the wave function is encoded in $\eta_{1,2}$. Consequently, a basis is constructed using three independent shell parameters, such that the sum of powers of $\eta_{1,2}$, $\xi_{1,2}$, and r_{12} are controlled by corresponding shell numbers Ω_A, Ω_B, and Ω_C

$$n_2 + n_3 \leq \Omega_A, \;\; n_4 + n_5 \leq \Omega_B, \;\; n_1 \leq \Omega_C, \tag{III.33}$$

and numerical convergence is attained by incrementing just one shell parameter, while keeping other fixed.

Matrix elements of the nonrelativistic Hamiltonian in this basis can be expressed in terms of direct and exchange integrals of the form

$$\begin{aligned} f_{\{n_i\}}(R) = R \int \frac{d^3 r_1}{4\,\pi} \int \frac{d^3 r_2}{4\,\pi} \, & \frac{e^{\alpha\,\eta_1 - \alpha\,\eta_2 - \alpha\,\xi_1 - \alpha\,\xi_2}}{r_{1A}\, r_{1B}\, r_{2A}\, r_{2B}} \\ & \times r_{12}^{n_1}\, \eta_1^{n_2}\, \eta_2^{n_3}\, \xi_1^{n_4}\, \xi_2^{n_5}, \end{aligned} \tag{III.34}$$

with non-negative integers n_i, which are the special case of f-integrals described in Section **??**.

Having constructed the Hamiltonian and overlap matrices, the energy and linear coefficients $c_{n_0 \ldots n_4}$ are determined by the secular equation,

$$\det\left[\left\langle n_1 \ldots n_5 \middle| H \middle| n_1' \ldots n_5' \right\rangle - E \left\langle n_1 \ldots n_5 \middle| n_1' \ldots n_5' \right\rangle\right] = 0. \tag{III.35}$$

It has to be solved separately for E_g and E_u. Consequently, to retrieve an exponentially small difference between eigenvalues for large internuclear distances, employment of extended-precision arithmetic is inevitable.

The generalized eigenproblem in Eq. (III.35) is solved with the help of the Shifted Inverse Power Method. At each iteration the linear system has to be solved to refine the initial eigenvalue estimation, which is done via calculation of the exact Cholesky factor of the $H - ES$ matrix, where H is the Hamiltonian and S the overlap matrix. A significant drawback of the applied basis is the fact that those matrices are dense, far from diagonally dominant and near-singular, especially for large R. This specific structure of matrices in the explicitly correlated exponential basis does not allow for straightforward application of iterative (e.g. Krylov-like) methods. Computation of the exact inverse Cholesky factor proved to be a suitable approach, providing cubic convergence.[4] A crucial advantage of this method is that the Cholesky factor has to be computed only once and can be reused in every iteration. The main drawback of performing full Cholesky factorization is its algorithmic complexity. It requires $n^3/3$ arithmetic operations in arbitrary precision, which eventually becomes a bottleneck of the whole calculation. Total computation time can be significantly reduced when Cholesky factorization is parallelized. We found that our implementation of procedure HSL_MP54 for dense Cholesky factorization from the HSL library [**? ?**] adopted to arbitrary precision performed best in terms of performance and accuracy.

Relying on our previous calculations of the Born-Oppenheimer potential for H_2 [38] and anticipating that variational calculations will follow one of the analytic results for the leading asymptotics of energy splitting, $\Delta E_{\mathrm{BCD}}(R) \sim\ R^3 e^{-2R}$ or $\Delta E_{\mathrm{HF}}(R) \sim\ R^{5/2} e^{-2R}$ with the coefficient of order of unity, the accuracy goal in decimal digits can be estimated as $\lceil \log_{10}(\Delta E) \rceil + n$. It is the number of correct digits in E_g and E_u required to obtain the difference between them on n last significant digits. In the extreme case of the internuclear distance $R = 57.5$ au, approximately 50 correct digits in the final numerical value of E_g and E_u are required. Consequently, solving generalized eigenvalue problems for E_g and E_u requires incorporation of arbitrary precision software. We have found the MPFR library [**?**] to be robust and provide the best performance among all the publicly available arbitrary-precision software.

1.5 Numerical results

It is crucial to properly choose the Ω parameters of the basis, in order to obtain sufficiently accurate exchange energy. If we assume $\Omega_B = \Omega_C = 0$, i.e. we allow only for a nontrivial dependence in η_1 and η_2, the energy splitting has a very low numerical convergence in Ω_A, and thus this shell parameter has to be sufficiently large to saturate the splitting. An essential feature of exponential function basis, other than the desired analytical behavior, is its exponential convergence to the complete basis set (CBS) limit, i.e. the $\log$ of differences of energies calculated for subsequent values of Ω are very well fitted to the linear function. By virtue of this property, extrapolation to the CBS limit is straightforward and reliable. Interestingly, we observe analogous behavior for the energy splittings, which entails,

$$\frac{\Delta E\left(\Omega_A\right) - \Delta E\left(\Omega_A - 1\right)}{\Delta E\left(\Omega_A - 1\right) - \Delta E\left(\Omega_A - 2\right)} = \mathrm{const}\,. \tag{III.36}$$

[4] To be exact, the proof that the convergence is in fact cubic, assumes that the value of the shift is also updated with each iteration, for more details see for instance the series of papers by M. Ostrowski [A. M. OSTROWSKI, On the convergence of the Rayleigh quotient iteration for the computation of the characteristic roots and vectors. I, II, III, IV, V and VI, Arch. Rational Mech. Anal., 1 (1958), pp. 233-241; 2 (1958/9), pp. 423-428; 3 (1959), pp. 325-340; 3 (1959), pp. 341-347; 3 (1959), pp. 472-481; 4 (1959), pp. 153-165.] and Jensen [https://www.jstor.org/stable/2156212]. In the actual implementation, updating the value of the spectral shift would be counterproductive because it would require additional factorizations, which are costly. On top of that, usually the actual, physical, eigenvalue is known apriori with good enough accuracy.

Consequently, extrapolation to the CBS limit can be performed by linear regression of the logarithm of energy splitting increments,

$$\log\left(\Delta E\left(\Omega_A\right) - \Delta E\left(\Omega_A - 1\right)\right) = \alpha - \beta\,\Omega_A. \tag{III.37}$$

The obtained coefficient β varies from $0.121(2)$ for $R = 20.0$, $\Omega_A = 40$ down to $0.0366(2)$ for $R = 57.5$, $\Omega_A = 145$.

At the largest considered nuclear distance of 57.5 au saturation was achieved with Ω_A as large as 145. This explains why previous numerical attempts were not successful. In fact, the only correct results were obtained in a previous work by one of us (KP) in Ref. [38], but those calculations were performed only for internuclear distances up to $R = 20$ au.

In contrast, numerical convergence in Ω_C is very fast. We performed calculations with increasing values of Ω_A and Ω_C shell parameters, but with $\Omega_B = 0$ up to $R = 57.5$. At first, saturation is achieved in the Ω_A parameter, and subsequently Ω_C is raised. Although such a basis has a multiplicative structure, a value as small as $\Omega_C = 4$ was sufficient to achieve the claimed numerical precision. Extrapolation is analogous as described above for the basis with $\Omega_C = 0$. Corresponding numerical results for bases with saturation in Ω_A and Ω_C are presented in the fourth column of Table III.1.

Table III.1: Dependence of energy splitting $\Delta E = E_u - E_g$ scaled by factor $R^{-5/2}e^{2R}$ on shell parameters at different internuclear distances R [au]. The first column presents ΔE as obtained with $\Omega_B = 0, \Omega_C = 0$, i.e. with no explicit correlation in the basis. The second is Δ, the difference in energy splitting between $\Omega_B = \Omega_C = 0$ basis and $\Omega_C \neq 0$ basis, and the third column is its value as extrapolated in Ω_C, still with Ω_B fixed at zero. The fourth column shows a correction δ to ΔE due to $\Omega_B \neq 0$, and the last column is the total energy splitting. Uncertainty of $\Delta E(\Omega_B = 0, \Omega_C = 0)$, Δ and δ come from extrapolation in Ω_A, Ω_C, and Ω_B, respectively, and were obtained as described in the text.

R	$\Delta E(\Omega_B = 0, \Omega_C = 0)$	Δ	$\Delta E(\Omega_B = 0)$	δ	ΔE
20.0	1.418 595 21(9)	0.138 969 8(18)	1.557 565 0(18)	-0.006 16(27)	1.551 41(27)
22.5	1.409 067 90(8)	0.140 756 3(20)	1.549 824 2(20)	-0.004 76(22)	1.545 06(22)
25.0	1.402 295 96(8)	0.142 648 3(22)	1.544 944 3(22)	-0.003 69(18)	1.541 25(18)
27.5	1.397 382 94(7)	0.144 560 8(24)	1.541 943 7(24)	-0.002 86(15)	1.539 09(15)
30.0	1.393 761 45(5)	0.146 451 2(26)	1.540 212 6(26)	-0.002 21(12)	1.538 00(12)
32.5	1.391 067 28(5)	0.148 290 4(28)	1.539 357 7(28)	-0.001 711(97)	1.537 646(97)
35.0	1.389 047 31(5)	0.150 069 3(30)	1.539 116 6(30)	-0.001 324(79)	1.537 792(79)
37.5	1.387 530 09(5)	0.151 780 1(32)	1.539 310 2(32)	-0.001 025(64)	1.538 285(64)
40.0	1.386 391 69(5)	0.153 422 3(34)	1.539 814 0(34)	-0.000 794(51)	1.539 020(51)
42.5	1.385 542 54(5)	0.154 995 7(35)	1.540 538 2(35)	-0.000 614(41)	1.539 924(41)
45.0	1.384 916 73(4)	0.156 503 7(37)	1.541 420 4(37)	-0.000 476(33)	1.540 945(33)
47.5	1.384 464 91(3)	0.157 947 4(39)	1.542 412 3(39)	-0.000 368(27)	1.542 044(27)
50.0	1.384 149 48(3)	0.159 332 5(41)	1.543 482 0(41)	-0.000 285(21)	1.543 197(21)
52.5	1.383 941 70(2)	0.160 660 9(44)	1.544 602 6(44)	-0.000 221(17)	1.544 382(18)
55.0	1.383 819 27(2)	0.161 931 6(45)	1.545 750 9(45)	-0.000 171(14)	1.545 580(15)
57.5	1.383 764 60(2)	0.163 109(31)	1.546 874(31)	-0.000 132(11)	1.546 742(33)

The only exception is the case of $R = 57.5$ au, for which only $\Omega_C = 3$ was technically feasible, which is reflected in higher uncertainty due to extrapolation in the Ω_C parameter. The limiting factor was the available computer memory of 2TB, which was exhausted by recursive derivation of integrals with extended-precision arithmetic.

The numerical convergence in Ω_B is relatively slow, but the crucial point is that the numerical significance of the basis functions with $n_4 + n_5 > 0$ becomes exponentially small in the limit of large internuclear distance R. Therefore, we calculate $\delta = R^{-5/2}e^{2R}\left[\Delta E - \Delta E\left(\Omega_B = 0\right)\right]$ using the single shell parameter Ω as in Eq. (III.32) for all values of internuclear distances up to $R = 35$, which was the upper limit set by the available computer memory. The resulting δ, as a function of R, is very well fitted to the exponential functions of the form $\alpha\, e^{-\beta\, R}$ with $\alpha = -0.0477(8)$ and $\beta = 0.1025(9)$, and we use this fit to obtain extrapolated δ for internuclear distances $R > 35$ au, as shown in Table I. This demonstrates that the correct asymptotics of the exchange energy can be obtained using basis functions with $n_4 + n_5 = 0$ only. Nevertheless, the influence of functions with $n_4 + n_5 > 0$ is included in order to obtain a complete numerical result for the exchange energy at individual values of R.

The final results for the splitting, presented in the last column of Table III.1, are obtained as a sum of $\Delta E(\Omega_B = 0)$ and δ. In view of the limitations of the available computer memory and reasonable computation times, we were able to perform calculations in $\Omega_B = 0$ basis for R up to 57.5 au. To illustrate the computational cost of these calculations, at $R = 57.5$ au, the largest internuclear distance presented, $\Omega_A = 145$, was required for saturation, which amounts to solving a dense eigenproblem in approximately 230 decimal-digit precision with basis size $N \sim 27500$.

1.6 Numerical fit of the asymptotic expansion

A brief analysis of numerical results gathered in Table III.1 and depicted in Fig. III.2 reveals that even after rescaling by a factor of $R^{-5/2}e^{2R}$ numerical data are still distant from γ in Eq. (III.8). Nevertheless, around $R = 35$ au monotonicity changes and convergence of $R^{-5/2}\, e^{2\,R}\, \Delta E(R)$ to the constant γ can be observed. In order to provide comprehensive analysis by performing a numerical fit, an important conclusion from the Herring-Flicker work [94] should be recalled, i.e. that the next asymptotic term should be of the relative order $1/\sqrt{R}$, not $1/R$. This conclusion is also supported by the derivation of Gor'kov and Pitaevskii presented in Sec. III. The considered relatively wide region of internuclear distances enforces accounting for at least 3 or 4 terms of asymptotic series to properly model the observed dependence. The result for the leading term depends on the length of the fitting expansion, but converges to the same value with an increasing number of points used for fitting, see Fig. III.3. Taking this into account, and the number of terms in the asymptotic series, we can estimate the leading coefficient to be $1.663(14)$, which is 2σ away from the Herring-Flicker value in Eq. (III.8), where we use the convention that the number in parentheses is the uncertainty denoted in the text by σ. This uncertainty is obtained by studying fits of various lengths to variable numbers of points and is chosen very conservatively. Because the original calculations in Refs. [93, 94] lack mathematical

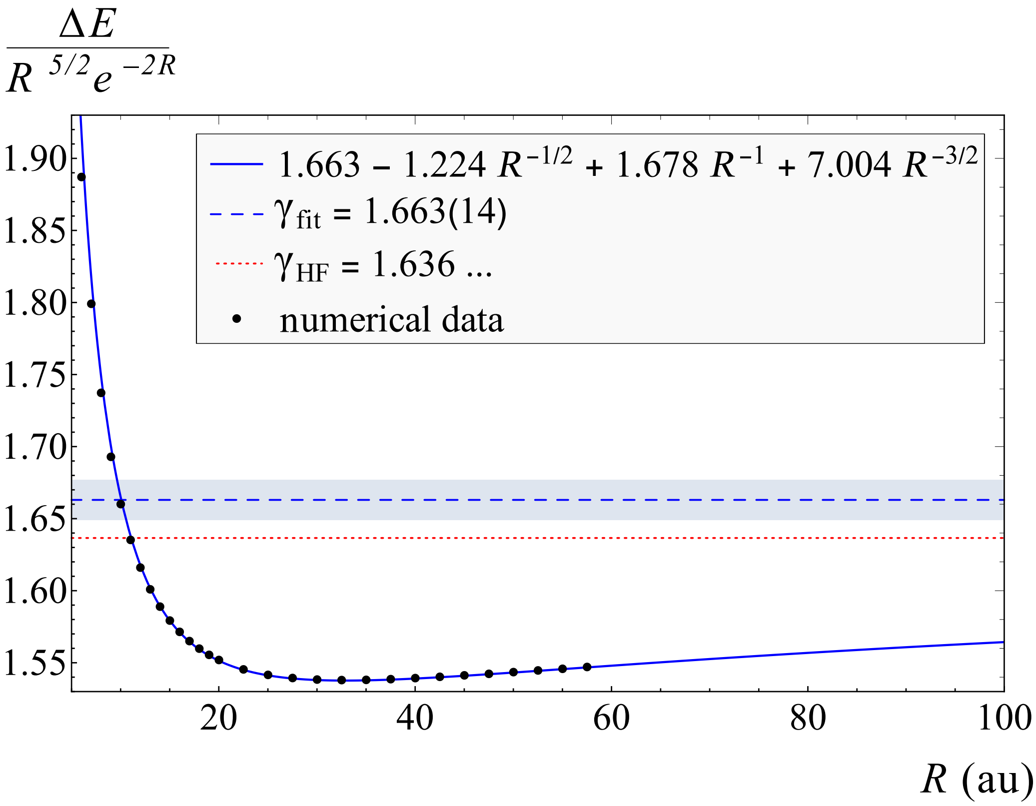


Figure III.2: Rescaled energy splitting $R^{-5/2}\, e^{2\,R}\, \Delta E$, fitted to numerical points in Table III.1 in the range $R = 20 - 57.5$ au, Herring and Flicker [94] asymptotics is the red horizontal dotted line, fitted γ is blue dashed line and light blue shaded region represents values within the uncertainty $\sigma = 0.014$ of γ. Results for $R \in (6, 19)$ au are taken from Ref. [38] for completeness but were not used for fitting. Values of higher order coefficients are presented without any uncertainties because they strongly depend on the length of the expansion. They are shown to represent the actual fitting function.

rigour and the asymptotic wave function is non-differentiable at $z_1 = -z_2$, the value of the asymptotics might be not fully correct.

Nonetheless, by assuming correctness of the Herring-Flicker value, which amounts to fixing $\gamma = \gamma_{\mathrm{HF}}$, and subsequent fitting in powers of $1/\sqrt{R}$, a coefficient for the next-to-leading, $R^2 e^{-2R}$, term can be estimated as $-0.66(7)$, which is significant, as conjectured by Hirschfelder and Meath [**?**]. This value is in disagreement with the work of Andreev [99], in which the next non-vanishing term is claimed to be $R^{3/2}\, e^{-2\,R}$.

It is perhaps more convenient to present numerical results and the fit as a function of $1/\sqrt{R}$, see Fig. III.4. Then it becomes more evident, that the calculated numerical values are sufficient to obtain the leading coefficient, and the polynomial fit should consist of at least 3 or 4 terms to properly model the numerical data.

Curiously, in the aforementioned $\Omega_B = \Omega_C = 0$ basis, the rescaled exchange splitting $R^{-5/2} e^{2R} \Delta E$ quickly and monotonically converges as a function of R, to a constant value of $\gamma_0 = 1.3835(2)$. Therefore, even in a basis with no powers of r_{12}, leading asymptotic

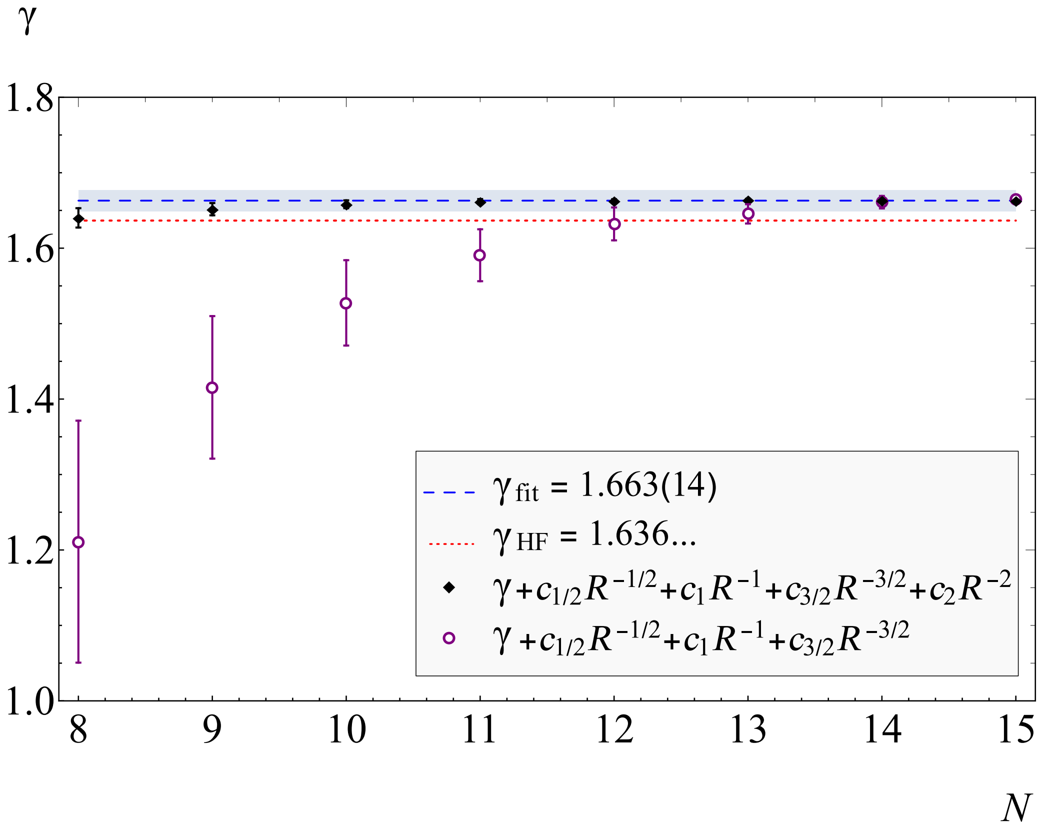


Figure III.3: Dependence of the leading coefficient in a fit to the rescaled energy splitting $R^{-5/2}\, e^{2\,R}\, \Delta E$, as a function of the number of last numerical data points used for fitting. Error bars represent standard deviation of the leading coefficient resulting from linear regression.

behavior could be achieved, although with the slightly smaller coefficient γ_0. Inclusion of higher powers of r_{12} brings this constant close to γ_{HF}, but even for the largest distances considered in the calculations, numerical points are still distant from the asymptotic constant, as presented in Fig. III.2.

Considering the result of Ref. [91], their leading asymptotics seems to be in significant disagreement with our numerical data, see Fig. III.5. This asymptotics, even with inclusion of a few higher order terms, cannot match our numerical data. Nevertheless, if one assumes the leading asymptotics of the form $R^3\, e^{-2R}$, although with the unknown coefficient, the results of the fit of a polynomial in $1/R$ strongly depend on the length of the fitting series and the number of points used for fitting. The obtained coefficients are abnormally large and have an alternating sign. This is an indication of improper choice of fitting function. If, nevetheless, one assumes $R^3 e^{-2R}$ asymptotics and fits a similar polynomial in $1/\sqrt{R}$ as in Fig. III.2 to the rescaled energy, one obtains

$$R^{-5/2}\, e^{2\,R}\, \Delta E = 0.000\,06(83) R^{1/2} + 1.662 - 1.212\, R^{-1/2} \\ + 1.632\, R^{-1} - 7.070\, R^{-3/2}\,. \tag{III.38}$$

The leading coefficient is consistent with 0, what is in disagreement with γ_{BDC} from

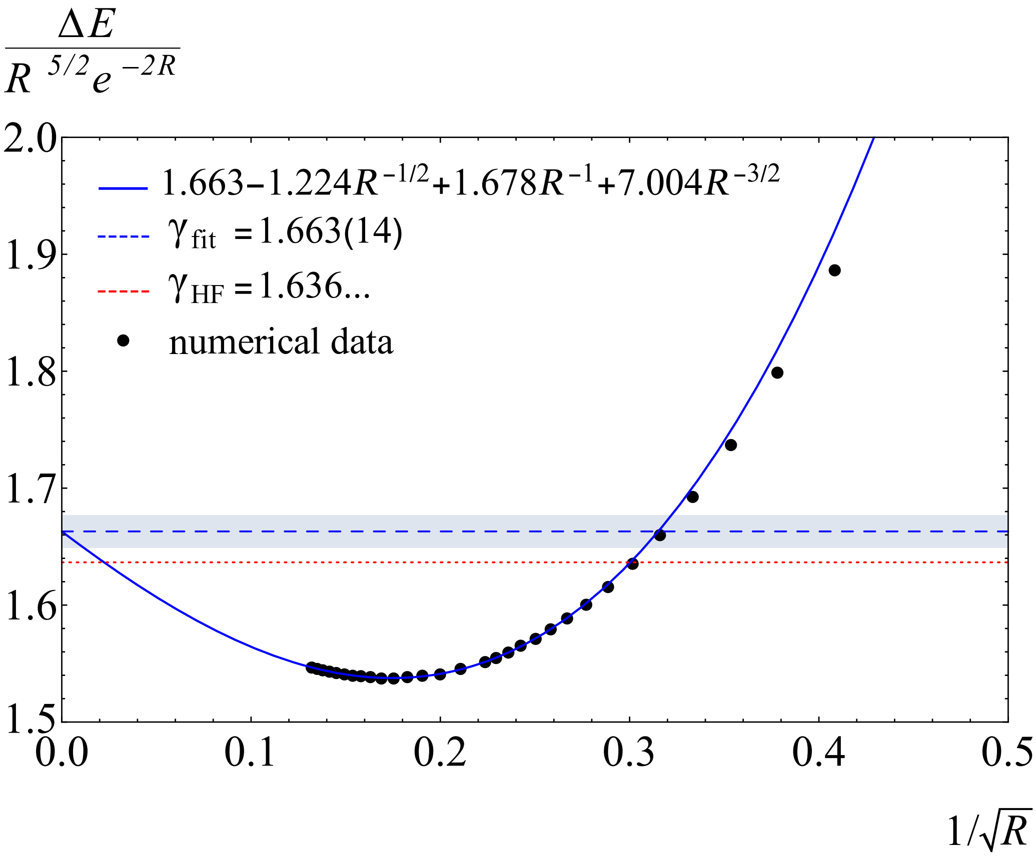


Figure III.4: Rescaled energy splitting $R^{-5/2}\, e^{2\,R}\, \Delta E$, fitted to numerical points in Table III.1 in the range $R = 20 - 57.5$ au, the same as in Fig. III.2, but represented as a function of $1/\sqrt{R}$.

Ref. [91]. This disagreement is even more pronounced when numerical results are confronted with the asymptotics of Ref. [91] in Fig. III.5.

1.7 Conclusions

The high numerical accuracy for the exchange energy is achieved owing not only to the correct asymptotic behavior of explicitly correlated exponential functions, but also due to the specific choice of the basis functions suggested by the significance of the internuclear axis neighborhood. Regardless of the relatively limited range of internuclear distances at $R \leq 57.5$ au, due to this high numerical accuracy, we were able to resolve the long-standing discrepancy between long-range asymptotics. Our results are in agreement with $\gamma\, R^{5/2}\, e^{-2\,R}$ asymptotics, although our numerically fitted γ is 2σ away from the Herring-Flicker value $\gamma_{\rm HF}$. Notably, fits of different lengths converge to the same γ, as shown in Fig. III.3, while the fit to $R^3\, e^{-2\,R}$ asymptotics gives a very small coefficient, consistent with 0 and in strong disagreement with $\gamma_{\rm BDC}$. This disagreement becomes more evident when the asymptotics from Ref. [91] is confronted with our numerical results in Fig. III.5.

In the future the Eq. (III.21) could be tackled numerically for fixed values of ξ to gain in-

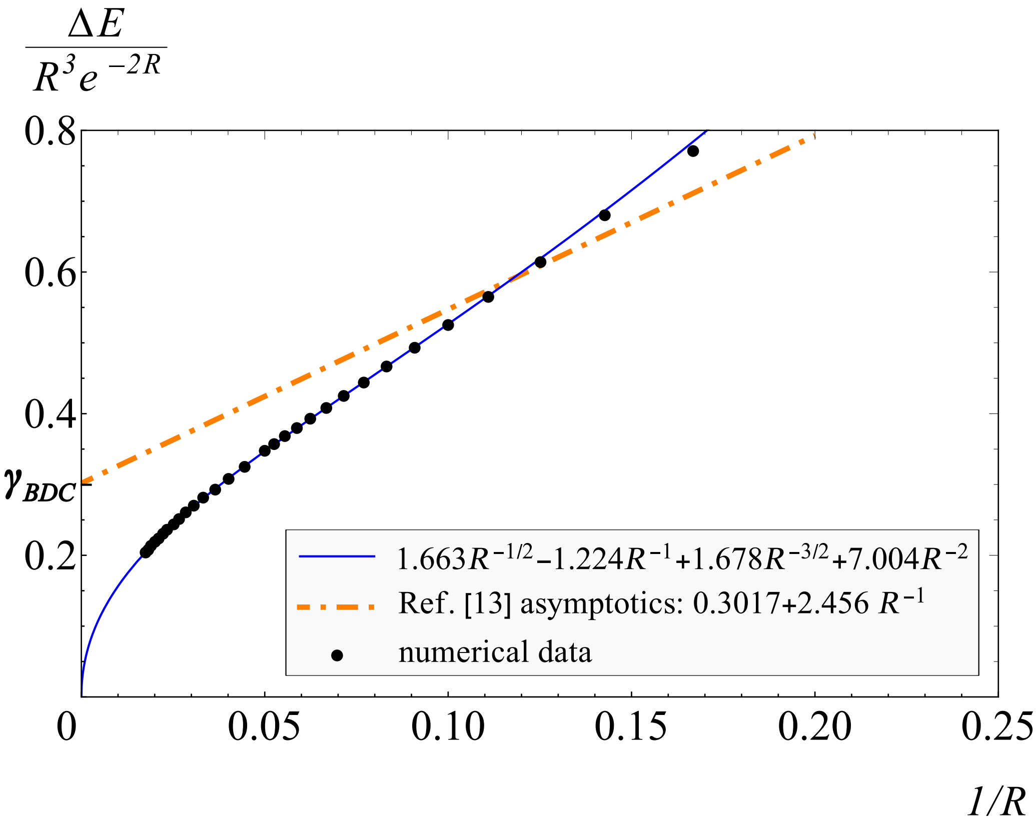


Figure III.5: Rescaled energy splitting $R^{-3}\, e^{2\,R}\, \Delta E$ fitted to numerical points in Table III.1 in the range $R = 20 - 57.5$ au, the same as in Fig. III.2, but presented as a function of $1/R$. Burrows-Dalgarno-Cohen asymptotics [91] is the dash-dotted orange line.

sight into the behavior of the wave functions. Even more readily though, we can can look at the difference of numerical gerade/ungerade eigenvectors. In the end our variational approach is relying on a large numerical cancellation to yield exponentially subdominant terms. It seems more suitable to look for more direct approaches to extracting the energy splitting. In particular the method based on the variational functional introduced in Ref. [104] seems to be easily implementable within our methodology.

To conclude, our numerical results revise the recent analytic derivations of the large-distance asymptotics and will provide a valuable benchmark for various calculations of interatomic interactions.

2 Excited electronic states of Σ^+ symmetry

The following Section is based on the work [A2] and partly on an unpublished data (for states with $n > 7$) and is devoted to calculations of high-accuracy Born-Oppenheimer potentials of hydrogen molecule states of Σ^+ symmetry. Calculations are based on Kolos-Wolniewicz basis and reach an unprecedented accuracy, typically varying from 12 to 15 digits, depending on the state and internuclear distance. For some of the states considered here, potential energy curves have already be considered, but are either much less accurate and are scattered among literature (majority was reported by Wolniewicz and collaborators). Here we present a unified and universal approach.

2.1 Introduction

Ab initio Born-Oppenheimer potentials have proven to be invaluable for the interpretation of spectroscopic data. Currently, transitions between rovibrational levels of $X\,^1\Sigma_g^+$ ground state for hydrogen molecule isotopologues are a subject of exhaustive investigations both from experimental [114–116] and theoretical [66, 117] standpoints, reaching the accuracy of 10^{-4} cm^{-1}. On the contrary, electronically excited states of the hydrogen molecule are much less studied, especially by theoretical methods. So far, calculations of Born-Oppenheimer (BO) potentials for excited Σ^+ states of H_2 were performed with full CI method [18, 19, 40], variational calculations with generalized GTOs [118], variational calculations with explicitly correlated gaussians (ECG) [119, 120] and more recently with free-complement local-Schrödinger-equation method (FC-LSE) [121]. The most accurate to date are variational calculations in an explicitly correlated exponential basis by Wolniewicz and co-workers [42, 122–125] and by Komasa *et al.* [119, 120] which, remarkably have remained unsurpassed for the last 20 years.

Among the plethora of H_2 excited states, of particular importance and long-standing interest is the $B\,1^1\Sigma_u^+$ state, the lowest of $^1\Sigma_u^+$ symmetry. It is easily accessible for spectroscopic measurements, through the allowed electric dipole transition from the $X\,1^1\Sigma_g^+$ ground state, therefore, it can be measured very accurately and serve as a calibration marker at XUV frequencies. Likewise, energies of states such as $EF\,2^1\Sigma_g^+$, $GK\,3^1\Sigma_g^+$, $B\,1^1\Sigma_u^+$ and $B'\,2^1\Sigma_u^+$ are of great spectroscopic interest, because they comprise intermediate states in multiphoton processes, which are crucial for investigations of doubly excited states, recognized as resonant states involved in the dynamics of preionization and predissociation [126–128].

Moreover, BO potentials comprise an essential input for Multichannel Quantum Defect theory analyses of Rydberg states, where the demand in accuracy is dictated by the goal accurady of the Rydberg series extrapolation. In the context of most recent experimental campaigns, an accuracy no worse than $0.001\,\mathrm{cm}^{-1}$ is required [129, 130], especially for the highly excited states. Accurate potentials are also important for studying *gerade*/*ungerade* mixing effects [131] beyond the BO approximation. Ultimately, accurate BO potentials may serve as a useful benchmark for less precise computational methods, electron-ion scattering experiments and numerous other applications [132–134]. We note that many previous calculations often come without estimation of uncertainties, making definitive comparisons rather difficult.

2.2 Symmetries and classification of states

The classification of the molecular wavefunction according to their symmetry properties is vital in determination of the selection rules. An attractive point of view of the short-range properties of the states of molecular hydrogen emerges from splitting the one-center

Table III.2: Mutually allowed discrete symmetries, classified by the values of nuclear spin.

Spin isomer	Ψ_{total}	ϕ_{el}	ϕ_{vib}	ϕ_{rot}	ϕ_{ns}	I	g_{ss}
Para- H_2 or T_2 (N even)	-1	1	1	1	-1	0	1
Ortho- H_2 or T_2 (N odd)	-1	1	1	-1	1	1	3
Ortho-D_2 (N even)	1	1	1	1	1	$0, 2$	3
Para-D_2 (N odd)	1	1	1	-1	-1	1	3

Table III.3: Coefficients mutliplying symmetrized spatial components of the total 2-electron wavefunction. Long dash in the g/u column denotes lack of $gerade/ungerade$ symmetry, i.e. diatomic system with asymmetric nuclei. Only two-electron states are considered, which entails that s, spin multiplicity, can only be either 1 (singlet) or 3 (triplet).

$\mathrm{mod}(\Lambda, 2)$	g/u	s	c_{direct}	$c_{\text{A}\leftrightarrow\text{B}}$	$c_{1\leftrightarrow 2}$	$c_{1\leftrightarrow 2,\text{A}\leftrightarrow\text{B}}$
0	g	1	1	1	1	1
0	g	3	1	1	-1	-1
0	u	1	1	-1	1	-1
0	u	3	1	-1	-1	1
0 or 1	–	1	2	0	2	0
0 or 1	–	3	2	0	-2	0
1	g	1	1	-1	1	-1
1	g	3	1	-1	-1	1
1	u	1	1	1	1	1
1	u	3	1	1	-1	-1

(united-atom) problem of helium-like atom into two centers. This is associated with lowering the spherical symmetry into the cylindrical one.

Total molecular wavefunction has to be symmetric with respect to exchange of two identical bosons and antisymmetric with respect to exchange of two identical fermions. In the context of homonuclear isotopomers of hydrogen molecule, the nuclei in the H_2 and T_2 are spin 1/2 fermions, whereas in D_2 the deuterons are the spin 1 bosons.

2.3 Method

In contrast to the $X\ 1\Sigma_g^+$ and $b\,^3\Sigma_u^+$ states, BO potentials for higher n exhibit much more complicated structure – a result of mutual avoided crossings and resonant interaction with the H^+H^- configurations, often resulting in double minima or bumps, rather than a smooth, single minimum Morse-like curve. This, in turn, implies the presence of strong configuration mixing in some regions of R, unlike the case of well-separated $X\,^1\Sigma_g^+$ and $b\,^3\Sigma_u^+$ states.

A crucial point of our computational method is that it relies on the fact that all the necessary matrix elements of the nonrelativistic Hamiltonian,

$$H = -\frac{\nabla_1^2}{2} - \frac{\nabla_2^2}{2} - \frac{1}{r_{1A}} - \frac{1}{r_{1B}} - \frac{1}{r_{2A}} - \frac{1}{r_{2B}} + \frac{1}{r_{12}} + \frac{1}{r_{AB}}, \tag{III.39}$$

can be readily constructed as a linear combination of f-integrals, see Section **??**.

Once all matrix elements are constructed in terms of f-integrals, the electronic energy is found as the nth lowest eigenvalue by refining an initial guess with inverse iteration method. This step is the most time consuming part of our computational method, because it scales as $\mathcal{O}(N^3)$, where N is the total size of the basis. Recently, interest in Aasen's algorithm [135] for indefinite matrix factorization has been revived due to a novel communication-avoiding variant [136], suitable for efficient parallelization on modern computer architectures.

In our calculations a custom implementation of this algorithm inspired by the PLASMA library [137] was utilized with custom vectorization of quad-double arithmetics based on Bailey's quad-double precision algorithms [138]. Incorporation of both the communication-avoiding variant of Aasen's factorization and vectorized quad-double arithmetics constitutes a very efficient implementation of dense matrix factorization – an essential component of the inverse iteration method with nonorthogonal bases. Extension to octuple precision arithmetics has proven sufficient to contend with near-singular matrices, ill-conditioning of which can be attributed to the presence of large powers of the r_{12} coordinate in the basis.

2.4 Results and discussion

energies are calculated for all possible symmetries of the Σ^+ manifold: $n^1\Sigma_g^+$, $n^3\Sigma_g^+$, $n^1\Sigma_u^+$, and $n^3\Sigma_u^+$, with $n \leq 7$ (26 states in total), with the exception of the ground $X\,{}^1\Sigma_g^+$ and $b\,{}^3\Sigma_u^+$ states, which were calculated elsewhere [38, 39] using special cases of the KW basis. The results are obtained on a grid of internuclear distances resembling logarithmic spacing in the range $R = 0.7 - 20.0$ au (72 points per state in total). It is sampled with denser spacing of 0.1 au in the region of $R = 4.0 - 6.0$ au, where potential curves demonstrate strong avoided crossing features and are subject to rapid changes as a function of R. Numerical results for BO energies, together with uncertainties originating purely from extrapolation to the complete basis set (CBS) limit are presented in the Appendix. Unsurprisingly, convergence for triplet states is better than for singlet, because the requirement of antisymmetry of total fermionic wavefunction generally results in less electron-electron correlation – well-known phenomenon of *correlation hole*. In Figs. III.7,III.10,III.12, and III.15 we compare pointwise accuracy of our potentials to the best known literature values.

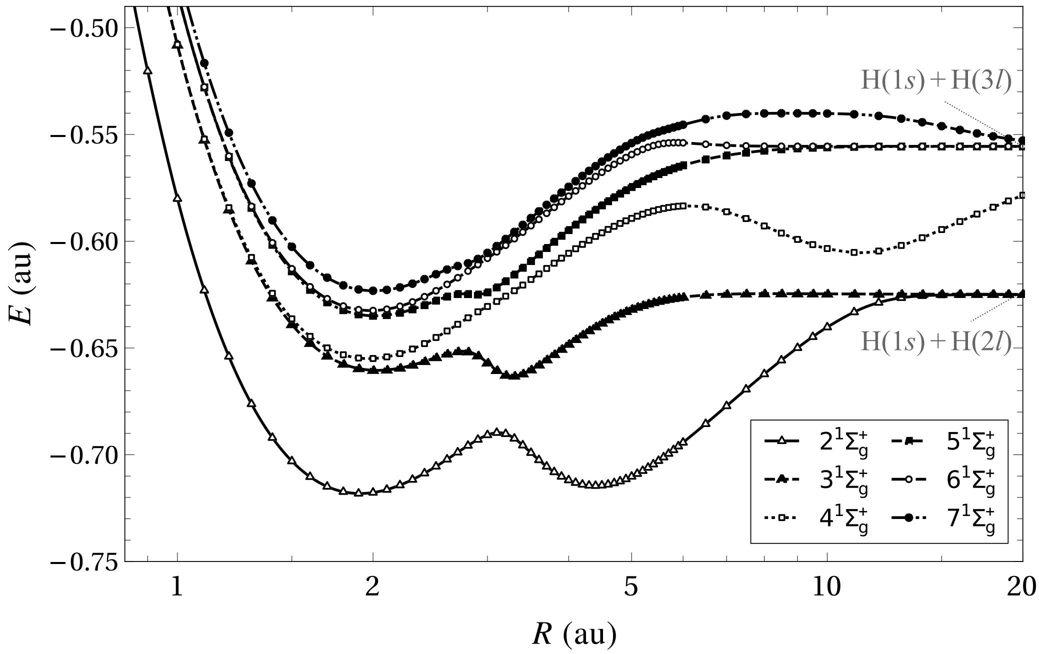


Figure III.6: BO potentials for $n^1\Sigma_g^+$ states, up to $n = 7$. In this scale the $X\ 1^1\Sigma_g^+$ ground state is not visible. The $GK\ 3^1\Sigma_g^+$ with $H\ 4^1\Sigma_g^+$ and $P\ 5^1\Sigma_g^+$ with $O\ 6^1\Sigma_g^+$ switch character from united atom $3d\sigma$ and $4d\sigma$ configurations to $3s$ and $4s$, respectively, exhibiting $< 1\,\mathrm{cm}^{-1}$ splitting around $R = 1.0$ au [122].

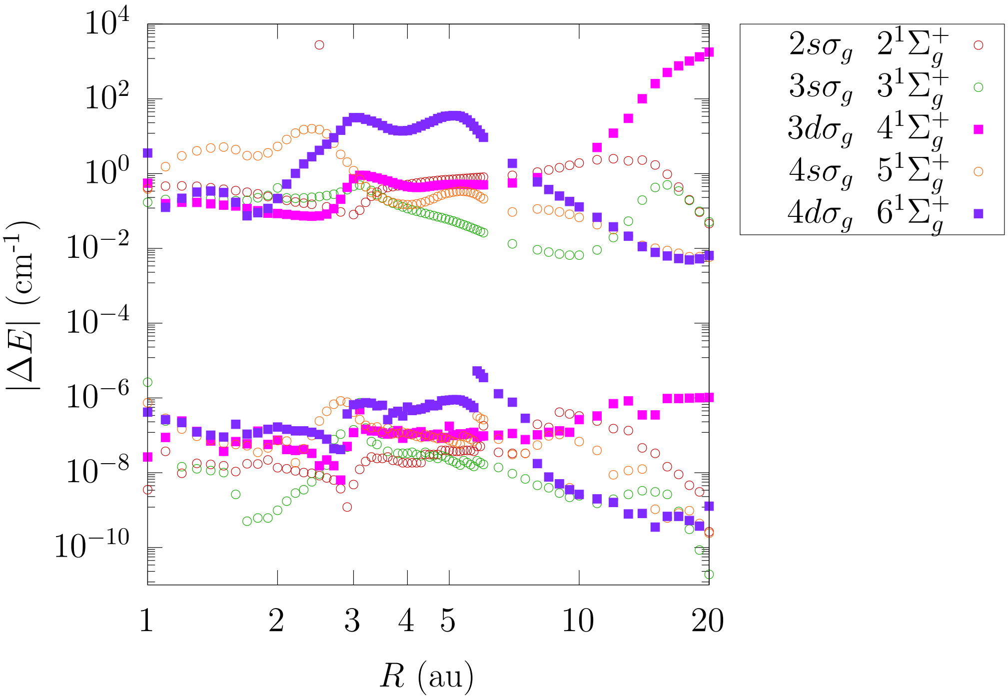


Figure III.7: Comparison of the pointwise accuracy of BO potentials with respect to best literature results for $n^1\Sigma_g^+$ states. Two series of data are color coded in the same manner, the upper ones are taken from Ref. [?] and ours data is lower.

Table III.4: Exemplary values of optimal nonlinear parameters for states and internuclear distances with high ionic component.

State	R	Sector 1				Sector 2			
		y	x	u	w	y	x	u	w
$B\,1^1\Sigma_u^+$	10.0	0.047	-0.447	0.338	0.468	-0.949	-1.263	1.052	1.226
$H\bar{H}\,4^1\Sigma_g^+$	12.0	0.000	-0.446	0.263	0.506	-0.807	-0.807	1.068	1.068
$6^1\Sigma_u^+$	15.0	0.079	-0.490	0.163	0.493	-0.863	-0.727	0.847	0.520
$7^1\Sigma_g^+$	20.0	-0.357	-0.858	0.276	0.692	-0.428	0.164	0.445	0.146

Table III.5: Exemplary values of optimal nonlinear parameters for $n = 7$ at various internuclear distances. Notice very small values of y,u in sector 1 and x,w in sector 2, corresponding to very diffuse (high n) highly excited atomic orbitals.

State	R	Sector 1				Sector 2			
		y	x	u	w	y	x	u	w
$7^1\Sigma_g^+$	2.0	0.000	-0.423	0.097	0.821	-0.080	-0.122	0.637	0.262
$7^3\Sigma_g^+$	4.0	0.000	-0.405	0.097	0.638	0.080	0.278	0.624	0.114
$7^1\Sigma_u^+$	6.0	-0.061	-0.514	0.146	0.619	-0.285	0.080	0.578	0.080
$7^3\Sigma_u^+$	8.0	0.047	-0.449	0.105	0.553	0.436	0.000	0.522	0.267

The irregularities and deviations from this prototype single minimum curve can be qualitatively understood in terms of many effects singly-excited character:

- Homogeneous perturbations,
- Interaction with doubly-excited (most notable example is probably in the Σ_g complex),
- Interaction with ionic curve,
- London dispersion interaction,
- Exchange effects,

From inspection of potential curves in Figures III.6, III.9, III.11 and III.14, one evident universal feature for all the considered states is the presence of principal minimum around 2 bohrs. Existence of a second minimum is mainly driven by the interaction of energy levels with purely ionic H^+H^- system. A modest drop in convergence rate can be noticed for the states: $EF\,2^1\Sigma_g^+$, $H\bar{H}\,4^1\Sigma_g^+$, $7^1\Sigma_g^+$ and $B\,1^1\Sigma_u^+$, $B''\bar{B}\,3^1\Sigma_u^+$, and $6^1\Sigma_u^+$ in regions of large R, where this interaction is most prevalent and configurations mix markedly. This observation is consistent with the optimal values that nonlinear parameters attain, see Table III.4 for exemplary values. For detailed analysis of ionic and covalent components we refer to Ref. [18, 19]. In Table III.5 we present exemplary values of optimal nonlinear parameters for $n = 7$ states. Evident asymmetry between parameters of first and second electron justifies the use of more flexible KW basis over its more symmetric special cases. We conjecture that the same basis type can be used as a remedy for the convergence rate of ionic states if our basis is augmented with a third scale sector, improving the representation of electron correlation, when both are localized around the same nucleus, similarly as it was performed in the calculations of HeH^+[139] BO potential and recognized as a feature of *in-out* electronic correlation in one-center, two-electron calculations of He [45].

All the considered states dissociate as H($1s$) + H(nl) with energies tending to the sum of its dissociation products as $R \to \infty$, see Figures III.6, III.9, III.11 and III.14. On the other hand, in the united atom limit, $R \to 0$, electronic configuration should approach those of He. Straightforward observation that the order of energies of atomic configurations He[^{1,3}L($1snl$)] is in general different than corresponding H($1s$) + H(nl) dissociation products, together with well-known theorem that the BO potential curves with the same symmetry cannot cross, implies that the character of the states must change in the region of intermediate R. The first qualitative approach aiming to predict such configuration mixing in terms of so-called correlation diagrams can be attributed to Mulliken [41], while a detailed discussion on configuration mixing and matching of Σ^+ manifolds electronic densities to the corresponding atomic orbitals was presented in the meticulous analysis by Corongiu and Clementi [18, 19, 40]. Here, we supplement this discussion with the help of Figure III.8, where we present accurate splittings between singlet and triplet energies approaching the united atom configuration, including ($1snf$) states which are split by values as small as $\sim 10^{-8}$ au.

The states of $^3\Sigma_g^+$ symmetry form the ($1sns$,nd) Rydberg series, and this singly-excited

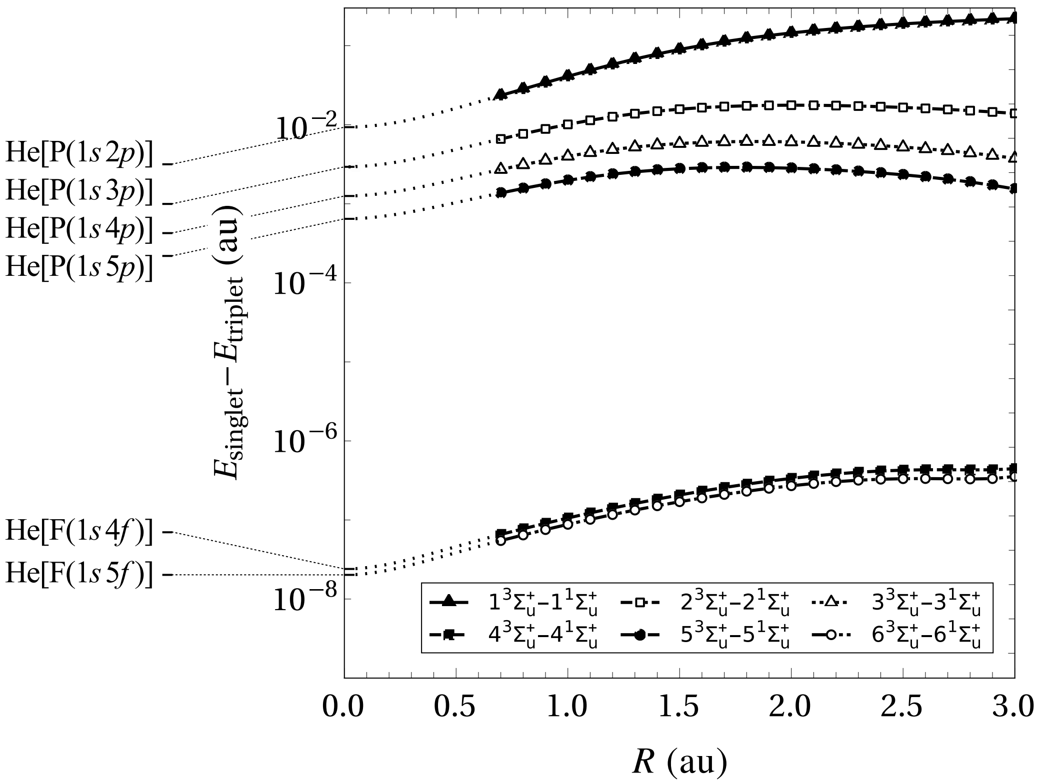


Figure III.8: Energy splittings between singlet and triplet $n\,\Sigma_u^+$ states at small internuclear distances. Labels on the y axis indicate values of energy differences between helium ${}^1L(1snl)$ and ${}^3L(1snl)$ states (here with L =P,F for the states under consideration). Dotted lines represent tentative assignments from calculated splittings to corresponding differences between united atom ($R \to 0$) energies from Ref. [140], which are in agreement with [19, 40].

character propagates from the united-atom limit to around the equilibrium distance $R \sim$ 2.0 au, where the singly-excited character transfer can be observed due to the avoided crossing.

For the sake of comparison with the most recent integral-free FC-LSE calculations by Nakashima and Nakatsuji [121], we refer to the definition of H-square, see Eq. (24) of Ref. [143],

$$\sigma^2_{FC-LSE} = \langle\Psi|\,(H-E)^2\,|\Psi\rangle, \tag{III.40}$$

which is utilized in Ref. [121] as a measure of wavefunction (and energy) accuracy. For convenience, we define a relative ratio p as,

$$p = \frac{E_{var} - E_{FC-LSE}}{\sigma^2_{FC-LSE}}, \tag{III.41}$$

where E_{var} denotes the variational energy result as obtained in this work and E_{FC-LSE} refers to results of the FC-LSE method from Ref. [121]. One observes, that in the case of the highly excited $7^3\Sigma_u^+$ state, p is much greater than 1 for the majority of points and varies significantly (up to $\sim$ 90) along with internuclear distance with no visible trend. In

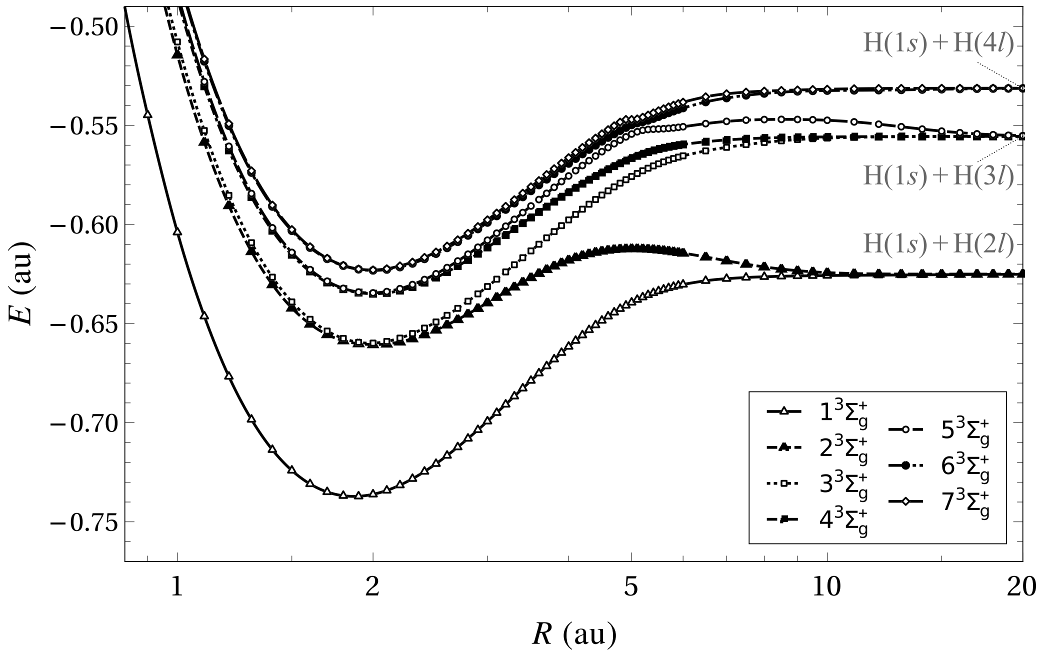


Figure III.9: BO potentials for $n^3\Sigma_g^+$ states, up to $n = 7$. Pairs of states $2 - 3$, $4 - 5$ and $6 - 7$ all anticross around the $R = 2.0$ au minima, conjointly changing the character from united atom $3d\sigma, 4d\sigma, 5d\sigma$ to $3s, 4s, 5s$, respectively.

contrast, another highly excited states available for the reference, such as $6^1\Sigma_u^+$ or $7^1\Sigma_g^+$, have $p > 1$ consistently in the region $R = 2.0 - 6.0$ au. For $n > 4$ and all symmetries, systematically, more than half of the points fall outside the range of confidence for triplet states, if H-square is given the interpretation of 1σ confidence interval. Therefore, we conclude that H-square vastly underestimates the actual uncertainty of wavefunctions (and of energies) obtained in Ref. [121], especially in case of triplet states and for large distances. Not surprisingly, a detailed comparison in Table III.6 of numerical results with their uncertainties for all the previous calculations for selected excited states at given distance of $R = 2.0$ au indicates that almost no previous calculations were able to correctly estimate numerical uncertainties.

2.5 Conclusions

We have demonstrated that a relative accuracy of 10^{-10} or better can be reached for BO energies of all the excited $n\,\Sigma^+$ states of H_2 up to $n = 7$, with at most 18 000 basis functions of explicitly correlated exponential basis. With a two-sector unrestricted Kolos-Wolniewicz basis, a rapid, exponential convergence towards the CBS limit is attained, even for exceptionally complicated electronic configurations of high singly-excited orbitals.

Adiabatic corrections are known to be of significant magnitude [42] and this work paves the way towards their accurate evaluation with method similar to that presented in Ref. [144]. Ultimately, because the results obtained in this work are at least 6 orders of magnitude more accurate than any other available in the literature, we believe that they will

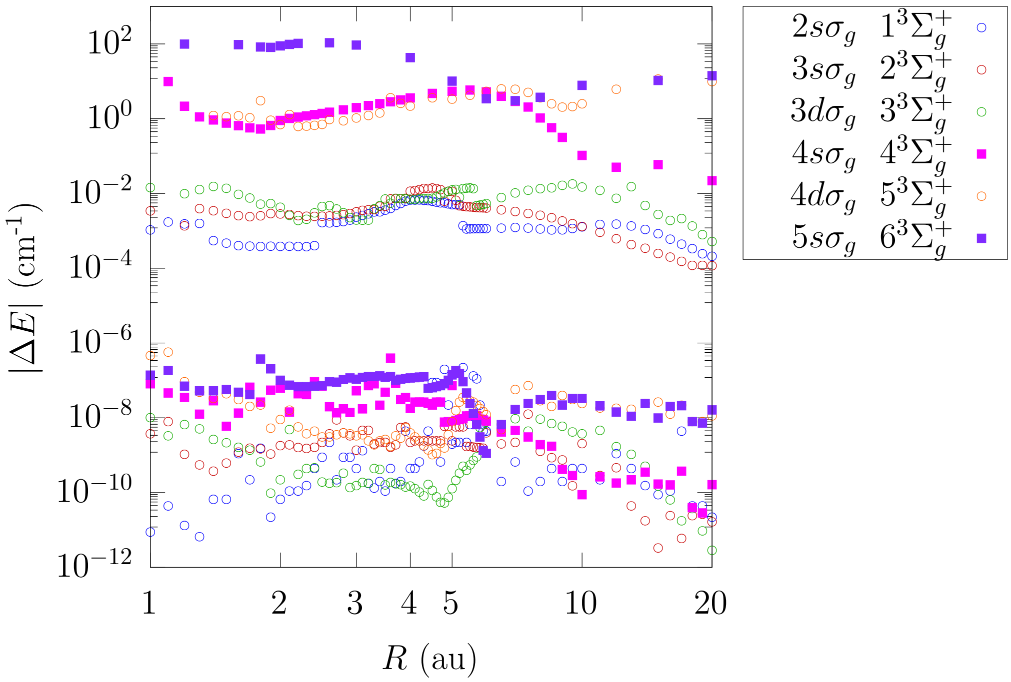


Figure III.10: Comparison of the pointwise accuracy of BO potentials with respect to best literature results for $n^3\Sigma_g^+$ states. Two series of data are color-coded exactly the same, the upper variant for $n = 1-3$ is from Ref. [124], $n = 4-5$ from Ref. [141], and $n = 6$ from Ref. [118], our data is lower at all points.

serve as a useful benchmark for less accurate computational methods. Moreover, our two-body two-center integrals with exponential functions can be used for any two-center systems, giving the possibility of achieving high-precision results for an arbitrary diatomic molecules. For the sake of conciseness, we do not present obtained data in the Thesis. The Born-Oppenheimer potentials, together with auxiliary data for states with principal quantum number $n \leq 7$ can be found in the Supplementary Material to the work [A2]. Newer, unpublished data for $n > 7$ can be obtained from the Author upon a reasonable electronic mail request.

3 Excited electronic states with $\Lambda > 0$

The following Section is based on the work [A3] and partly on an unpublished data. It is devoted to the extension of the computational scheme of variational Born-Oppenheimer potential utilizing Kolos-Wolniewicz basis to the case of nonzero Λ. Results presented here, owing to the choice of the basis set, reach an unprecedented accuracy and for many states are the first results ever.

In the work [A2] we have performed calculations of Born-Oppenheimer (BO) potentials for excited states of all $n\,\Sigma^+$ symmetries with $n \leq 7$, for which we obtained the accuracy exceeding all the previously known results by 3-4 orders of magnitude. In Section

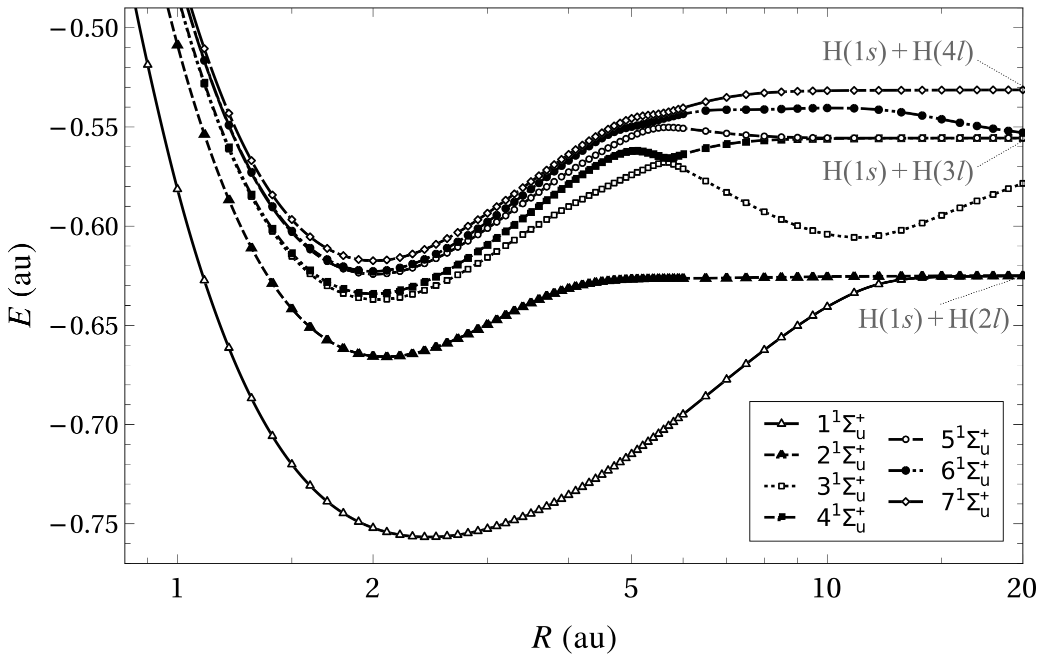


Figure III.11: BO potentials for $n^1\Sigma_u^+$ states, up to $n = 7$.

we extend those calculations to Π, Δ, and Φ excited states with the relative accuracy of at least 10^{-9} for internuclear distances of 0.01 – 20 au. Some of these states have already been investigated in the literature. Namely, the most significant and accurate results at that time were obtained primarily in a series of works by Kołos, Wolniewicz, and Rychlewski [49, 145–148], using the explicitly correlated exponential basis, called Kołos-Wolniewicz (KW) basis functions [37]. Their results, however, disagreed with experimental values for Δ states. Jeziorski *et al.* pointed out in Ref. [149] that the angular factor for these states in Ref. [49] was incomplete. This was verified and later corrected by Wolniewicz in Ref. [150]. It lowered BO curves by a few cm^{-1} for singlet and less than 1 cm^{-1} for triplet Δ_g states and resolved discrepancies with the experimental data available at those times.

Another method, based on explicitly correlated gaussian (ECG) functions, was employed in Ref. [151, 152] to obtain a potential curve for $C^1\Pi_\mathrm{u}$ $(n = 1)$. The most recent contributions to the ab-initio Potential Energy Curves (PEC) of H_2 consist of a Free-Complement local Schrödinger equation method developed by Nakatsuji and collaborators [153–157] with potential curves for Σ, Π, Δ, and Φ states. In this Section we not only improve upon all the results present in the literature by a few orders of magnitude, but also calculate many higher excited states of Π, Δ, and Φ symmetries and finally draw attention to possible further applications of Kolos-Wolniewicz basis.

3.1 Angular factors

Expansion of the type in Eq. (II.13) is valid only for the states of Σ^+ symmetry. Extension of the KW basis to states of higher angular momentum requires the introduction of

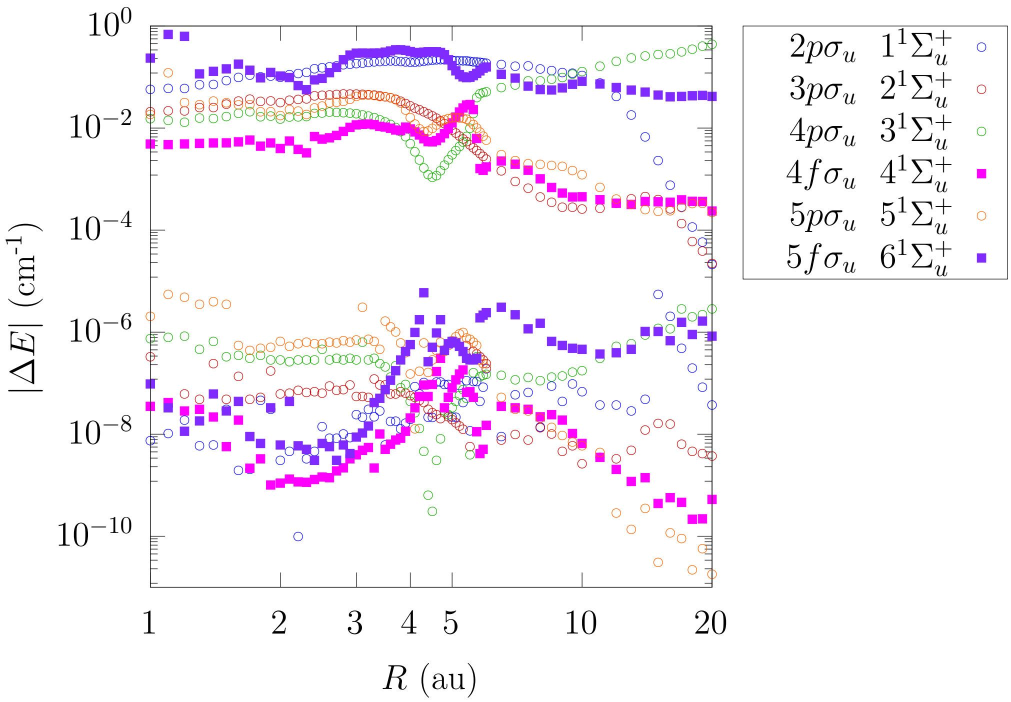


Figure III.12: Comparison of the pointwise accuracy of BO potentials with respect to best literature results for $n^1\Sigma_u^+$ states. Two series of data are color-coded exactly the same, the upper series for $n = 1 - 6$ is taken from Ref. [42], our data is lower.

angular factors. The electronic state of a diatomic molecule is, among other symmetries, characterized by $|\Lambda|$ – an absolute value of the eigenvalue of the $\vec{n}\cdot\vec{L}$ operator, where $\vec{n}$ is a normalized vector parallel to the internuclear axis and $\vec{L}$ is the electronic angular momentum operator. In order to enforce proper angular symmetry for $\Lambda \neq 0$ we construct symmetric, traceless l–th rank tensors,

$$\begin{aligned}
\chi_1^i &= \rho_1^i \text{ for } \Pi, \\
\chi_{11}^{ij} &= \rho_1^i\rho_1^j - \frac{1}{2}\delta_\perp^{ij}\,\rho_1^2 \text{ for } \Delta, \\
\chi_{12}^{ij} &= \rho_1^{(i}\rho_2^{j)} - \delta_\perp^{ij}\vec{\rho}_1\cdot\vec{\rho}_2 \text{ for } \Delta, \\
\chi_{111}^{ijk} &= \rho_1^i\rho_1^j\rho_1^k - \frac{1}{3}\rho_1^2\,\rho_1^{(k}\delta^{ij)} \text{ for } \Phi, \\
\chi_{112}^{ijk} &= \rho_1^{(i}\rho_1^j\rho_2^{k)} - \frac{1}{3}\rho_1^2\,\rho_2^{(k}\,\delta^{ij)} - \frac{2}{3}\vec{\rho}_1\cdot\vec{\rho}_2\,\rho_1^{(k}\,\delta^{ij)} \text{ for } \Phi,
\end{aligned} \tag{III.42}$$

where $\rho^i = r^i - n^i\,\vec{n}\,\vec{r}$, $\delta_\perp^{ij} = \delta^{ij} - n^i\,n^j$, $\vec{n} = \vec{R}/R$, and (ijk) denotes symmetrization of indices. Such tensors represents irreducible representations of SO(2) rotations (around the internuclear axis) in the coordinate space. Consequently, the total wavefunction for

Table III.6: Comparison of calculated BO energies (hartrees) for selected states at internuclear distance of 2 bohrs (vicinity of first minimum). Long dash indicates no data available for given method. Underlined digits present an improvement over previous most accurate result.

Method	Ref.	BO energy (hartrees)
State: $EF\,2^1\Sigma_g^+$		
Full CI	[18, 19, 40]	-0.717 68
FC-LSE	[121]	-0.717 724 7(96)
ECG	[120]	-0.717 715 240
KW	[123],[42]	-0.717 715 096
KW	This work	-0.717 715 $\underline{279\,148\,71}$(3)
Method	Ref.	BO energy (hartrees)
State: $H\bar{H}\,4^1\Sigma_u^+$		
Full CI	[18, 19, 40]	-0.634 09
FC-LSE	[121]	-0.634 105(21)
GGTOs	[118]	-0.634 098 15
KW	[123],[42]	-0.634 101 622 0
KW	This work	-0.634 101 $\underline{640\,058\,24}$(1)
Method	Ref.	BO energy (hartrees)
State: $7\,^3\Sigma_u^+$		
Full CI	[18, 19, 40]	$-0.618\,97$
FC-LSE	[121]	$-0.618\,207(64)$
KW	This work	$-0.618\,9\underline{69\,968\,931}(3)$

Π, Δ, and Φ states, corresponding to $\Lambda = 1, 2$, and 3, respectively, is expanded as

$$
\begin{aligned}
\Phi_\Pi^i &= \sum_{\{n\}}^{\Omega} c_{\{n\}} \hat{S}_{AB}^{\pm} \hat{S}_{12}^{\pm} \chi_1^i \Phi_{\{n\}}, \\
\Phi_\Delta^{ij} &= \sum_{\{n\}}^{\Omega} c_{\{n\}} \hat{S}_{AB}^{\pm} \hat{S}_{12}^{\pm} \chi_{11}^{ij} \Phi_{\{n\}} + \sum_{\{n\}}^{\Omega'} c'_{\{n\}} \hat{S}_{AB}^{\pm} \hat{S}_{12}^{\pm} \chi_{12}^{ij} \Phi'_{\{n\}}, \\
\Phi_\Phi^{ijk} &= \sum_{\{n\}}^{\Omega} c_{\{n\}} \hat{S}_{AB}^{\pm} \hat{S}_{12}^{\pm} \chi_{111}^{ijk} \Phi_{\{n\}} + \sum_{\{n\}}^{\Omega'} c'_{\{n\}} \hat{S}_{AB}^{\pm} \hat{S}_{12}^{\pm} \chi_{112}^{ijk} \Phi'_{\{n\}}.
\end{aligned}
\tag{III.43}
$$

Angular factors with even higher values of Λ could be implemented in an analogous manner. Altough in KW basis one should expect significant accuracy loss, due to very lengthy expression for matrix elements, which range over many orders of magnitude. On the other hand, states corresponding to high values of Λ should be sufficiently approximable by simple polarization models, because those in such states any interaction with the $1s$ electron or the ionic core will be very weak and in the language of singly-excited orbitals only

$l \geq \Lambda$ are involved. In other words for high values of Λ, Hund's case (b) is usually not a good approximation.

In the evaluation of matrix elements with the above functions, repeated Cartesian indices in bra and ket are summed over, and the resulting expression is a linear combination of f-integrals with various sets of $\{n\}$, which are defined as

$$f_{\{n\}}(R) = R \int \frac{d^3 r_1}{4\,\pi} \int \frac{d^3 r_2}{4\,\pi}\, \frac{e^{-w_1\, r_{12} - u\,\xi_1 - w\,\xi_2 - y\,\eta_1 - x\,\eta_2}}{r_{1A}\, r_{1B}\, r_{2A}\, r_{2B}}\, r_{12}^{n_0-1} \eta_1^{n_1} \eta_2^{n_2} \xi_1^{n_3} \xi_2^{n_4}. \tag{III.44}$$

Efficient recursive evaluation of these integrals is the subject of Refs. [36, 53, 158], and also outlined in Section **??**.

The expressions for matrix elements tend to get very lenghty for states with $\Lambda > 0$. Even those for the Hamiltonian with wavefunctions of the Π symmetry are too lengthy to be reported here. Crucially though, with symbolic algebra packages such as Mathematica[159] their derivation can be efficiently automated. Nevertheless, we have explicitly checked that our construction of angular factors yields the same linear combinations of f-integrals, as with the use of either real or complex angular factors introduced by Jeziorski *et al.* in Ref. [149]. In practical calculations, due to the length of these formulas, evaluation of matrix elements dominates the computation time for Δ and Φ symmetry, even at moderate basis sizes.

In pioneering calculations of the lowest gerade Δ states, namely J and $S\,^1\Delta_\mathrm{g}$ and j and $s\,^3\Delta_\mathrm{g}$, by Kołos and Rychlewski [146, 148] and later by Wolniewicz [49, 150], the $\pi\pi$ terms were not included (the χ_{12} angular factor), as hinted by Jeziorski *et al.* [149]. Its inclusion improves the adiabatic energies by a few cm^{-1} for $J^1\Delta_\mathrm{g}$ and $S^1\Delta_\mathrm{g}$ states and tenths of cm^{-1} for triplet $j^3\Delta_\mathrm{g}$ and $s^3\Delta_\mathrm{g}$ states, as demonstrated in subsequent work by Wolniewicz [150]. Together with the evaluation of nonadiabatic coupling by Yu and Dressler [160], the apparent discrepancy with experimental values for dissociation energies of H_2 and D_2 [161, 162] has been resolved.

3.2 Results

In work [A3] we have calculated BO energies for $1-4\,\Pi$ and $1-3\,\Delta$ and $1-2\,\Phi$ states, and additionally $3\,^1\Phi_\mathrm{u}$, and $3\,^3\Phi_\mathrm{u}$ states (38 in total) in 81 points of a nonuniform grid spanned within $R \in (0.01, 20.0)$ au. In order to test the capability of the exponential basis, we have selected the $I^1\Pi_\mathrm{g}$, $i^3\Pi_\mathrm{g}$, $C^1\Pi_\mathrm{u}$, and $c^3\Pi_\mathrm{u}$ states ($n=1$), for which we have ventured to exceptionally large bases consisting of two sectors with their own nonlinear parameters: JC(21,19) (54648 basis functions in total) in the range $R = 0.01 - 6.0$ au, and KW(18,16) (53998 basis functions in total) in the range $R = 6.5 - 20.0$ au. This allowed us to achieve 15 or more significant digits in the range $R = 0.7 - 20\,au$, and can be regarded as the state-of-the-art of our current computational approach.

In the remaining cases, calculations were performed with smaller bases, obtained by incrementing Ω of both sectors by 1 until the extrapolated energies reached uncertainty no worse than 10^{-9} at all distances. This usually required the use of the JC(14,12) basis in the range $0.01-6.0$ au and the KW(12,10) basis in $6.5-20.0$ au. To reduce the computational cost of calculations with Δ and Φ symmetries, both sectors having different angular factor were set to carry the same nonlinear parameters. This significantly reduced the number of f-integrals required for calculations of matrix elements.

All the potential curves have a well-pronounced single minimum around $R = 2$ au and exhibit strong features of anticrossings and curve interactions in the region $R = 4-8$ au, which are associated with the configuration mixing. Those interactions have a trend to become weaker with the increasing angular momentum of the excited electron. Due to the high accuracy of the calculated potential, the dominating electronic configuration can be deduced from comparison to energies of helium atom excited states and of an infinitely separated hydrogen H($1s$) – H(nl) atoms. In particular, we observe, by reaching internuclear distances as small as $R = 0.01$ au, that the energies smoothly evolve to the corresponding value of the excited He atom [163]. It follows from analysis of curves that each highly excited molecular state is dominated by a single atomic $1snl$ configuration at both the united atom and the dissociation limit. The nl configuration at both of those limits is usually not the same; therefore, in such cases, when considering fixed n in the molecular term (i.e., the n-th eigenvalue of the BO molecular Hamiltonian), a character change of the excited electron has to occur at least once along the PEC. Understanding of the electronic character of a molecule in terms of singly excited $1snl$ atomic configurations originates from the pioneering works on molecular binding theory of Hund, Mulliken and many others [164–166] and can be qualitatively described with the correlation diagrams [167]. Detailed analysis of electronic characters along the PECs is out of scope of the current report and here we mainly focus on the computational aspects and accuracy comparison with previous ab-initio results. For a meticulous analysis of electronic configuration evolution as a function of n and R, we refer to the extensive analysis of Corongiu and Clementi [20].

3.2.1 States of Π symmetry

Although the basis for the Π state could in principle be built with a single sector, use of the second sector with different nonlinear parameters has proven to be advantageous. Primarily, it clearly makes the basis more flexible with the introduction of another set of nonlinear parameters. Secondarily, multi-sector bases are routinely utilized in atomic calculations with Hylleraas bases, where the largest sector spans the most diffuse length scales with nonlinear parameters bounded from below by $\sqrt{-2\,m\,E}$, and subsequent sectors aim to improve the shorter scale range to the nucleus. Optimal values of parameters obtained in the present calculations for H_2 suggest that spanning more diffuse functions is usually energetically more important than the short-range motion in the vicinity of the nuclei, and the introduction of a second sector seems especially relevant in the regions without the domination of a single electronic configuration.

Our numerical results for $1-4\ \Pi$ states are plotted in Fig. III.17, raw numerical data is moved to Appendix for better readability. In order to compare with the previous results of Refs. [49, 151, 157, 168] we select $R = 2$ au and present value of potentials in Table

III.7. To test capabilities of our method, we have also evaluated a few Π_u states with $n = 5, 6, 10$ at a single point $R = 2.0$ au.

In Ref. [168] an alternative approach to solving the Schrödinger equation in terms of stochastic evaluation of the path integral with the Schrödinger potential was introduced as an energy estimator. In general these results were in good agreement with previous results. However, few σ discrepancy was observed for the $I^1\Pi_g$ state, for which their initial result of -0.659 515 9(3) appeared to be discrepant by a few σ with the variational result $-0.659\,515\,055\,5$ of Wolniewicz [49]. Curiously enough, by taking four times larger statistical sample, more specifically four times more integration paths in the generalized Feynman-Kac method (GFK), they tightened the result to -0.659 515 54(6), thus suggesting a significant improvement over the result of Wolniewicz. Comparison of both results with ours reveals that result of Ref. [168] overshoots the variational limit by almost the same amount as the difference between our result and that of Wolniewicz. This indicates that the convergence of the GFK method to the exact energy is much slower than anticipated and the extrapolation uncertainty was much too optimistic.

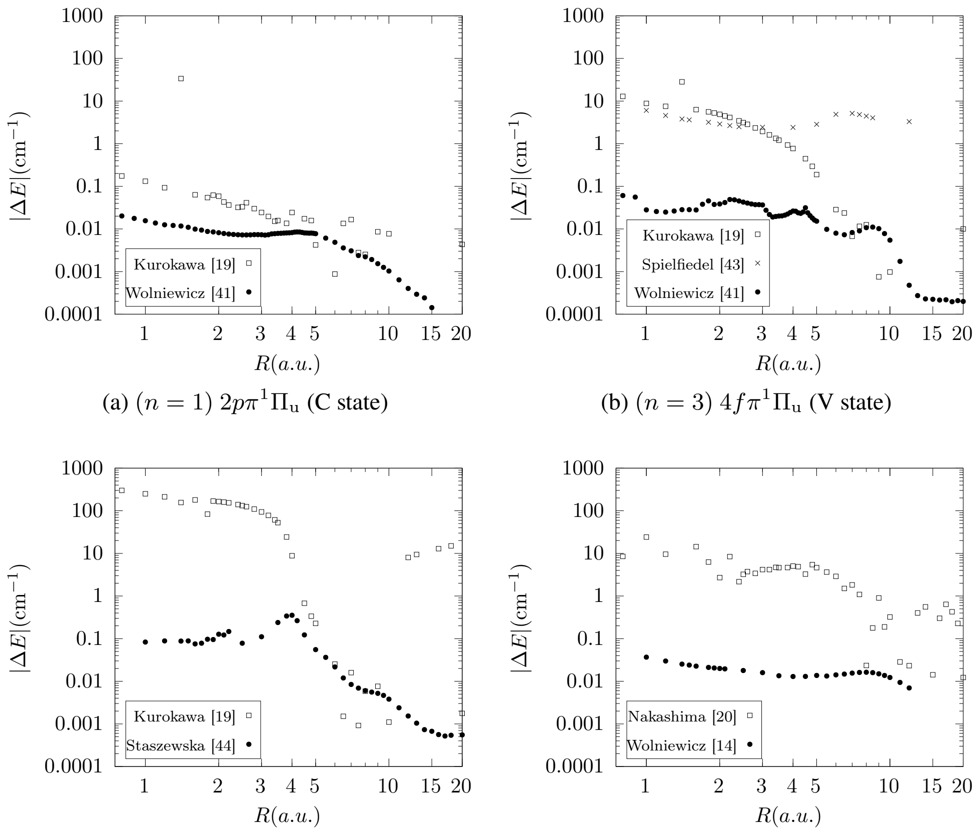
Table III.7: Comparison of BO energy near minimum for selected Π states.

Method/basis size	R/Bohr	E/hartree	Ref.
		I state (n =1) $\mathbf{1s\sigma_g 2p\pi_g}$ $^1\mathbf{\Pi_g}$	
KW/75	2.0	$-0.659\,511\,60$	[145]
JC(5,3)/140	2.0	$-0.659\,512\,139$	This work
KW/193	2.0	$-0.659\,515\,055\,5$	[49]
JC(6,4)/272	2.0	$-0.659\,515\,272$	This work
GFK	2.0	$-0.659\,515\,54(6)$	[168]
JC(21,19)/53636	2.0	$-0.659\,515\,\underline{340\,754\,017}(6)$	This work
		C state (n=1) $\mathbf{1s\sigma_g 2p\pi_u}$ $^1\mathbf{\Pi_u}$	
KW/150	1.952	$-0.718\,366\,655$	[147]
ECG/149	1.952	$-0.718\,367\,778$	[151]
JC(5,0.280,0.745,3, 0.618,0.675)/168	1.952	$-0.718\,367\,796\,214$	This work
KW/449	1.952	$-0.718\,367\,979$	[48]
ECG/600	1.952	$-0.718\,368\,027$	[152]
JC(8,6)/917	1.952	$-0.718\,368\,027\,687$	This work
JC(21,19)/53636	1.952	$-0.718\,368\,0\underline{30\,147\,144\,23}(7)$	This work
		D state (n=2) $\mathbf{1s\sigma_g 3p\pi_u}$ $^1\mathbf{\Pi_u}$	
CI/50	2.0	$-0.655\,035$	[169]
KW/80	2.0	$-0.655\,299\,82$	[47]
KW/150	2.0	$-0.655\,325\,841$	[147]
FC-LSE[a]/1050	2.0	$-0.655\,328\,191$	[157]
JC(6,4)/316	2.0	$-0.655\,328\,203$	This work

Continued on next page

Table III.7 – *Continued from previous page*

Method/basis size	R/Bohr	E/hartree	Ref.
KW/724	2.0	$-0.655\,328\,261$	[170]
JC(7,5)/552	2.0	$-0.655\,328\,266\,813$	This work
JC(8,6)/917	2.0	$-0.655\,328\,274\,470$	This work
JC(14,12)/9080	2.0	$-0.655\,328\,\underline{276\,407}(7)$	This work
V state (n=3) $\mathbf{1s\sigma_g 4f\pi_u\ {}^1\Pi_u}$			
KW	2.0	$-0.633\,939$	[169]
MRCI/173	2.0	$-0.632\,582\,84$	[171]
MRCI/284	2.0	$-0.634\,045\,91$	[172]
FC-LSE^a/1050	2.0	$-0.634\,036\,945$	[157]
KW/724	2.0	$-0.634\,058\,929$	[170]
JC(8,6)/917	2.0	$-0.634\,059\,096\,079$	This work
JC(14,12)/9080	2.0	$-0.634\,05\underline{9\,104\,699\,22}(8)$	This work
D' state (n=4) $\mathbf{1s\sigma_g 4p\pi_u\ {}^1\Pi_u}$			
KW	2.0	$-0.632\,391$	[169]
MRCI/284	2.0	$-0.632\,606\,24$	[172]
FC-LSE^a/1050	2.0	$-0.632\,669\,650$	[157]
KW/724	2.0	$-0.632\,670\,21$	[170]
JC(8,6)/917	2.0	$-0.632\,670\,221\,022$	This work
JC(14,12)/9080	2.0	$-0.632\,670\,2\underline{22\,456}(6)$	This work
(n=5) $\mathbf{1s\sigma_g 5f\pi_u\ {}^1\Pi_u}$			
FC-LSE^a/1050	2.0	$-0.621\,700\,378$	[157]
JC(8,6)/917	2.0	$-0.622\,727\,031$	This work
KW(12,10)/9191	2.0	$-0.622\,\underline{727\,143\,343}(3)$	This work
(n=6) $\mathbf{1s\sigma_g 5p\pi_u\ {}^1\Pi_u}$			
FC-LSE^a/1050	2.0	$-0.620\,612\,4$	[157]
JC(8,6)/917	2.0	$-0.622\,010\,993$	This work
JC(14,12)/9080	2.0	$-0.622\,\underline{011\,008\,773}(5)$	This work
(n=10) $\mathbf{1s\sigma_g 7f\pi_u\ {}^1\Pi_u}$			
Full-CI/320	2.0	$-0.603\,59$	[20]
KW(8,6)/1749	2.0	$-0.612\,873\,187\,073$	This work
KW(14,12)/17816	2.0	$-0.6\underline{12\,873\,232\,0}(1)$	This work
(n=10) $\mathbf{1s\sigma_g 7p\pi_u\ {}^3\Pi_u}$			
Full-CI/320	2.0	$-0.605\,11$	[20]
KW(8,6)/1749	2.0	$-0.613\,021\,263\,099$	This work
KW(14,12)/17816	2.0	$-0.6\underline{13\,021\,373\,965}(5)$	This work



(a) $(n = 1)\ 2p\pi^1\Pi_\mathrm{u}$ (C state)

(b) $(n = 3)\ 4f\pi^1\Pi_\mathrm{u}$ (V state)

(c) $(n = 3)\ 5d\pi^3\Pi_\mathrm{g}$ (w state)

(d) $(n = 2)\ 4d\delta^1\Delta_\mathrm{g}$ (S state)

Figure III.18: Comparison of BO energies with resepct to the literature values for selected Π and Δ states as a function of R.

In Fig. III.18, we have plotted the difference between our results and that of Refs. [156, 157, 170, 172, 173] as a function of R for a few selected Π states differing in the singlet/triplet and gerade/ungerade symmetry, as well as in the character of the excited electron. Considering the energy differences between our results and those of Refs. [49, 151, 157] for various Π states as a function of R, we conclude that rather old results of Wolniewicz [170] for $1 - 4^1\Pi_\mathrm{u}$ states are accurate to at least 0.1 cm^{-1}. Interestingly, the agreement with Ref. [157] within ~ 1 cm^{-1} accuracy is observed for the $1, 2\ \Pi$ states of p and d character. In contrary the discrepancy is much bigger for the states dominated by the configurations with higher l, where the discrepancy reaches even hundreds of cm^{-1}, see Fig III.18c. Most likely it is due to the poor representation of singly-excited configurations with large values of l, especially of f, g, and h character, and could be associated with the absence of terms proportional to $\mathrm{H(1s)} - \mathrm{H}(n = 4)$ in the initial function of their method. This absence is already noted by the Authors of Ref. [157].

3.2.2 States of Δ symmetry

Table III.8: Comparison of BO energy Δ states at $R = 2.0\,au$. To the Authors' best knowledge, these are all the ab-initio results of Δ symmetry available in the literature. δ is the difference with respect to the best available result.

Method/basis size	R/Bohr	E/hartree	δ/cm^{-1}	
		J state (n=1) $\mathbf{1s\sigma_g 3d\delta_g\ {}^1\Delta_g}$		
Full-CI/320	2.0	$-0.657\,53$	10.57	[20]
FC-LSE	2.0	$-0.657\,565(52)$	2.89	[156]
VMC	2.0	$-0.657\,577\,61(4)$	0.12	[168]
GFK	2.0	$-0.657\,578\,0(3)$	0.04	[168]
KW/394	2.0	$-0.657\,578\,084\,4$	0.02	[150]
JC(6,4)/316	2.0	$-0.657\,578\,102\,4$	0.016	This work
JC(16,14)/16233	2.0	$-0.657\,578\,\underline{175\,516}(2)$	0.0	This work
		j state (n=1) $\mathbf{1s\sigma_g 3d\delta_g\ {}^3\Delta_g}$		
Full-CI/320	2.0	$-0.657\,59$	10.27	[20]
FC-LSE	2.0	$-0.657\,658(29)$	-4.65	[156]
KW/394	2.0	$-0.657\,636\,708\,8$	0.02	[150]
JC(6,4)/316	2.0	$-0.657\,636\,722\,7$	0.016	This work
JC(16,14)/9080	2.0	$-0.657\,636\,\underline{796\,522}(2)$	0.0	This work
		S state (n=2) $\mathbf{1s\sigma_g 4d\delta_g\ {}^1\Delta_g}$		
FC-LSE	2.0	$-0.633\,651(40)$	-2.65	[156]
KW/70	2.0	$-0.633\,607\,617$	6.87	[148]
KW/394	2.0	$-0.633\,638\,424\,0$	0.11	[150]
JC(8,6)/917	2.0	$-0.633\,638\,871$	0.012	This work
JC(14,12)/16233	2.0	$-0.633\,638\,\underline{926\,5}(2)$	0.0	This work
		s state (n=2) $\mathbf{1s\sigma_g 4d\delta_g\ {}^3\Delta_g}$		
FC-LSE	2.0	$-0.633\,697(25)$	-5.72	[156]
KW/70	2.0	$-0.633\,657\,867$	2.87	[148]
KW/394	2.0	$-0.633\,670\,563\,6$	0.08	[150]
JC(14,12)/9080	2.0	$-0.633\,670\,\underline{925\,50}(8)$	0.0	This work
		(n=1) $\mathbf{1s\sigma_g 4f\delta_u\ {}^1\Delta_u}$		
Full-CI/320	2.0	$-0.633\,93$	0.91	[20]
MRCI^b/284	2.0	$-0.633\,923\,21$	2.40	[172]
JC(6,4)/272	2.0	$-0.633\,934\,070$	0.016	This work
JC(14,12)/9080	2.0	$-0.633\,934\,\underline{144\,964}(1)$	0.0	This work

Our numerical results for $1-3\,\Delta$ states are presented in the Appendix, and are shown in Fig. III.19. Moreover, in Table III.8. we compare our results for Δ symmetry at $R = 2.0$ au (vicinity of the minimum) with all the ab-initio results available in the literature.

Comparison reveals that Wolniewicz's results for J and $S\ ^1\Delta_\mathrm{g}$ and j and $s\ ^3\Delta_\mathrm{g}$ states are accurate up to 0.1 cm^{-1}, which is roughly the uncertainty he had originally assigned to his calculations [150]. This Table reveals that for the S state, the basis JC(14,12) even with different parameters for both sectors, gives rather slow convergence to the CBS limit; therefore, the JC basis is far from optimal for this state. By virtue of high accuracy of our curves we can unambigously assign state configurations by direct comparison with helium values [163]. In particular $1, 2, 3\,\Delta_\mathrm{g}$ and $1, 2, 3\,\Delta_\mathrm{u}$ states start at $R = 0$ as $1s3d$, $1s4d$, $1s5d$, $1s4f$, $1s5f$, and $1s6f$, respectively and this configurations propagate at least up to $R = 5$ au, with the exception of $3\,\Delta_\mathrm{g}$ states which sharply switch to $1s5g$ configuration at $R \sim 0.5$ au.

3.2.3 States of Φ symmetry

Table III.9: Comparison of BO energy of Φ states at $R = 2.0\,au$ with, to the Authors' best knowledge, the only ab-initio results available in the literature for this symmetry. Underlined digits present an improvement with respect to the previous best value.

Method/basis size	$E/\mathrm{hartree}$	$E/\mathrm{hartree}$
	$(n=1)$ $\mathbf{1s\sigma_g 4f\phi_u\ ^1\Phi_u}$	$(n=1)$ $\mathbf{1s\sigma_g 4f\phi_u\ ^3\Phi_u}$
Full-CI/320, Ref. [20]	$-0.633\,72$	$-0.633\,72$
FC-LSE[a], Ref. [156]	$-0.633\,746(24)$	$-0.633\,746(24)$
JC*(5,3)/140	$-0.633\,733\,620$	$-0.633\,733\,849$
JC*(15,13)/12240[b]	$-0.633\underline{733701792}(6)$	$-0.633\,7\underline{33\,908\,758}(2)$
	$(n=1)$ $\mathbf{1s\sigma_g 4g\phi_g\ ^1\Phi_g}$	$(n=1)$ $\mathbf{1s\sigma_g 4g\phi_g\ ^3\Phi_g}$
Full-CI/320, Ref. [20]	$-0.622\,61$	$-0.622\,61$
FC-LSE[a], Ref. [156]	$-0.622\,53(17)$	$-0.622\,53(17)$
JC*(5,3)/140	$-0.622\,625\,783$	$-0.622\,625\,783$
JC*(15,13)/11832[c]	$-0.622\,6\underline{28\,438\,589}(3)$	$-0.622\,6\underline{28\,439\,218}(3)$
	$(n=3)$ $\mathbf{1s\sigma_g 6h\phi_u\ ^1\Phi_u}$	$(n=3)$ $\mathbf{1s\sigma_g 6h\phi_u\ ^3\Phi_u}$
Full-CI/320, Ref. [20]	$-0.613\,77$	$-0.613\,77$
JC*(5,3)/140	$-0.616\,525\,695\,795$	$-0.616\,525\,695\,796$
JC*(15,13)/12240[d]	$-0.61\underline{6\,525\,704\,654\,9}(2)$	$-0.61\underline{6\,525\,704\,656\,4}(2)$

Our numerical results for $1-2\,\Phi$, and $3\,\Phi_\mathrm{u}$ states are presented in the Appendix, the R-dependence is shown in Fig. III.20. In the literature Φ states were calculated only in Ref. [156] using the Free Complement local Schrödinger equation (FC-LSE) method of Nakashima and Nakatsuji [154] and in Ref. [20] using the Full-CI method. In this latter work the results were presented only for a few selected states and at specific points corresponding to the energy minimum and dissociation limit, $R = 2$ au and $R = 100$ au, respectively. Consequently, in Table III.9 we present a comparison to those results at the curve minimum $R = 2$ au. It appears, that for the Φ state, FC-LSE functions do not span the complete Hilbert space with their choice of initial spatial functions. The deviation is slightly smaller than $1\,\mathrm{cm}^{-1}$, and thus larger than the uncertainty estimates. Ultimately though, direct comparison with experimental data is cumbersome, because for such highly excited states the Rydberg electron decouples from the nuclear axis due to nonadiabatic effects and Λ is no longer a good quantum number.

Due to high angular momentum, the curves are very regular. The difference between neighbouring states propagates almost unchanged from those of helium values [163] at $R = 0$ up to around $R = 5$ au. The singly-excited characters of $1, 2\,\Phi_\mathrm{g}$ and $1, 2, 3\,\Delta_\mathrm{u}$ states start at $R = 0$ as $1s5g$, $1s6g$, $1s4f$, $1s5f$, and $1s6f$, respectively and this configurations propagate at least up to $R = 5$ au, with the exception of $3\,\Phi_\mathrm{u}$ states which sharply switch to $1s6h$ configuration at $R \sim 0.3$ au.

3.3 Summary and Conclusions

The Γ symmetry and states with even higher values of Λ can be easily implemented in an analogous manner, although then, 3 or more angular generators are required. In practice it would probably suffer from significant numerical erosion already observed with Φ. On the other hand such states should be pretty easily approximated by relatively simple polarization models. $\Lambda > 4$ entails $l \geq 4$, therefore already all the Γ states should be nonpenetrating to very good approximation. For high Λ Hund's case (b) is not the best starting point due to l-recoupling.

In order to compare our results with the plethora of transitions measured with accuracy reaching $\sim 0.001\,\mathrm{cm}^{-1}$, theoretical values of relativistic, QED, adiabatic, and nonadiabatic corrections are necessary. The importance of the latter is arguably the most significant due to strong nonadiabatic couplings, because in contrast to the well-isolated $X\,^1\Sigma_\mathrm{g}^+$ ground state, energy differences of BO energies between neighboring excited states can be as small as a few cm^{-1}, thus a large magnitude of couplings between adiabatic states is expected[160]. As the principal number increases, one should rather speak of vibronic states and abandon the concept of a series of vibrational states belonging to just one adiabatic PEC.

In recent years explicitly correlated Gaussian (ECG) functions have achieved a great success in high-precision calculations of hydrogen molecule isotopologues, ranging in applications from BO energy [151, 174] and nonadiabatic corrections [175, 176] to relativistic [177–179] and QED [180, 181] corrections. All those calculations, however, were limited to the electronic $X^1\Sigma_\mathrm{g}^+$ ground state.

In the present work we have demonstrated that the Kołos-Wolniewicz bases still find a niche in high-accuracy variational calculations of excited states of a diatomic two-electron molecule, especially for the states with high angular momentum. Alongside with our previous calculations of Σ^+ states [182], present calculations reconcile with all the previous *ab-initio* calculations of BO potentials of H_2 by elucidating the actual accuracy of the former calculations. Numerical uncertainty of Born-Oppenheimer potentials has been alleviated from a level of a few to the millionth parts of cm^{-1}; hence, we have laid the foundation for the evaluation of further corrections to the energy levels, lack of knowledge of which currently hinders comparison with state-of-the-art spectroscopic results.

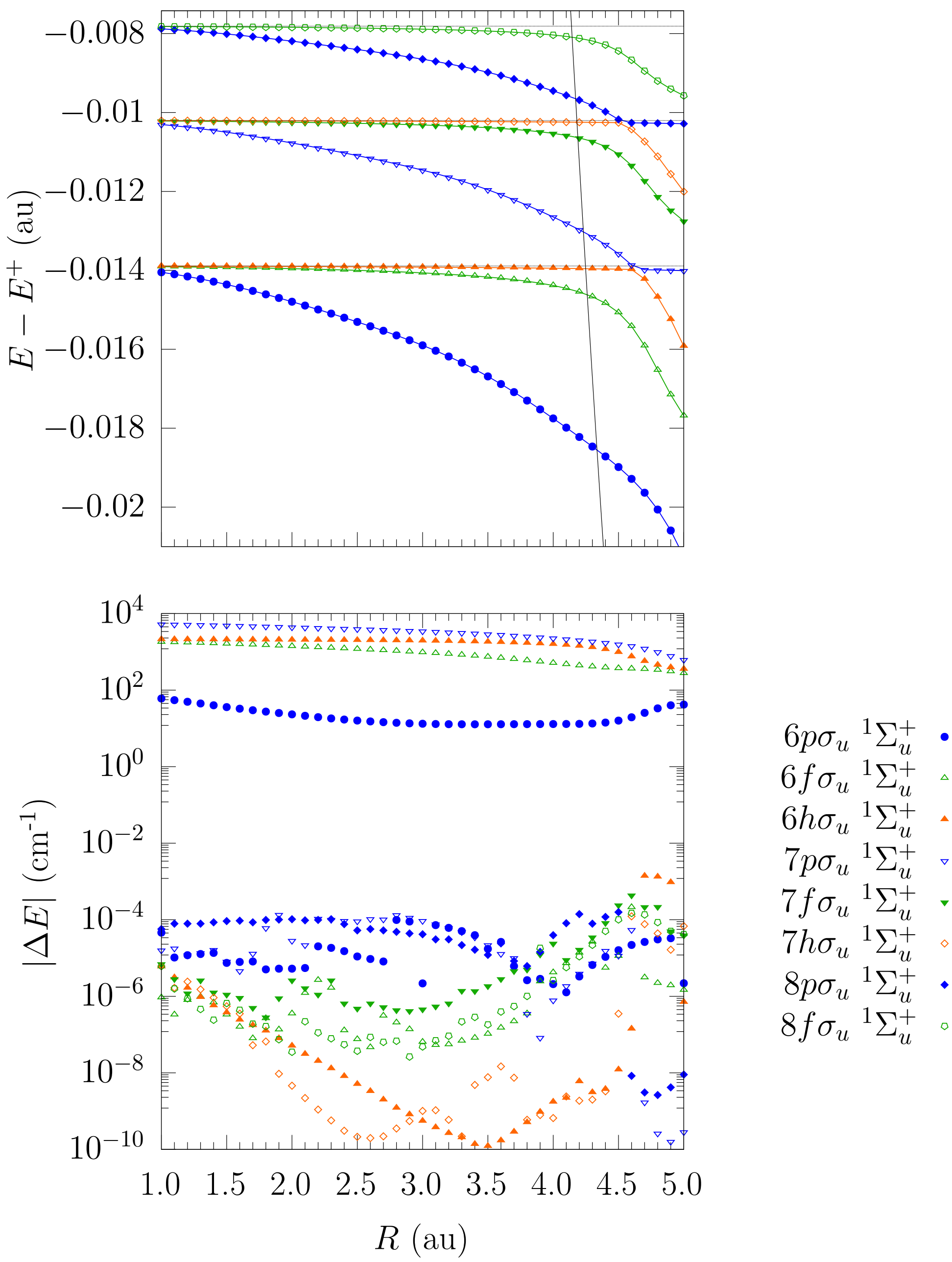


Figure III.13: Pointwise accuracy of unpublished BO potentials with respect to best literature results for higher $^1\Sigma_u^+$ states. (right bottom: sorted by increasing $n = 7, \ldots, 14$). The literature data [142] is color-coded exactly the same but is significantly higher on the bottom accuracy panel. The energy of the lowest doubly-excited diabatic state of this symmetry, $2s\sigma_g 2s\sigma_u$ changes much more rapidly with R and is presented as near vertical line (long-dash, top panel). It interacts with singly-excited configuration of Rydberg states, causing the electrostatic perturbation around $R = 4$ au associated with the observed loss of single-particles character or those abiabatic curves. Especially the outer minimum of $3^1\Sigma_u^+$ can be attributed due to the interaction with $(2p\sigma_u 2s\sigma_g)$, because the singly-excited configuration would approach the $n = 3$ dissociation limit from above.

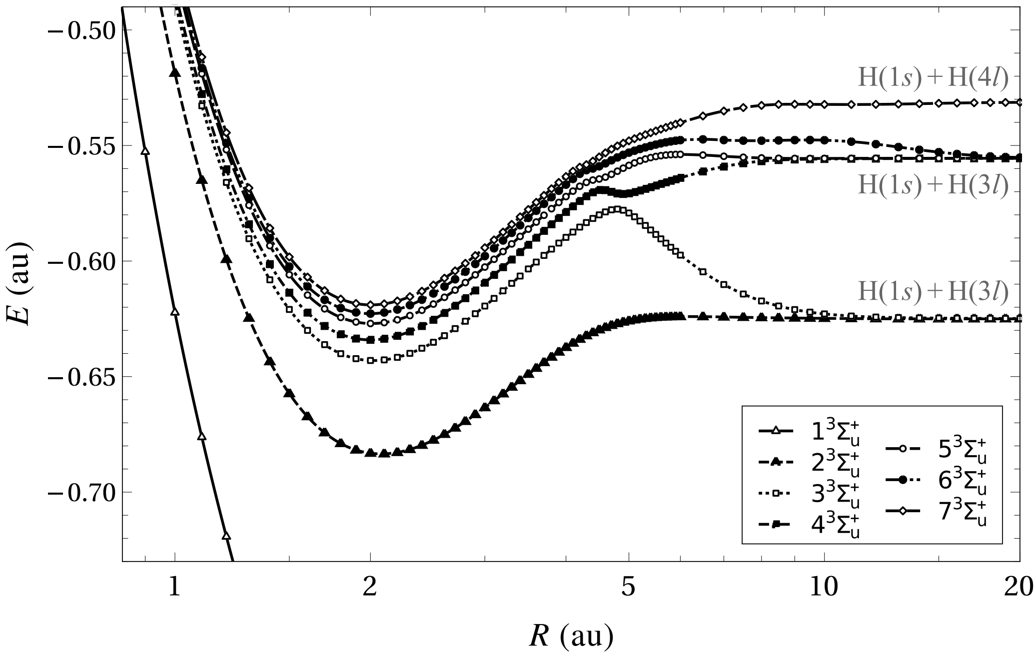


Figure III.14: BO potentials for $n^3\Sigma_u^+$ states, up to $n = 7$, partial curve for $b\,1^3\Sigma_g^+$ from Ref. [39] is shown for reference.

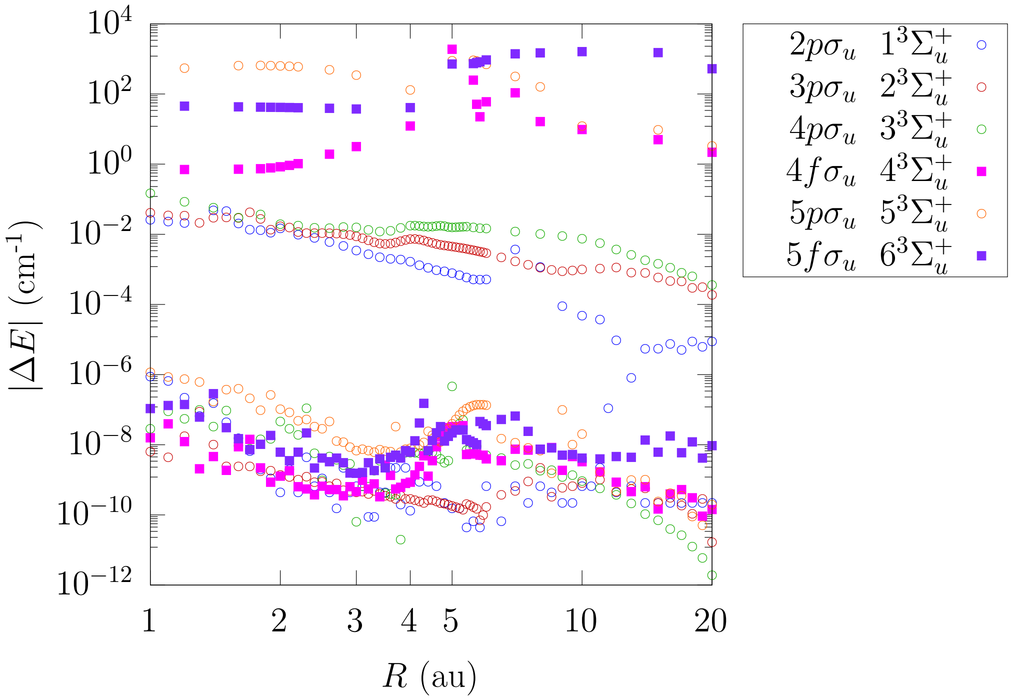


Figure III.15: Comparison of the pointwise accuracy of BO potentials with respect to best literature results for $n^3\Sigma_u^+$ states. Two series of data are color-coded exactly the same, the upper series for $n = 1 - 3$ is from Ref. [124] and for $n = 4 - 6$ from Ref. [118], our data is lower.

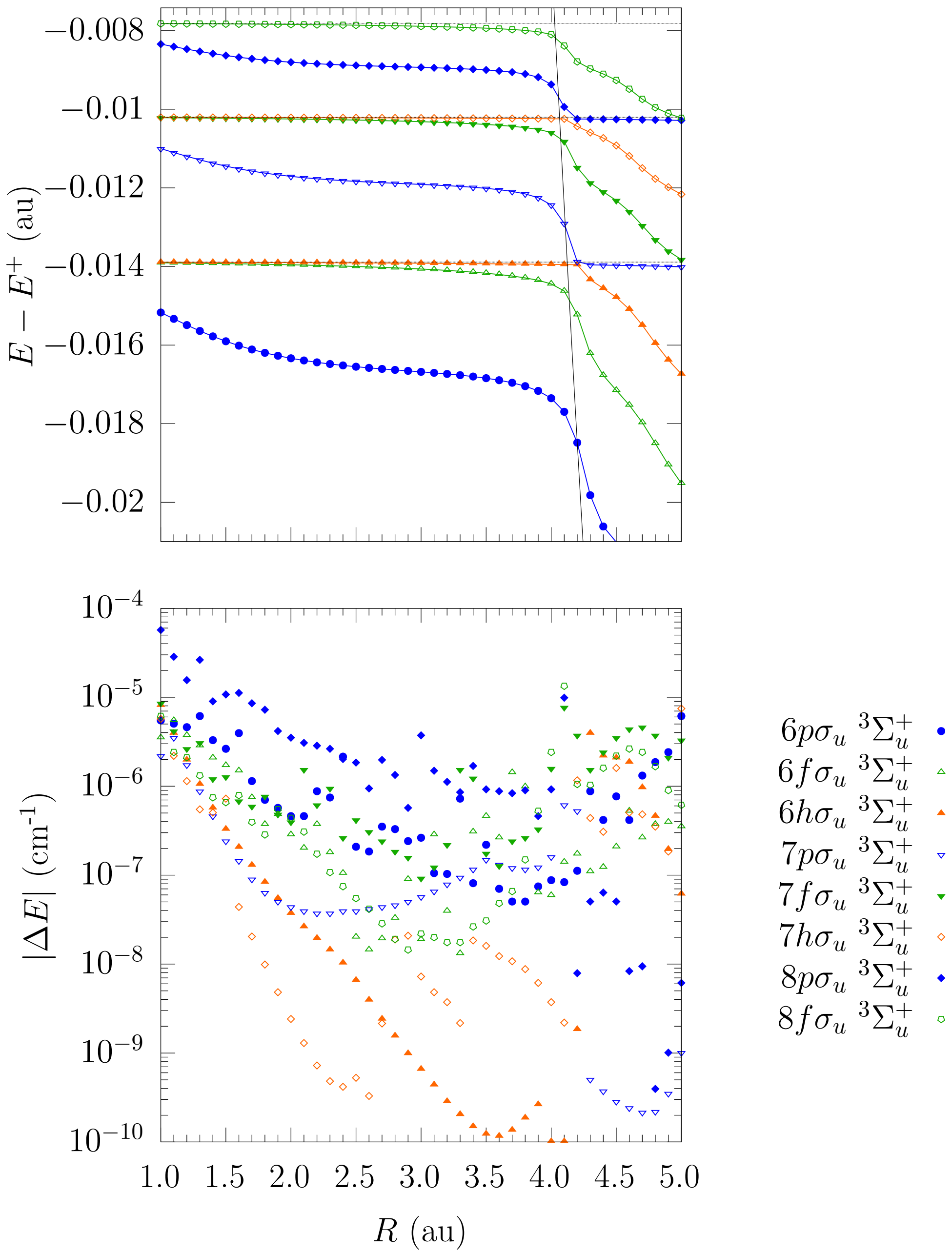


Figure III.16: Pointwise accuracy of unpublished BO potentials with respect to best literature results for higher $^3\Sigma_u^+$ states (right bottom: sorted by increasing $n = 7, \dots, 14$). The literature data is color-coded exactly the same but is significantly higher on the bottom accuracy panel. The energy of the doubly-excited diabatic state of this symmetry changes much more rapidly with R and is presented as near vertical line (long-dash, top panel). A rapid change in the dE/dR can be observed around $R = 4$ au due to the electrostatic perturbation between doubly- ($2p\sigma_u 2n\sigma_g$) and singly-excited character, which induces secondary $p - h$ and $p - f$ mixing.

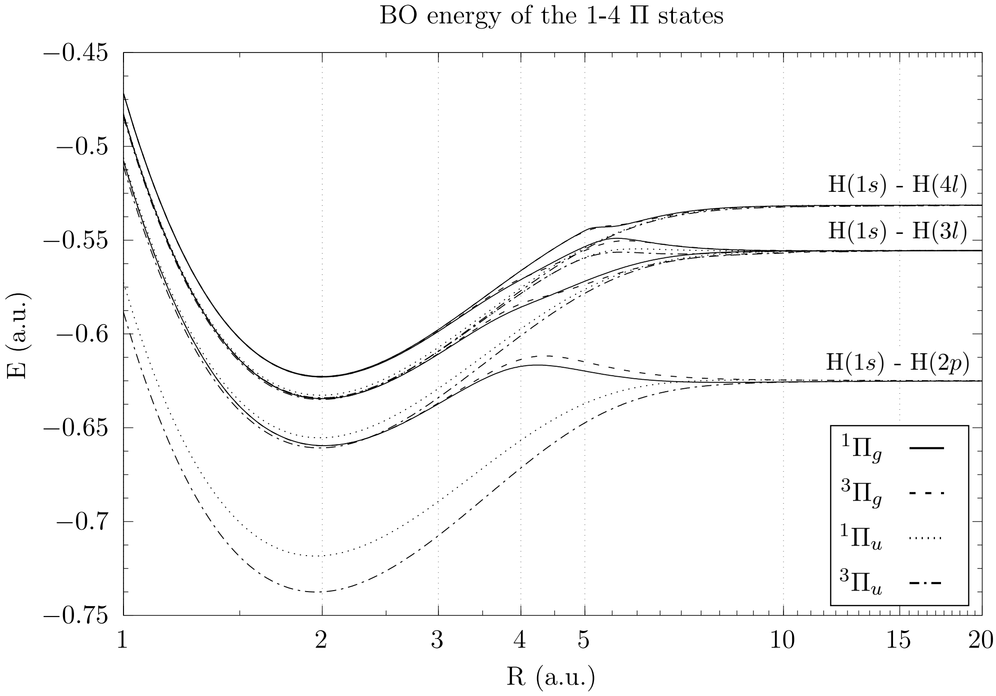


Figure III.17: BO potential for $n = 1..4$ Π states.

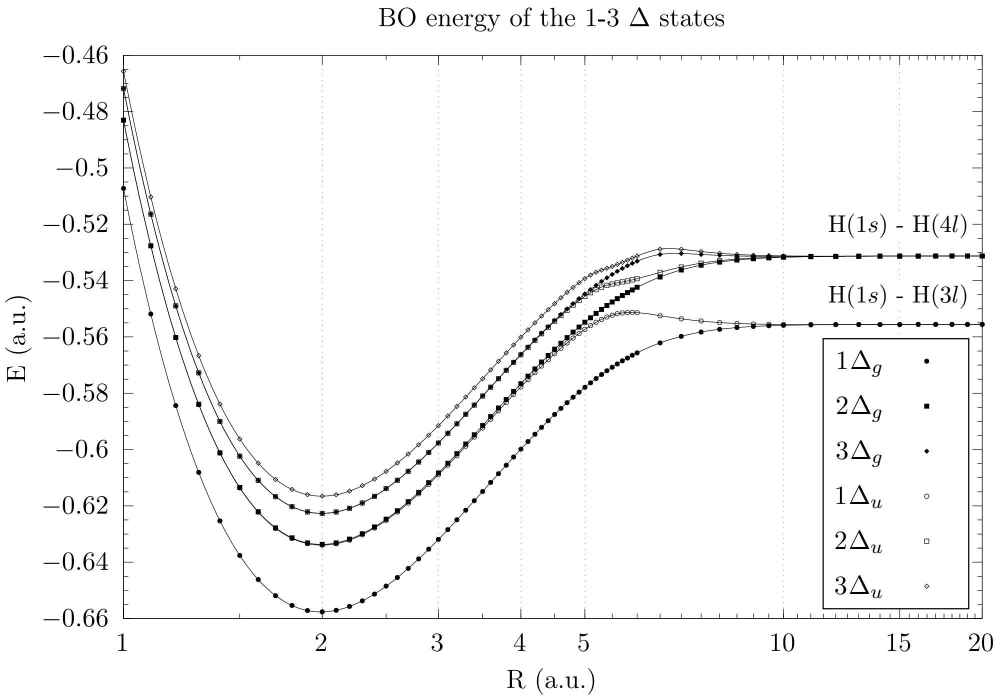


Figure III.19: BO potential for $n = 1..3$ Δ states. The difference between singlet and triplet states for specific gerade/ungerade symmetry and fixed n is indistinguishable on this scale. It amounts to a few cm^{-1} at all distances, peaking at around $R = 3$ au, where it reaches $\sim 15\,cm^{-1}$ for $1\,\Delta_g$.

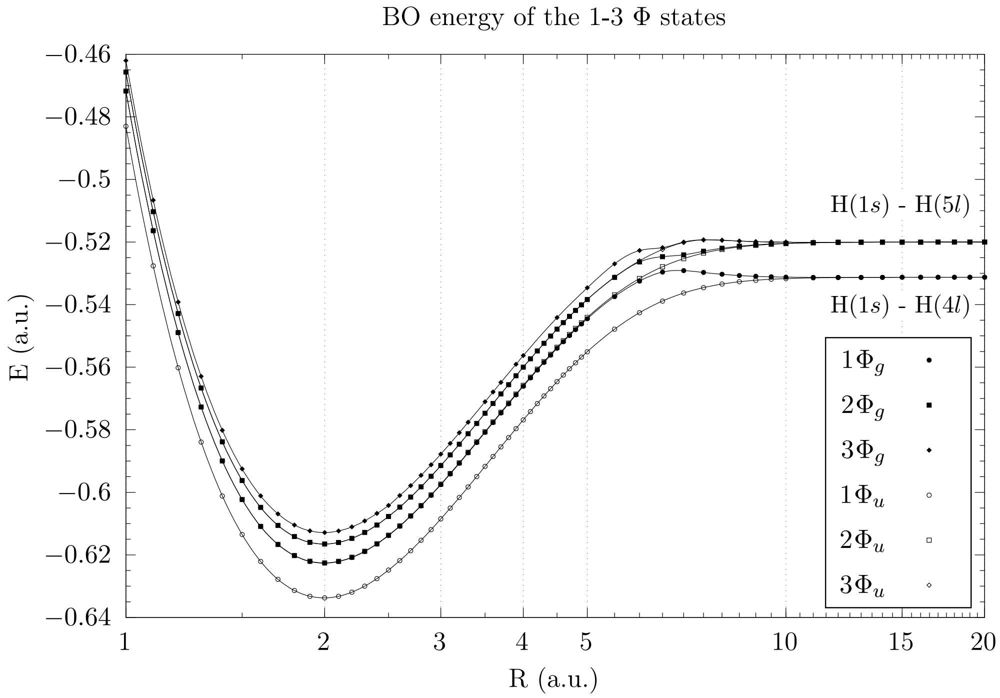


Figure III.20: BO potential for $n = 1..3$ Φ states. The difference between singlet and triplet states for specific gerade/ungerade symmetry and fixed n is indistinguishable on this scale.

CHAPTER IV

ADIABATIC AND NONADIABATIC NONRELATIVISTIC CORRECTIONS

This Chapter presents unpublished results concerning generalization of computational method to heteronuclear systems in general Kolos-Wolniewicz basis. The capability of our method is illustrated by obtaining highly accurate diagonal adiabatic corrections for $B\,^1\Sigma_u^+$, and $EF, GK, H\bar{H}, P, O\,^1\Sigma_g^+$ states.

Although not performed here, we outline the computational approach to offdiagonal couplings, which are required for instance, for solving the strongly-perturbed structure of vibronic $^1\Sigma_g^+$ manifold with the coupled equation approach.

1 Nonadiabatic Perturbation Theory (NAPT)

Since nonrelativistic energy is the largest contribution, the accuracy demand is also very high, reaching relative precision 10^{-13}. For this purpose the most accurate results come from fully nonadiabatic variational four-body calculations in naJC basis [183–186]. Those calculations however are computationally very demanding and have to address each rovibrational state separately and the concept of PEC is abandoned.

For the calculations of the finite nuclear mass effects on the rovibrational spectra one does not have to rely solely on fully nonadiabatic methods. Such effects can be accounted for perturbatively by virtue of recent formulation of Nonadiabatic Perturbation Theory (NAPT) [187, 188]. The starting point of NAPT is the partition of full molecular wavefunction Ψ,

$$\Psi(\mathbf{r}_1,\mathbf{r}_2,\mathbf{R}) = \psi(\mathbf{r}_1,\mathbf{r}_2)\chi(\mathbf{R}) + \delta\Psi_{\mathrm{na}}(\mathbf{r}_1,\mathbf{r}_2,\mathbf{R}), \tag{IV.1}$$

with the usual factorization into electronic and vibrational part stemming from adiabatic approximation and a remainder, which is by definition orthogonal with respect to integration over electronic degrees of freedom $\langle\delta\Psi_{\text{na}}|\,\psi\rangle_{\text{el}} = 0$.

As a starting point one considers full molecular Schrödinger equation,

$$\left[H_{\text{el}} + H_n - E^{(2)}\right] |\psi\chi + \delta\Psi_{\text{na}}\rangle = 0, \tag{IV.2}$$

with some freedom to how the partition into electronic and nuclear Hamiltonian is made. Although most convenient choice is to define H_{el} as the one diagonalizing the electronic adiabatic basis, so that

$$H_{\text{el}} |\psi\rangle = \mathcal{E}_{\text{el}} |\psi\rangle\,. \tag{IV.3}$$

Then the equation is partitioned it as follows,

$$\left[(H_{\text{el}} - \mathcal{E}_{\text{el}}) + (\mathcal{E}_{\text{el}} + H_n - E^{(2)})\right] |\psi\chi + \delta\Psi_{\text{na}}\rangle = 0, \tag{IV.4}$$

because then the action of $(H_{\text{el}} - \mathcal{E}_{\text{el}})$ on ψ vanishes and one can formally solve for $|\delta\Psi_{\text{na}}\rangle$,

$$\begin{aligned}|\delta\Psi_{\text{na}}\rangle =& \mathcal{R}' \left[\mathcal{E}_{\text{el}} + H_n - E^{(2)}\right] |\psi\chi + \delta\Psi_{\text{na}}\rangle \\ =& \mathcal{R}' H_n |\psi\chi\rangle + \mathcal{R}' \left[\mathcal{E}_{\text{el}} + H_n - E^{(2)}\right] |\delta\Psi_{\text{na}}\rangle\end{aligned} \tag{IV.5}$$

To obtain corrections to energy, we reach for the partitioned molecular Schrödinger equationand multiply it from the left by ψ and integrate over electronic degrees of freedom,

$$\langle\psi|\,\mathcal{E}_{\text{el}} + H_n - E^{(2)}\,|\psi\chi\rangle_{\text{el}} + \langle\psi|\,H_n\,|\delta\Psi_{\text{na}}\rangle_{\text{el}}\,. \tag{IV.6}$$

To progress further we have to utilize the actual form of H_n, which unveils the central difficulty behind NAPT calculations – the fact that $\boldsymbol{\nabla}_R$ acts both on ψ and χ. With the use of identities $\langle\psi|\,\boldsymbol{\nabla}_R\,|\psi\rangle =$ and $\langle\psi|\,\boldsymbol{\nabla}_{\text{el}}\,|\psi\rangle = 0$ we obtain one of the central formulas behind NAPT methodology,

$$\left[\mathcal{E}_{\text{el}} + \mathcal{E}^{(2,1)} + H_n - E^{(2)}\right] |\chi\rangle = -\,\langle\psi|\,H_n\,|\delta\Psi_{\text{na}}\rangle_{\text{el}}\,, \tag{IV.7}$$

with $\mathcal{E}^{(2,1)}$ identified as the adiabatic correction to the nuclear motion,

$$\mathcal{E}^{(2,1)} = \langle\psi|\,H_n\,|\psi\rangle\,, \tag{IV.8}$$

with

$$\langle\phi_{\text{el}}|\,\nabla_R^2\,|\phi_{\text{el}}\rangle_{\text{el}} = -\left\langle\vec{\nabla}_R\phi_{\text{el}}\middle|\,\vec{\nabla}_R\phi_{\text{el}}\right\rangle, \tag{IV.9}$$

by virtue of $\vec{\nabla}_R\,\langle\phi_{\text{el}}|\,\phi_{\text{el}}\rangle = 0$, because electronic wavefunction is normalized to a constant. The wavefunction correction is then found as,

$$|\delta\phi_{\rm na}\rangle = |\phi_{\rm el}\delta\chi\rangle + \mathcal{R}'\left[\mathcal{E}_{\rm el} + H_n - \mathcal{E}_a - \delta\mathcal{E}_{na}\right]|\phi_{\rm el}\chi + \delta\phi_{\rm na}\rangle\,, \tag{IV.10}$$

with $\delta\phi_{\rm na}$ neglected in the right-hand side ket, one obtaines the lowest order.

In the context of NAPT, the NRQED expansion of the bound state energy in the fine structure constant α, cf Eq. (**??**), the expansion coefficients $E^{(k)}$ themselves not admit an expansion in the mass ratio m/μ_n and we found it convenient to use the notation $E^{(k,l)}$, for a coefficient in front of $\alpha^k m\ (m/\mu_n)^l$.

With the aim to provide most accurate prediction of rovibrational transitions, NAPT-based $E^{(2,2)}$ results are now deprecated in favor of fully nonadiabatic results obtained with naJC basis [183–186]. Nevertheless, due to substantial computational cost of fully nonadiabatic calculations, they have not covered all rovibrational levels for all the isotopologues (total number of which is on the order of a few hundreds per isotopologue) and $E^{(2,2)}$ still provides the best estimate of the nonrelativistic energy for higher rovibrational states [189].

2 Shifted $\tilde{\nabla}$ operator

As outlined in the Introduction, we are operating in the t-parametrized reference frame, where $t \in (0,1)$ specifies center of reference frame along internuclear axis. In particular, $t = 1/2$ corresponds to the geometrical midpoint between nuclei and $t = \frac{M_A}{M}$ to the CNM coordinates. Then, vectors $\vec{R}_A$ and $\vec{R}_B$ point at nucleus A and B, respectively,

$$\begin{aligned}\vec{R}_A &= (1-t)\vec{R},\\ \vec{R}_B &= -t\vec{R},\end{aligned} \tag{IV.11}$$

and i-th electron position vector attached to appriopriate nucleus A or B is,

$$\begin{aligned}\vec{r}_{iA} &= \vec{r}_i - (1-t)\vec{R},\\ \vec{r}_{iB} &= \vec{r}_i + t\vec{R},\end{aligned} \tag{IV.12}$$

where $\vec{r}_i$ stands for i-th electron position vector in reference frame with geometrical center.

From the point of view of adiabatic and nonadiabatic corrections the t-parametrized form of nuclear Hamiltonian is of central importance,

$$H_n = -\frac{1}{2\mu_n}\tilde{\nabla}^2 - \frac{1}{2M}\nabla^2_{\rm el}, \tag{IV.13}$$

with nuclear reduced mass $\mu_n = (1/M_A + 1/M_B)^{-1}$ and $M = M_A + M_B$ begin total nuclear mass and

$$\tilde{\vec{\nabla}} = \vec{\nabla}_R - \left(t - \frac{M_A}{M}\right)\vec{\nabla}_{\rm el}, \tag{IV.14}$$

with $\vec{\nabla}_{el} = \sum_{i=1}^{N} \vec{\nabla}_i$, running over N electrons. Althought not evident from Eq. (IV.14), action of $\tilde{\vec{\nabla}}$ on electronic wavefunction is t-invariant.

In t-parametrized reference frame we have,

$$
\begin{aligned}
\nabla_R R^n &= nR^{n-1}\hat{R},\\
\nabla_R^2 \hat{R} &= \frac{2}{R},\\
\nabla_R r_{iA} &= (1-t)\,\hat{r}_{iA},\\
\nabla_R r_{iB} &= -t\,\hat{r}_{iB},\\
\nabla_R \hat{r}_{iB} &= -2t\frac{1}{r_{iB}},\\
\nabla_R^2 \hat{r}_{iA} &= 2(1-t)\frac{1}{r_{iA}},\\
\nabla_R^2 \hat{r}_{iB} &= -2t\frac{1}{r_{iB}},
\end{aligned}
\tag{IV.15}
$$

In particular, the choice $t = \frac{M_A}{M_B}$ entails $\tilde{\vec{\nabla}} = \vec{\nabla}_R$ and absence of the $\vec{\nabla}_R \cdot \vec{\nabla}_{\rm el}$ operator, which simplifies the computations.

3 Nonadiabatic corrections

According to NAPT, the leading order nonadiabatic correction to the energy of a molecular level would result [190],

$$E^{(2)}_{\rm na} = \langle \Psi | H_n \mathcal{R}' H_n | \Psi \rangle, \tag{IV.16}$$

where the $\mathcal{R}' \equiv \frac{1}{(\mathcal{E}_{\rm el} - H_{\rm el})'} = \sum_n \frac{1 - |\phi_{\rm el}\rangle\langle\phi_{\rm el}|}{\mathcal{E}_{\rm el} - \mathcal{E}_n}$ is the reduced resolvent. Within NAPT one proceeds perturbatively with adiabatic approximation as the zeroth order ansatz for the total molecular wavefunction, $|\Psi\rangle = |\phi_{\rm el}\chi\rangle$

After integrating out the electronic degrees of freedom, instead of including those corrections to the molecular level energy on the level of nuclear wavefunctions perturbatively by summing appriopriate expectation values, one can alternatively solve nuclear Schrödinger equation in a corrected potential and R-dependent effective masses as,

$$\left[-\frac{1}{R^2}\frac{\partial}{\partial R}\frac{R^2}{2\mu_{\|}(R)}\frac{\partial}{\partial R} + \frac{J(J+1)}{2\mu_{\perp}(R)R^2} + \mathcal{Y}(R)\right]\tilde{\chi}_J(R) = E\tilde{\chi}_J(R), \tag{IV.17}$$

where

$$\mathcal{Y}(R) = \mathcal{E}_{\rm el}(R) + \mathcal{E}_{\rm a} + \delta\mathcal{E}_{\rm na}(R). \tag{IV.18}$$

and

$$\begin{aligned} \frac{1}{2\mu_{\parallel}(R)} &= \frac{1}{2\mu_n} + \mathcal{W}_{\parallel}(R), \\ \frac{1}{2\mu_{\perp}(R)} &= \frac{1}{2\mu_n} + \mathcal{W}_{\perp}(R). \end{aligned} \tag{IV.19}$$

$$\mathcal{W}_{\parallel} \equiv \frac{1}{\mu_n^2}\frac{1}{R^2}\Big\langle \vec{R}\cdot\tilde{\vec{\nabla}}\phi_{\rm el}\Big|\mathcal{R}'\Big|\vec{R}\cdot\tilde{\vec{\nabla}}\phi_{\rm el}\Big\rangle, \tag{IV.20}$$

$$\mathcal{W}_{\perp} \equiv \frac{1}{2\mu_n^2}\left(\delta_{ij} - \frac{R^iR^j}{R^2}\right)\langle\tilde{\nabla}^i\phi_{\rm el}|\mathcal{R}'|\tilde{\nabla}^j\phi_{\rm el}\rangle, \tag{IV.21}$$

$$\delta\mathcal{E}_{\rm na}(R) \equiv \mathcal{U}(R) + \left(\frac{2}{R} + \frac{\partial}{\partial R}\right)\left[\mathcal{V}(R) + \delta\mathcal{V}(R)\right], \tag{IV.22}$$

$$\mathcal{U}(R) \equiv \langle H_n\phi_{\rm el}|\mathcal{R}'|H_n\phi_{\rm el}\rangle, \tag{IV.23}$$

$$\mathcal{V}(R) \equiv \frac{1}{\mu_n R}\left\langle H_n\phi_{\rm el}|\mathcal{R}'|R^i\tilde{\nabla}^i\phi_{\rm el}\right\rangle. \tag{IV.24}$$

and $\delta\mathcal{V}(R)$ which arises from third order of NAPT, but contributes to the μ_n^{-2} order, ought to be defined as[1],

$$\delta\mathcal{V}(R) \equiv \frac{\partial_R\mathcal{E}_{\rm el}}{2\mu_n^2R^2}\left\langle R^i\tilde{\nabla}^i\phi_{\rm el}\big|(\mathcal{R}')^2\big|R^j\tilde{\nabla}^j\phi_{\rm el}\right\rangle \tag{IV.25}$$

It is worth noting that including corrections to effective masses directly in the nuclear equation, rather than perturbatively, also admixtures some effects from higher order in $\frac{m}{\mu_n}$.

We also point out that the action of radial part of $\tilde{\nabla}$ on $\phi_{\rm el}$ scales as $\mu_n^{1/4}$ therefore effective order of correction from $\mathcal{W}_{\parallel}$ is $\mu_n^{-3/2}$ rather than μ_n^{-2} [187, 191]. As a result, estimates of higher order nonadiabatic effects ought to be of relative order $(m/\mu_n)^{1/2}$ with respect to the leading order corrections, rather than $(m/\mu_n)^1$.

Ultimately, the nondiabatic corrections in the second order enter not only through the additional contribution to the effective potential $\mathcal{Y}(R)$ in which nuclear dynamics needs to be solved, but also as the modification of effective reduced nuclear masses.

3.1 Implementation in Kołos-Wolniewicz basis

Here we present implementation of nonrelativistic nonadiabatic corrections in general Kolos-Wolniewicz basis for reference frame centered on any point along the internuclear axix. The implementation is substantially different previously performed in the Explicitly Correlated Gaussian (ECG) basis [190].

[1] The multiplicative dependence of $\delta\mathcal{V}(R)$ on $\partial_R\mathcal{E}_{\rm el}$ implies its blowup as $R \to 0$

We recall the definition of an auxiliary vector u (see also Eq. (32) of Ref. [192]).

$$u_k \equiv \langle \Psi_k | \partial_R \phi_{\rm el} \rangle = \sum_l \left(\mathcal{A}_{kl} v_l + \mathcal{N}_{kl} \partial_R v_k \right). \tag{IV.26}$$

By applying the $\mathbf{\nabla}_R$ to Schrödinger equationwe have,

$$\vec{\nabla}_R \phi_{\rm el} = \mathcal{R}' \vec{\nabla}_R (V) \phi_{\rm el}, \tag{IV.27}$$

and in t-parameterized reference frame we have

$$\vec{\nabla}_R (V) = \sum_i^N \left[-Z_A \left(1-t\right) \frac{\vec{r}_{iA}}{r_{iA}^3} + t Z_B \frac{\vec{r}_{iB}}{r_{iB}^3} \right] - Z_A Z_B \frac{\vec{R}}{R^3}. \tag{IV.28}$$

This expression, however, involves integrals with negative second powers of the interparticle coordinates which, though recently have become managable in the ECG basis, remain very problematic to evaluate in the Kolos-Wolniewicz basis.

Hence, instead of utilizing the formula (IV.27), we take the advantage of explicit R-dependence of KW basis functions and obtain an action of ∂_R by direct differentiation of coresponding matrix elements, formulas for which can be conveniently expressed in terms of f-integrals.

Nevertheless, evaluation of the action of $\partial_R \vec{v}$ is still required, and it is probably most conveniently obtained indirectly by differentiation of the Schrödinger equation [144],

$$\partial_R \vec{v} = \mathcal{R}' \left(\partial_R \mathcal{H} - \mathcal{E}_{\rm el} \partial_R \mathcal{N} \right) \vec{v} - \frac{1}{2} \vec{v} (\vec{v}^T \partial_R \mathcal{N} \vec{v}) \tag{IV.29}$$

In view of the different form of H_n in the center of mass system, given by Eq. (IV.13), we explicitly separate the purely electronic part from the auxiliary vector w, originally defined by Eq. (34) of Ref. [192],

$$w_l \equiv \langle \Psi_l | \nabla_R^2 \phi_{\rm el} \rangle = \sum_k \left(\mathcal{N}_{lk} \partial_R^2 + \frac{2}{R} \mathcal{N}_{lk} \partial_R + 2 \mathcal{A}_{lk} \partial_R + C_{lk} \right) v_k, \tag{IV.30}$$

$$y_l \equiv \langle \Phi_l | \nabla_{\rm el}^2 \phi_{\rm el} \rangle = \sum_k C_{lk}^{(\rm el)} v_k, \tag{IV.31}$$

with

$$\begin{aligned} C_{kl} &\equiv \langle \Psi_k | \nabla_R^2 \Psi_l \rangle, \\ C_{kl}^{(\rm el)} &\equiv \langle \Psi_k | \nabla_{\rm el}^2 \Psi_l \rangle. \end{aligned} \tag{IV.32}$$

An auxiliary vector w requires the knowledge of $\partial_R^2 \vec{v}$. Analogously to $\partial_R \vec{v}$, it can be obtained by direct double differentiation of the Schrödinger equation,

$$\begin{aligned}\partial_R^2\vec{v} = \mathcal{R}'\Big[&2\left(\partial_R\mathcal{H} - \partial_R\mathcal{E}_{\rm el}\mathcal{N} - \mathcal{E}_{\rm el}\partial_R\mathcal{N}\right)\partial_R\vec{v} \\ &+ \left(\partial_R^2\mathcal{H} - \mathcal{E}_{\rm el}\partial_R^2\mathcal{N} - 2\partial_R\mathcal{E}_{\rm el}\partial_R\mathcal{N}\right)\vec{v}\Big] \\ &- \left(\partial_R\vec{v}^T\mathcal{N}\partial_R\vec{v} + 2\partial_R\vec{v}^T\partial_R\mathcal{N}\vec{v} + \frac{1}{2}\vec{v}^T\partial_R^2\mathcal{N}\vec{v}\right)\vec{v}\end{aligned} \tag{IV.33}$$

where the term proportional to $\vec{v}$ is obtained by utilizing the auxiliary condition, $\partial_R^2\left(\vec{v}^T\mathcal{N}\vec{v}\right) = 0$. Accordingly, the potentials $\mathcal{U}(R)$, $\mathcal{V}(R)$ and $\delta\mathcal{V}(R)$ are expressed in terms of auxiliary vectors as,

$$\mathcal{U}(R) = \frac{1}{4\mu_n^2}w^T\mathcal{R}w + \frac{1}{2\mu_n M}w^T\mathcal{R}y + \frac{1}{4M^2}y^T\mathcal{R}y, \tag{IV.34}$$

$$\mathcal{V}(R) = -\frac{1}{2\mu_n^2}u^T\mathcal{R}w - \frac{1}{2\mu_n M}u^T\mathcal{R}y, \tag{IV.35}$$

$$\delta\mathcal{V}(R) = \frac{1}{2\mu_n^2 R^2}\,\partial_R\mathcal{E}_{\rm el}\,u^T\mathcal{R}^T\mathcal{N}\mathcal{R}u \tag{IV.36}$$

By virtue of t-invariant action of $\tilde{\nabla}$ on $\phi_{\rm el}$, the potentials $\mathcal{W}_{||}$, $\mathcal{W}_{\perp}$, and $\delta\mathcal{V}$ have the same functional form independently from chosen value of t.

4 Adiabatic correction

In the previous Section we have identified $\mathcal{E}^{(2,1)}$ as the adiabatic correction to the nuclear motion,

$$\mathcal{E}^{(2,1)} = \langle\psi|\,H_n\,|\psi\rangle\,, \tag{IV.37}$$

which is given as an expectation value of zeroth order nuclear Hamiltonian and modifies the effective potential in which the eigenproblem of nuclear wavefunction is solved,

$$\mathcal{E}^{\rm ad} \equiv \mathcal{E}^{(2,1)} = \langle\psi|\,H_n\,|\psi\rangle = -\frac{1}{2\mu_n}\langle\psi|\,\tilde{\nabla}^2\,|\psi\rangle - \frac{1}{2M}\langle\psi|\,\nabla_{\rm el}^2\,|\psi\rangle\,. \tag{IV.38}$$

Due to the t-invariance of the $\tilde{\nabla}$ operator it is independent from the reference frame. In can be expressed in terms of auxiliary quantities introduced in previous Section as,

$$\mathcal{E}^{\rm ad} = -\frac{1}{2M}\vec{v}^T\mathcal{B}_{\rm el}\vec{v} + \frac{1}{2\mu_n}\left[\vec{v}^T\mathcal{B}\vec{v} + (\partial_R\vec{v})^T\mathcal{N}(\partial_R\vec{v}) + 2(\partial_R\vec{v})^T\mathcal{A}\vec{v}\right] \tag{IV.39}$$

this method requires solving a resolvent equation within the same symmetry, thus $\partial_R\vec{v}$, Eq. (**??**) acquires contributions from *all* states within the symmetry block of the reference state. In Table IV.1 we present the potential of this computational method as applied to a few $^1\Sigma^+$ states and plot the R-behaviour of the diagonal adiabatic correction on Fig. IV.1. The diagonal adiabatic correction is asymptotically dominated by the centrifugal term as[193] $\frac{L(L+1)-2\Lambda^2}{2\mu_n R^2}$, as $R \to 0$, where L pertains to the orbital angular momentum in the united-atom limit, which is well visible in the plots, as the result of s and d singly-excited character transfer near $R = 1$ au.

Table IV.1: $\mu_n/m\mathcal{E}^{(2,1)}$ in au for a few $^1\Sigma^+$ states. Due to rescaling by a factor of μ_n/m, those are valid for all isotopologues. Results up to $R = 5$ au are calculated with nonsymmetric James-Coolidge basis ($\Omega \leq 15$). For larger R, we use unrestricted Kolos-Wolniewicz basis ($\Omega \leq 13$).

R	EF $2^1\Sigma_g^+$	GK $3^1\Sigma_g^+$	H$\bar{H}$ $4^1\Sigma_g^+$	P $5^1\Sigma_g^+$	O $6^1\Sigma_g^+$	B $1^1\Sigma_u^+$
0.7	0.93608697(2)	0.8840863(6)	13.05395453(4)	0.867841(7)	13.0419501(2)	4.9712287717(7)
0.8	0.891741254(10)	0.8405170(3)	10.143135347(6)	0.824431(6)	10.13116939(8)	3.9806660212(9)
0.9	0.850442076(6)	0.8000357(2)	8.1384388(2)	0.784053(4)	8.126475(2)	3.295531817(2)
1.0	0.81248023(2)	0.7644172(3)	6.69911(3)	0.7543(2)	6.691(2)	2.801648851(2)
1.1	0.777860953(8)	5.626764(2)	0.729112(2)	5.61450(2)	0.713254(4)	2.4339855671(9)
1.2	0.746446900(8)	4.8078827(3)	0.6980830(2)	4.796183(6)	0.682758(3)	2.153176612(2)
1.3	0.718037907(6)	4.16791252(10)	0.6702102(2)	4.156458(3)	0.655109(3)	1.934160176(3)
1.4	0.692415307(6)	3.65806177(8)	0.6450723(2)	3.646887(3)	0.630167(3)	1.760281639(3)
1.5	0.669367111(5)	3.24536492(6)	0.6224583(2)	3.234570(2)	0.607752(2)	1.620057837(3)
1.6	0.648703260(4)	2.90686465(5)	0.60220076(9)	2.896624(2)	0.587716(2)	1.505320078(3)
1.7	0.630267081(4)	2.62625302(4)	0.58418870(10)	2.616866(2)	0.569975(2)	1.410109177(3)
1.8	0.613947608(4)	2.39183571(4)	0.56839725(7)	2.383834(2)	0.5545608(10)	1.329996977(3)
1.9	0.599697974(3)	2.19532801(4)	0.55494351(6)	2.189715(2)	0.5416965(8)	1.261655863(4)
2.0	0.587567959(3)	2.03127508(4)	0.54420189(5)	2.030076(2)	0.5319798(7)	1.202574150(4)
2.1	0.577765703(2)	1.89713286(3)	0.53705388(4)	1.904773(2)	0.5267969(5)	1.150857690(4)
2.2	0.570779841(2)	1.79443103(3)	0.53546493(3)	1.821515(2)	0.5293439(3)	1.105083284(4)
2.3	0.567631252(2)	1.73235534(2)	0.543917548(8)	1.807147(2)	0.547407114(5)	1.064185001(4)
2.4	0.5704162398(9)	1.73760617(4)	0.57328089(2)	1.94487901(5)	0.6017482(5)	1.027363795(4)
2.5	0.5835400857(3)	1.8811041(2)	0.65228279(5)	2.504289(6)	0.754632(2)	0.994015790(4)
2.6	0.6166724373(3)	2.3425190(6)	0.86469139(8)	4.32430(3)	1.217622(3)	0.963676713(4)

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Table IV.1 – *Continued from previous page*

R	EF $2^1\Sigma_g^+$	GK $3^1\Sigma_g^+$	H$\bar{H}$ $4^1\Sigma_g^+$	P $5^1\Sigma_g^+$	O $6^1\Sigma_g^+$	B $1^1\Sigma_u^+$
2.7	0.6921680594(5)	3.469443(2)	1.4730061(2)	8.48527(7)	2.737144(3)	0.935980411(4)
2.8	0.863961788(8)	5.204101(2)	3.205939(3)	10.87046(2)	6.71721(8)	0.910629232(4)
2.9	1.26063267(4)	5.678069(2)	6.381124(2)	9.91848(3)	8.4000(2)	0.887373811(4)
3.0	2.1266756(2)	4.7203101(3)	6.481648(10)	6.916837(6)	4.43450(5)	0.865999854(4)
3.1	3.5053297(4)	4.5665729(8)	3.6258875(2)	3.144052(2)	2.203350(6)	0.846319772(4)
3.2	4.1823836(3)	4.4358421(5)	2.0183443(9)	1.435515(2)	1.452392(6)	0.828167460(5)
3.3	3.23751111(7)	3.11776478(7)	1.3981006(5)	0.8514093(8)	1.175611(3)	0.811394983(5)
3.4	2.09329687(2)	1.82465281(8)	1.1464138(2)	0.6426557(4)	1.050738(2)	0.795870319(5)
3.5	1.46143538(2)	1.14370784(7)	1.02827349(6)	0.5597955(3)	0.9820251(5)	0.781475680(5)
3.6	1.168344313(3)	0.84262694(5)	0.96353491(2)	0.5240557(2)	0.93756982(3)	0.768106094(5)
3.7	1.026967242(2)	0.71079233(3)	0.92284595(5)	0.5082148(2)	0.9052585(3)	0.755668141(5)
3.8	0.950078129(5)	0.65156821(2)	0.89433621(6)	0.50177368(8)	0.8799086(4)	0.744078755(6)
3.9	0.901780216(6)	0.62496390(2)	0.87270689(7)	0.50023517(7)	0.8590578(4)	0.733264111(6)
4.0	0.867122840(7)	0.614003347(7)	0.85535469(8)	0.50147106(6)	0.8414343(5)	0.723158568(6)
4.1	0.839586500(7)	0.611008970(5)	0.84087506(8)	0.50436869(5)	0.8263602(5)	0.713703704(6)
4.2	0.816182515(7)	0.612234202(4)	0.82844203(9)	0.50828480(5)	0.8135178(5)	0.704847436(6)
4.3	0.795475919(8)	0.615695487(4)	0.81753808(8)	0.51281204(5)	0.8028817(4)	0.696543222(7)
4.4	0.776746438(8)	0.620253133(3)	0.80783299(9)	0.51767629(5)	0.7947474(4)	0.688749377(7)
4.5	0.75961352(2)	0.625203240(4)	0.7991283(2)	0.52269180(2)	0.7898412(3)	0.681428438(8)
4.6	0.743861205(9)	0.630089473(2)	0.79133093(9)	0.52774155(5)	0.78953020(7)	0.674546643(8)
4.7	0.729353312(9)	0.634613064(2)	0.78443271(9)	0.53276734(5)	0.7961725(2)	0.668073465(8)
4.8	0.715991990(10)	0.638587159(2)	0.77849440(9)	0.53776149(5)	0.8136730(5)	0.661981208(9)

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Table IV.1 – *Continued from previous page*

R	EF $2^1\Sigma_g^+$	GK $3^1\Sigma_g^+$	H$\bar{H}$ $4^1\Sigma_g^+$	P $5^1\Sigma_g^+$	O $6^1\Sigma_g^+$	B $1^1\Sigma_u^+$
4.9	0.703697222(10)	0.641910578(2)	0.77362238(9)	0.54275625(5)	0.8482644(10)	0.656244680(10)
5.0	0.69239709(2)	0.644549318(2)	0.76994252(10)	0.54780986(4)	0.909297(2)	0.650840879(10)
5.1	0.68202346(4)	0.646520772(2)	0.7675711(2)	0.55299020(4)	1.008963(5)	−−
5.2	0.67251056(4)	0.6478790446(6)	0.7665871(2)	0.55835752(4)	1.157796(6)	−−
5.3	0.66379443(4)	0.6487013502(7)	0.7670067(2)	0.56394882(4)	1.350620(8)	0.63642379(4)
5.4	0.65581337(6)	0.6490761614(2)	0.7687649(5)	0.56976557(4)	1.54413(2)	−−
5.5	0.64850845(3)	0.6490936544(2)	0.7717082(2)	0.57576625(4)	1.655607(4)	0.62813304(3)
5.6	0.64182353(6)	0.6488387832(4)	0.7755903(5)	0.58186448(5)	1.6220712(3)	−−
5.7	0.63570619(6)	0.6483869002(3)	0.7800903(4)	0.58793300(5)	1.466956(5)	−−
5.8	0.63010734(8)	0.6478015751(4)	0.7848300(4)	0.59381290(5)	1.271812(2)	0.6173851(9)
5.9	0.62498170(8)	0.6471341079(6)	0.7894089(4)	0.59932745(5)	1.100264(2)	0.6142038(5)
6.0	0.62028767(2)	0.64642420405(5)	0.79344108(4)	0.60429887(6)	0.9731652(6)	0.6112045(5)
6.5	0.60206972(2)	0.6430036241(4)	0.79695699(10)	0.61674828(5)	0.73827105(2)	0.59864106(5)
7.0	0.59021862(2)	0.6404097632(6)	0.7752075(2)	0.60965576(4)	0.67405799(3)	0.58947403(3)
7.5	0.58260714(3)	0.638536740(2)	0.7484428(2)	0.59664576(2)	0.63565965(2)	0.58307405(4)
8.0	0.57809527(2)	0.637117802(2)	0.7264909(2)	0.58657515(2)	0.611966597(3)	0.57909372(4)
8.5	0.57620103(8)	0.635992382(2)	0.7096472(3)	0.5802949426(6)	0.597892747(5)	0.57745704(4)
9.0	0.5769360(2)	0.635083523(2)	0.6965838(3)	0.5764831073(10)	0.589539434(9)	0.57837298(5)
9.5	0.58071969(4)	0.634360878(2)	0.6864722(3)	0.574098615(2)	0.58453739(2)	0.58233139(4)
10.0	0.58821690(3)	0.633824902(2)	0.6789289(2)	0.57252505(2)	0.581490596(8)	0.58995458(4)
11.0	0.614470183(4)	0.63349390(2)	0.6683829(10)	0.5703044(3)	0.57799383(2)	0.615537445(5)
12.0	0.638771725(5)	0.63520620(6)	0.6476144(10)	0.56820315(4)	0.57531346(2)	0.63771513(3)

Continued on next page

Table IV.1 – *Continued from previous page*

R	EF $2^1\Sigma_g^+$	GK $3^1\Sigma_g^+$	H$\bar{H}$ $4^1\Sigma_g^+$	P $5^1\Sigma_g^+$	O $6^1\Sigma_g^+$	B $1^1\Sigma_u^+$
13.0	0.646476207(6)	0.642714(2)	0.612091(8)	0.5663319765(10)	0.572839198(7)	0.64364308(3)
14.0	0.65848735(7)	0.6609656(3)	0.585657(3)	0.564919776(5)	0.570725986(4)	0.64974935(4)
15.0	0.66356483(4)	0.66989515(4)	0.5720651(10)	0.56386339(2)	0.568961221(2)	0.65236479(3)
16.0	0.64442804(4)	0.6518554(2)	0.565399(3)	0.56302754(5)	0.5674730788(3)	0.64361436(2)
17.0	0.63104882(4)	0.63817107(8)	0.561972(4)	0.56233621(9)	0.566204822(2)	0.63561394(9)
18.0	0.62666136(3)	0.6331403(4)	0.560129(4)	0.5617511(2)	0.565115246(3)	0.63203238(7)
19.0	0.625456346(9)	0.63129459(2)	0.5591346(6)	0.5612503(4)	0.564172993(5)	0.63056321(5)
20.0	0.625128261(3)	0.630395445(5)	0.5586138(8)	0.5608182(7)	0.563353431(8)	0.62981561(5)

5 Nonadiabatic couplings

5.1 Radial couplings

For the sake of setting up coupled equations and diabetization of quantum defects we are interested in calculation of the first-, $\langle\phi'|\frac{d}{dR}|\phi\rangle$, and second-order, $\langle\phi'|\frac{d^2}{dR^2}|\phi\rangle$, radial coupling elements between two adiabatic electronic states.

To the best of our knowledge the actual implementation of such couplings is usually performed according to one of three ways,

- by commuting derivatives over R with the electronic Hamiltonian, thus obtaining terms $\sim \nabla_R(V)$,
- direct implementation of the action of the R-derivative on constant basis functions,
- numerical implementation of ∂R by its action on PECs,

We recall the formula for the R-derivative of the eigenvector, Eq. (IV.29),

$$\partial_R\vec{v} = \mathcal{R}'_n\left(\partial_R\mathcal{H} - \mathcal{E}_{\mathrm{el}}\partial_R\mathcal{N}\right)\vec{v} - \frac{1}{2}\vec{v}(\vec{v}^T\partial_R\mathcal{N}\vec{v}), \tag{IV.40}$$

where by $\vec{v}$ we denote the eigenvector (vector of linear coefficients) pertaining to the n-th eigenvalue, $\mathcal{E}_n$, and $\mathcal{R}'_n$ pertains to the reduced resolvent with the n-th eigenstate projected-out.

First-order radial coupling

First-order radial coupling, $\langle\phi'|\frac{d}{dR}|\phi\rangle$, between two adiabatic electronic states can be represented as,

$$\langle\phi'|\frac{d}{dR}|\phi\rangle = \vec{v}^{T\prime}\left(\mathcal{N}\partial_R\vec{v} + \mathcal{A}\vec{v}\right), \tag{IV.41}$$

where $\mathcal{A}_{kl} = \langle\Psi_k|\,\vec{v}(\partial_R\Psi_l)\rangle$ and $\vec{v'}$ pertains to the n'-th eigenstate. The first term arises from differentiation of the linear coefficients vector while keeping the basis functions constant as a functions of R and vice-versa for the second term – the basis functions are differentiated with respect to R, while the linear coefficients are kept constant with respect to R.

We take the advantage of the representation of reduced resolvent as a weighted sum over all the eigenstates of electronic Hamiltonian,

$$\mathcal{R}'_n = \sum_{i\neq n}\frac{1-|i\rangle\langle i|}{\mathcal{E}_n - \mathcal{E}_i} \tag{IV.42}$$

and the orthogonality of adiabatic states,

$$\langle i \mid n \rangle \sim \delta_{in}, \tag{IV.43}$$

so that after the multiplication from the left by $\vec{v'}^T$, the radial coupling expectation value simplifies to,

$$\vec{v'}^{\mathrm{T}} \partial_R \vec{v} = \frac{\vec{v'}^T \left(\partial_R \mathcal{H} - \mathcal{E}_n \partial_R \mathcal{N} \right) \vec{v}}{\mathcal{E}_n - \mathcal{E}_{n'}}. \tag{IV.44}$$

Then first-order radial coupling is given by,

$$\vec{v'}^{\mathrm{T}} \partial_R \vec{v} + \vec{v'}^{\mathrm{T}} \mathcal{A} \vec{v} = \vec{v'}^T \left(\frac{\partial_R \mathcal{H} - \mathcal{E}_n \partial_R \mathcal{N}}{\mathcal{E}_n - \mathcal{E}_{n'}} + \mathcal{A} \right) \vec{v} \tag{IV.45}$$

This representation explicitly manifests the sensitivity of radial coupling matrix element to the proximity in energy between two given adiabatic states.

Eq. (IV.45) is then employed as a working formula and the matrices $\partial_R \mathcal{H}$, $\partial_R \mathcal{N}$ and $\mathcal{A}$ can be straighforwardly implemented in Kolos-Wolniewicz basis. Crucially, this way of computation does not require solving the resolvent equation.

As of present, the best accuracy of such of diagonal couplings we have reached is $\sim 10^{-8}$ and is a few orders lower than accuracy of energy. The dependence of radial couplings on the basis and its convergence is yet to be investigated and presented elsewhere.

Second-order radial coupling

In second-order radial coupling element, $\langle \phi' | \frac{d^2}{dR^2} | \phi \rangle$, the most problematic term

$$\begin{aligned} \partial_R^2 \vec{v} = \mathcal{R}'_n \Big[& 2 \left(\partial_R \mathcal{H} - \partial_R \mathcal{E}_n \mathcal{N} - \mathcal{E}_n \partial_R \mathcal{N} \right) \partial_R \vec{v} \\ & + \left(\partial_R^2 \mathcal{H} - \mathcal{E}_n \partial_R^2 \mathcal{N} - 2 \partial_R \mathcal{E}_n \partial_R \mathcal{N} \right) \vec{v} \Big] \\ & - \left(\partial_R \vec{v}^T \mathcal{N} \partial_R \vec{v} + 2 \partial_R \vec{v}^T \partial_R \mathcal{N} \vec{v} + \frac{1}{2} \vec{v}^T \partial_R^2 \mathcal{N} \vec{v} \right) \vec{v} \end{aligned} \tag{IV.46}$$

can be simplified when left-multiplied by another eigenvector $\vec{v}'$,

$$\begin{aligned} \vec{v'}^{\mathrm{T}} \partial_R^2 \vec{v} = \frac{1}{\mathcal{E}_n - \mathcal{E}_{n'}} \Big[& 2 \vec{v'}^{\mathrm{T}} \left(\partial_R \mathcal{H} - \partial_R \mathcal{E}_n \mathcal{N} - \mathcal{E}_n \partial_R \mathcal{N} \right) \partial_R \vec{v} \\ & + \vec{v'}^{\mathrm{T}} \left(\partial_R^2 \mathcal{H} - \mathcal{E}_n \partial_R^2 \mathcal{N} - 2 \partial_R \mathcal{E}_n \partial_R \mathcal{N} \right) \vec{v} \Big], \end{aligned} \tag{IV.47}$$

but in contrary to the first-order case, here in the first term one cannot infer orthogonality of $\partial_R \vec{v}$, and in general it admits contributions from whole symmetry block.

Angular couplings

Angular couplings are identified as $L_{ij}(R)$, see Eq. (**??**) and Ref. [**?**]. These couplings give rise to the heterogeneous perturbations in the spectra and are the only elements which couple states with $\Delta\Lambda = \pm 1$ in the standard coupled equations setting, see Section **??**. From the computational point of view, those elements are rather simple expectation values and angular factors can be easily expressed in terms of elliptic coordinates and resultantly as appropriate f-integrals, therefore its implementation in KW basis is expected to be straightforward, but as of yet we do not have any preliminary results.

5.1.1 Diabetization

In some problems it is more convenient to work with diabatic states well-defined setting for the variational caluclations, especially with the assumed Born-Oppenheimer approximation, because it is uniquely defined as the basis which diagonalizes the electronic Hamiltonian,

$$\forall_R \langle \Psi_k | \mathbf{H}_{\mathrm{el}} | \Psi_l \rangle_{\mathrm{el}} = 0, \tag{IV.48}$$

Here we illustrate the diabetization of adiabatic PEC. The in the sense of Lichten and Smith[**? ?**], so that the diabatic representation (ϕ^d) is defined by,

$$\forall_R \langle \phi_k^d | \mathbf{T}_N | \phi_l^d \rangle_{\mathrm{el}} = 0, \tag{IV.49}$$

Clearly, such a transformation can be represented by a unitary matrix $\mathbf{C}$ (pointwise, with different matrix $\mathbf{C}$ for each value of R),

$$\phi^d = \Psi \cdot \mathbf{C}, \tag{IV.50}$$

with Ψ denoting adiabatic basis.

According to the definition of diabatic basis, we demand

$$\langle \phi_1 | \mathbf{B} | \phi_2 \rangle = \langle \Psi_1 | \mathbf{C}^{-1} \mathbf{B} \mathbf{C} | \Psi_2 \rangle \tag{IV.51}$$

Utilizing the actual form of $\mathbf{B} = \hat{R} \cdot \mathbf{P}_N$ we have,

$$\langle \mathbf{C}\Psi_1 | \frac{d\mathbf{C}}{dR} + \mathbf{B}\mathbf{C} | \Psi_2 \rangle \tag{IV.52}$$

and from arbitrariness of Ψ_1 and Ψ_2 we have a first order linear equation for matrix $\mathbf{C}$,

$$\frac{d\mathbf{C}}{dR} + \mathbf{B} \cdot \mathbf{C} = 0, \tag{IV.53}$$

with boundary condition most conveniently chosen as $\mathbf{C}(R_0) = \mathbf{I}$, where $R_0 = 0$ seems to be the best choice, because then it can be connected to known united-atom limit, which are unmixed, thus $d(0) = 0$.

Hereafter we assume pure two-state mixing. Since matrix $B(R)$ is antisymmetric, we have,

$$\mathbf{B} = \begin{pmatrix} 0 & d(R) \\ -d(R) & 0 \end{pmatrix} \tag{IV.54}$$

with $d(R) \equiv \langle \Psi_1 | d/dR | \Psi_2 \rangle$. Now, with

$$\mathbf{C} = \begin{pmatrix} c_{11} & c_{12} \\ c_{21} & c_{22} \end{pmatrix}, \tag{IV.55}$$

Eq. (IV.53) reads

$$\begin{pmatrix} c'_{11} & c'_{12} \\ c'_{21} & c'_{22} \end{pmatrix} = d(R) \begin{pmatrix} -c_{21} & -c_{22} \\ c_{11} & c_{12} \end{pmatrix}, \tag{IV.56}$$

which appears to give four first order linear differential equations, straightforward to be solved numerically.

These, however, can be simplified to a single one by utilizing the unitarity of $\mathbf{C}$, which can be parametrized by a mixing angle θ,

$$\mathbf{C} = \begin{pmatrix} \cos(\theta) & \sin(\theta) \\ -\sin(\theta) & \cos(\theta) \end{pmatrix}, \tag{IV.57}$$

which entails

$$\frac{d\theta(R)}{dR} = d(R), \tag{IV.58}$$

so that

$$\theta(R) = \int_{R_0}^{R} d(R')dR' + \theta(R_0), \tag{IV.59}$$

with convenient choice of boundary condition $\theta(R_0 = 0) = 0$[2] because this has a clear physical meaning of unmixed united-atom limit states. This choice is most convenient if there is no another another anticrossing in the region $R \in (0, R_c)$, with R_c begin the value of R at which the interaction between adiabatic curves is maximal. On the other hand a $\theta(R_0) = 0$ with some very large R_0 can be used, especially when collision problem is at hand, however in practice the mixing of the character in the asymptotes prevails at least a few tens of Bohr radii[Wolniewiczasymp].

Then, properties of diabatized states, such as energy, can be retrieved from those calcu-

[2] Provided we have the advantage of accurate values of $d(R)$ at such a small values of R, so that the propagation from R_0 is feasible. Otherwise an arbitary R_0 within the interesting range of R can be chosen and the boundary conditions for $d(R)|_{R=R_0}$ can be attained by iteratively solving the differential equation and employing the bisection method to converge to the correct boundary value.

lated with adiabatic basis, with weights $\sim |c_{ij}|^2$,

$$\begin{pmatrix} E(\phi_1) \\ E(\phi_2) \end{pmatrix} = \begin{pmatrix} |c_{11}|^2 E(\Psi_1) + |c_{21}|^2 E(\Psi_2) \\ |c_{12}|^2 E(\Psi_1) + |c_{22}|^2 E(\Psi_2) \end{pmatrix} = \begin{pmatrix} \cos^2(\theta) E(\Psi_1) + \sin^2(\theta) E(\Psi_2) \\ \sin^2(\theta) E(\Psi_1) + \cos^2(\theta) E(\Psi_2) \end{pmatrix} \tag{IV.60}$$

In case of H_2 we have the advantage of availability of highly accurate ab-initio d/dR couplings between adiabatic states. Therefore they can be used as $d(R)$ directly. The influence of the accuracy of d/dR matrix elements as well as two-state mixing assumption on the quality of final deperturbed diabatic curves remains to be investigated.

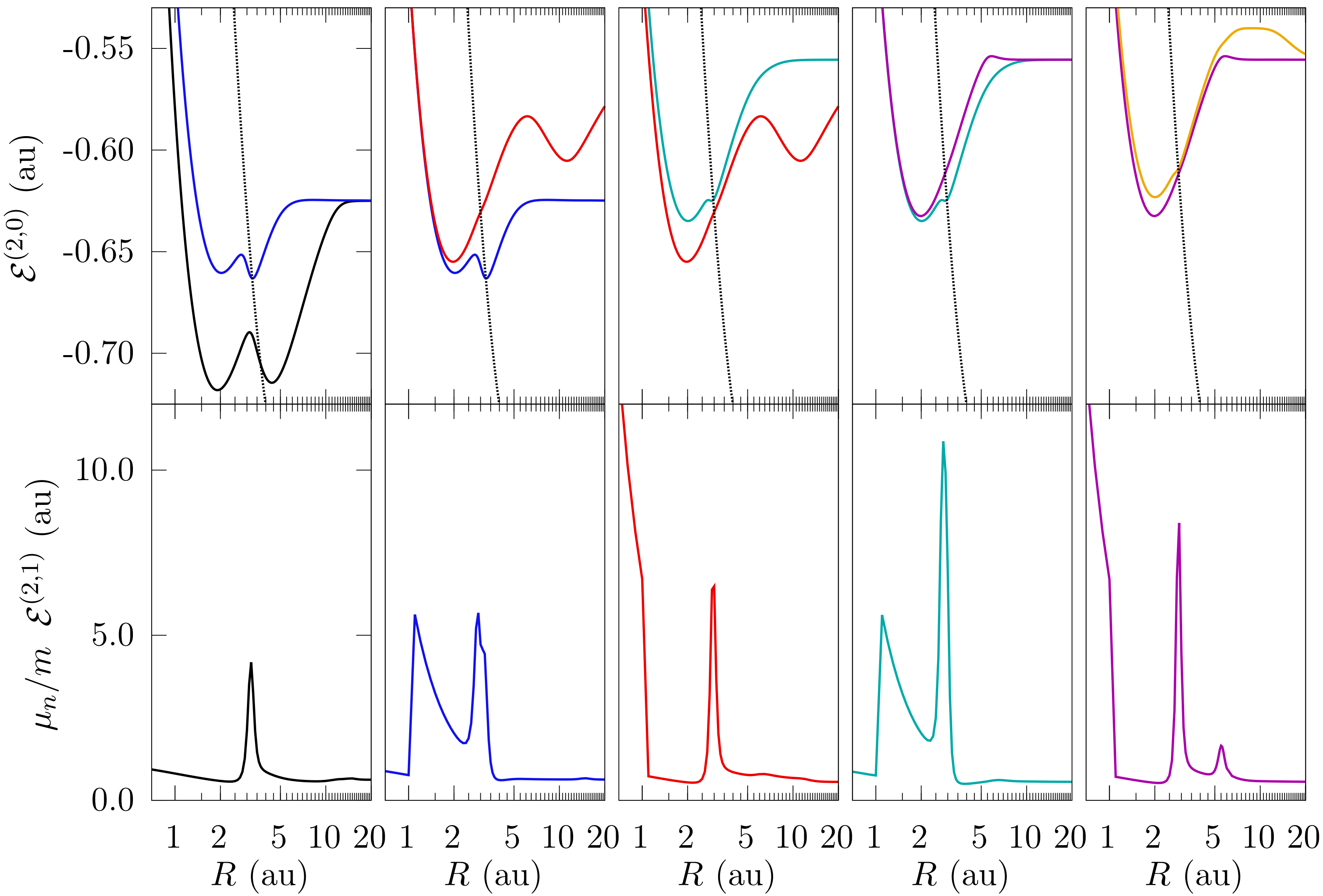

Figure IV.1: Diagonal adiabatic correction (lower panels), for EF (black), GK (blue), $H\bar{H}$ (red), P (aquamarine), and O (purple) ${}^1\Sigma_g^+$ states together with BO energies for reference (upper panels). The dotted near vertical line (black) is the lowest member of the doubly-excited resonances of this symmetry, $(1s\sigma_u)(2p\sigma_u)$ [194**? ?**], strongly electrostatically perturbing the evolution of singly-excited configurations. Notice sharp change in the behaviour of this correction between EF-GK and P-O around $R = 1$ au associated with avoided crossing and rapid $3s, 3d$ and $4s, 4d$ singly-excited character change.

CHAPTER V

RELATIVISTIC AND QUANTUM ELECTRODYNAMIC CORRECTIONS

1 Nonrelativistic Quantum Electrodynamics (NRQED)

It seems plausible to use Dirac bispinors as a starting point for the perturbative calculations of higher-order corrections. Especially in view of analytic solution of the Dirac equation in the Coulomb field. This however poses various problems. When a Dirac operator of two particles is constructed directly as acting on the tensor product of those particle vector spaces it is known to have no bound spectrum. In other words, Dirac equation is essentially a single particle equation and in the solution to the Coulomb problem the field is treated as external. In particular transformation into the center of mass motion and attempting to describe the motion as effective single particle with reduced mass does not work the same as with Schrödinger operators. Therefore, one should resort to the field-theoretic description.

1.1 Foldy-Wouthuysen transformation

There is however another way, one can try to identify which terms couple upper and lower components of the Dirac bispinor and try to perform a unitary transformation which would result in electrons decoupled from positrons, so that their evolution can be effectively described by simpler Schrödinger-Pauli equation. This central idea behind Foldy-

Wouthouysen transformation can be written as,

$$\Psi' = e^{iS}\Psi, \tag{V.1}$$
$$i\partial_t\Psi' = H'\Psi' = \left\{e^{iS}\left[H_0 - i\partial_t\right]e^{-iS}\right\}\Psi' \tag{V.2}$$

with

$$e^{iS}He^{-iS} = \sum_{k=0}^{\infty}\frac{i^k}{k!}\left[S,\ldots,[S,H]\ldots\right] \tag{V.3}$$

which pivots on the choice of operator S such that in the transformed frame, the terms mixing upper and lower component of the bispinors are eliminated, such that

$$\mathcal{O}' = 0 \text{ (up to terms } \sim \alpha^n) \tag{V.4}$$

It is known how to contruct this transformation up to desired order n, but its form eliminating $\mathcal{O}$ to all orders in α is not known in general. In practical derivations the FW transformation is often constructed as a sequence of FW transformations eliminating $\mathcal{O}$ order by order in α [195, 196].

We start with the spin 1/2 particle, minimally coupled to the EM field.

$$\left[(i\gamma^\mu\partial_\mu - e\gamma^\mu A_\mu - m + \frac{\kappa e}{4m}\sigma^{\mu\nu}F_{\mu\nu}\right]\Psi = 0 \tag{V.5}$$

$$\sigma^{\mu\nu} = \frac{i}{2}\left[\gamma^\mu, \gamma^\nu\right] \tag{V.6}$$

In the context of atomic physics, we assume the EM fields to be spatially slowly varying with resepect to the size of an atom, which jusitifies neglecting higher-order derivatives of EM field vector potential.

$$H_{\text{Dirac}} = \boldsymbol{\alpha\pi} + \beta m + eA^0 \tag{V.7}$$

We choose the operator S conveniently, such that

$$S = -\frac{i}{2m}\left[\beta\boldsymbol{\alpha\pi} - \frac{\beta}{3m^2}(\boldsymbol{\alpha\pi})^3 + \frac{1}{2m}\left[\boldsymbol{\alpha\pi}, eA^0 - i\partial_t\right]\right] \tag{V.8}$$

The Hamiltonian is then partitioned as,

$$H_0 = \mathcal{O} + \mathcal{E} + \beta m. \tag{V.9}$$

with the term $\mathcal{O}$ which mixes upper and lower components of bispinor and $\mathcal{E}$ (and βm)

do not,

$$\mathcal{O} = \boldsymbol{\alpha}\boldsymbol{\pi}_\beta, \tag{V.10}$$

$$\mathcal{E} = eA_0 - \frac{\kappa e}{2m}\beta\boldsymbol{\sigma}\mathbf{B}, \tag{V.11}$$

where $\boldsymbol{\pi}_\beta = \mathbf{p} - e\mathbf{A} - \frac{ie\kappa}{2m}\beta\mathbf{E}$.

After a fair amount of algebra, one arrives at transformed Hamiltonian

$$\begin{aligned} H_{FW} \;=\; & e\,A^0 + \frac{\pi^2}{2\,m} - \frac{e}{4\,m}\,\sigma^{ij}\,B^{ij} - \frac{\pi^4}{8\,m^3} + \frac{e}{16\,m^3}\{\sigma^{ij}\,B^{ij},\,p^2\} \\ & -\frac{e}{8\,m^2}\Big(\vec{\nabla}\cdot\vec{E}_\parallel + \sigma^{ij}\,\big\{E^i_\parallel,\,p^j\big\}\Big) + \frac{e^2}{2\,m^2}\,\sigma^{ij}\,E^i_\parallel\,A^j \\ & +\frac{i\,e}{16\,m^3}\,[\,\sigma^{ij}\,\{A^i,\,p^j\}\,,\,p^2] + \frac{e^2}{8\,m^3}\,\vec{E}^2_\parallel + \frac{3\,e}{32\,m^4}\,\{p^2\,,\,\sigma^{ij}\,E^i_\parallel\,p^j\} \\ & +\frac{5}{128\,m^4}\,[p^2,[p^2,e\,A^0]] \\ & -\frac{3}{64\,m^4}\,\Big\{p^2\,,\,\nabla^2(e\,A^0)\Big\} + \frac{1}{16\,m^5}\,p^6\,, \end{aligned} \tag{V.12}$$

where $\vec{E}_\parallel = -\vec{\nabla}A^0$ and

$$\sigma^{ij} \;=\; \frac{1}{2i}\big[\sigma^i,\sigma^j\big]\,, \quad B^{ij} = \partial^i A^j - \partial^j A^i\,. \tag{V.13}$$

In order to encode the information about internal structure of particles the minimal coupling prescription is substituted by the combination of F_1 and F_2 form factors (sometimes called Dirac and Pauli form factors, respectively), which allow most general form of the interaction allowed by the QED symmetry. For a spin 1/2 fermion, it reads,

$$\gamma^\mu A_\mu(q) \to \left[\gamma^\mu F_1(q^2/m^2) + \frac{i\sigma_{\mu\nu}q^\nu}{2m}\kappa F_2(q^2/m^2)\right] A_\mu(q), \tag{V.14}$$

with the normalization of the form factors, $F_1(0) = 1$ and $F_2(0) = 1$.

$$\langle r_E^2\rangle = \frac{3}{4m^2}\left[1 + 2\kappa + 8F_1'(0)\right], \tag{V.15}$$

$$\langle r_M^2\rangle = \frac{3}{4m^2}\left[1 + \frac{8}{1+\kappa}\left(F_1'(0) + \kappa F_2'(0)\right)\right], \tag{V.16}$$

$$\langle r_E^4\rangle = \frac{60}{m^4}F_1''(0), \tag{V.17}$$

1.2 Effective Hamiltonians

The NRQED is an effective field theory, designed to provide an accurate description of the low-energy nonrelativistic particles. By construction, the theory has to admit all possible interactions within the symmetry expected within the low-energy regime (which is usually also of lower symmetry). The formulation is perturbative, meaning that bound state energies admit an expansion in the fine-structure constant α,

$$E(\alpha) = \alpha^2 E^(2)) + \alpha^4 E^{(4)} + \alpha^5 E^{(5)} + \alpha^6 E^{(6)} + \alpha^7 E^{(7)} + \dots, \tag{V.18}$$

with $E^{(k)}$ being the contribution to the $\alpha^k m$ order of theory, with m being the electron mass. The strucutre of the $E^{(k)}$ might be quite a complicated function of m, nuclear charges, but also powers of $\ln \alpha$, which are characteristic to QED corrections [17].

With the transformed H_{FW} the energy corrections to the bound states are identified as the energy shift with respect to unperturbed Hamiltonian which brings it onto the energy shell,

$$G(E) \equiv \frac{1}{E - H_{\text{eff}}} \tag{V.19}$$

where $H_{\text{eff}} = H_0 + \Sigma(E)$ and $\Sigma(E)$ is irreducible two-particle interaction operator, which includes multiphoton exchanges.

The correction to the energy level is then a shift of the pole of $G(E)$, so that it admits an expansion,

$$\delta E = \langle\Psi|\, \Sigma(E_0)\, |\Psi\rangle + \langle\Psi|\, \Sigma(E_0) \frac{1}{(E_0 - H_0)'} \Sigma(E_0)\, |\Psi\rangle + \dots, \tag{V.20}$$

2 Relativistic corrections in Born-Oppenheimer approximation

The leading order relativstic correction, $E^{(4)}$, can be exactly separated into spin-free and spin-dependent part[197] and is given as the expectation value with molecular wave function of,

$$H^{(4)} = -\sum_a \frac{p_a^4}{8m_a} - \frac{1}{2}\sum_{a,b,a\neq b} \frac{z_a z_b}{m_a m_b} p_a^i\, d_{ab}^{ij}\, p_b^j + \quad z_a\, z_b \sum_a \left(\frac{1}{m_a} + \frac{\delta s_x}{m_a}\right) \delta^{(3)}(r_{ab}), \tag{V.21}$$

with $d_{ab}^{ij} = \frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i r_{ab}^j}{r_{ab}^3}$ and $\delta s = 0$ for nuclear spin $I = 0, 1$ and $\delta s = 1$ for $I = 1/2$.

$$H_{\text{rel}} = -\frac{1}{8}(p_1^4 + p_2^4) - \frac{1}{2} p_1^i \left(\frac{\delta^{ij}}{r_{12}} + \frac{r_{12}^i r_{12}^j}{r_{12}^3}\right) p_2^j + \pi\delta(\mathbf{r}_{12}) + \frac{\pi}{2}\sum_{i,X} \delta(\mathbf{r}_{iX}) \tag{V.22}$$

the spin dependent part of the Breit-Pauli Hamiltonian can be neglected in the context of the ground electronic state ($^1\Sigma_g^+$) of H_2 for which $S = 0$ and its expectation value vanishes.

Here we merely highlight the core differences of the method used in Ref. [h2rel] with respect to previous attempts.

[move this to a proper place as a footnote] Unfortunately, as of current date, it is not known how the linear interelectronic cusp can be generalized to more than 2-electron ECG basis.

To achieve good numerical convergence and high accuracy, it was pivotal to use the ECG basis augmented with the linear cusp – $(1 + \frac{r_{12}}{2}$ factor. Use of the EVI

Standard scheme [**?**],

$$
\begin{aligned}
4\pi\delta(\mathbf{r}_{iX}) =& 4\pi\left[\delta(\mathbf{r}_{iX})\right]_r + \left\{\frac{2}{r_{iX}}, H-\mathcal{E}\right\}, \\
4\pi\delta(\mathbf{r}_{12}) =& 4\pi\left[\delta(\mathbf{r}_{12})\right]_r + \left\{\frac{1}{r_{12}}, H-\mathcal{E}\right\}, \\
p_1^4 + p_2^4 =& \left[p_1^4 + p_2^4\right]_r + 4\left\{\mathcal{E}-V, H-\mathcal{E}\right\} + 4(H-\mathcal{E})^2,
\end{aligned}
\tag{V.23}
$$

where $\mathbf{r}_{iX}$ pertains to any electron-nucleus coordinate and

$$
\begin{aligned}
4\pi\left[\delta(\mathbf{r}_{iX})\right]_r =& \frac{4}{r_{iX}}(\mathcal{E}-V) - \sum_k \vec{p_k}\frac{2}{r_{iX}}\vec{p_k}, \\
4\pi\left[\delta(\mathbf{r}_{12})\right]_r =& \frac{4}{r_{iX}}(\mathcal{E}-V) - \sum_k \vec{p_k}\frac{1}{r_{12}}\vec{p_k}, \\
\left[p_1^4 + p_2^4\right]_r =& 4(H-\mathcal{E})^2 - 2p_1^2p_2^2,
\end{aligned}
\tag{V.24}
$$

For the exact wave function Ψ solves the electronic Schrödinger equation $(\mathcal{E} - H)\Psi = 0$, therefore EVI holds $\langle\Psi|\ldots|\Psi\rangle = \langle\Psi|\left[\ldots\right]_r|\Psi\rangle$. In general, for arbitrary operator Q, $\langle\Psi|\left\{Q, H-\mathcal{E}\right\}|\Psi\rangle = 0$. Nevertheless, for an approximate wavefunction $\tilde{\Psi}$, the expectation value of such commutator does not vanish, but clearly, converges to zero in the limit $\tilde{\Psi} \to \Psi$. In practice, the operator Q can be chosen such that the rate of the numerical convergence of the regularized form is much faster, than *direct* evaluation of the expectation value.

The rECG basis with the standard regularization scheme requires integrals with up to three odd indices. Such integrals can be evaluated with the gausext quadrature described in the Section 3. Due to the cancellations within the modified scheme however, all the integrals with three odd powers of interparticle distances do not appear in the matrix elements with rECG functions. This observation is of crucial importance concerning the computational cost of rECG method for the relativistic correction. Resultantly, calculations with the basis as big as $N = 1024$ were feasible. The relative pointwise accuracy of the $\mathcal{E}^{(4)}$ was better than 10^{-7} cm^{-1}. The final relative uncertainty is assumed to be smaller than 10^{-6} cm^{-1}, which results from the chosen density of points at which $\mathcal{E}^{(4)}(R)$ was evaluated, together with the uncertainty resulting from its interpolation.

The 2017 results for the leading relativistic corrections turned out to be incompatible with the previous one from 2009, by Piszczatowski et al. [198], cf. Table V.1. The 2009 calculations partially relied on the former calculations by Wolniewicz [199], which were performed in Kolos-Wolniewicz basis with the use the method pioneered by Wolniewicz, which relied on the generalized Neumann expansion of r_{12}^{-2} in terms of Gegenbauer polynomials[200].

Table V.1: Comparison of $E^{(4,0)}$ contribution to $D_0(\mathrm{H}_2)$. Intriguingly, the newest rECG-based result with the best control over the numerical uncertainties seem to be closer to the first-ever result of Wolniewicz.

Authors	Method	$\delta_{\mathrm{rel}} D_0(\mathrm{H}_2)$
Wolniewicz (1993) [199]	KW	-0.533 0
Piszczatowski et al. (2009) [198]	ECG+KW	-0.531 9(3)
Puchalski et al. (2017) [68]	rECG	-0.533 121(1)

3 Relativistic recoil corrections

With fully nonadiabatic approach one has to abandon the concept of effective electronic potentials in which the nuclear dynamics is solved and the corrections have to be calculated (involving computationally heavy optimization of thousands of parameters of 4-body wave function) for each rovibrational state separately. For this reason fully nonadiabatic values for relativistic corrections has only be obtained with the naECG method for a few rovibrational states. Despite substantial computational effort a concurent scheme utilizing naJC basis is presently being developed [1].

Leading-order relativistic recoil corrections

The following summarizes recent work [201], which was the main part of P. Czachorowski's Ph. D. Thesis [179]. The motivation for calculations of the $E^{(4,1)}$ – leading relativistic recoil correction – emerged as a consequence of surprising conclusion stemming from the 2017 reevaluation of Born-Oppenheimer relativistic correction by M. Puchalski *et al.* [68](outlined in previous Section). The 2017 recalculation of $E^{(4,0)}$ utilized the rECG basis functions together with clever use of EVI, to provide well-converged highly-accurate value of this correction. Resultantly, it revealed that previous, 2009 calculations [198], were much less accurate than claimed and good agreement with experimental value of dissociation energy of H_2, D_0 (H_2) was fortuitous.

According to a combined NRQED and NAPT expansion[179, 201], the leading order relativistic recoil correction to the effective electronic potential can be represented as

$$\mathcal{E}^{(4,1)}(R) = \frac{1}{\mu_n}\left[\langle \nabla_R \Psi_{\mathrm{rel}} | \nabla_R \Psi\rangle - \langle \Psi_{\mathrm{rel}} | \nabla^2_{\mathrm{el}} |\Psi\rangle\right] + \langle \Psi | H^{(4,1)}_M |\Psi\rangle \,, \tag{V.25}$$

where $|\Psi_{\mathrm{rel}}\rangle$ is the relativistic correction to the nonrelativistic wavefunction,

$$|\Psi_{\mathrm{rel}}\rangle = \mathcal{R}' H^{(4,0)} |\Psi\rangle \,, \tag{V.26}$$

[1] J. Komasa *private communication*

and $H_M^{(4,1)}$ is the effective relativistic Hamiltonian in the first order of m/μ_n,

$$H_M^{(4,1)} = -\frac{1}{4\mu_n}\sum_{a=1,2}\nabla_a^i\left(\frac{\delta^{ij}}{r_{aA}}+\frac{r_{aA}^i r_{aA}^j}{r_{aA}^3}-\frac{\delta^{ij}}{r_{aB}}-\frac{r_{aB}^i r_{aB}^j}{r_{aB}^3}\right)\nabla_R^j, \tag{V.27}$$
$$+\frac{1}{4\mu_n}\sum_{a=1,2}\nabla_a^i\left(\frac{\delta^{ij}}{r_{aA}}+\frac{r_{aA}^i r_{aA}^j}{r_{aA}^3}+\frac{\delta^{ij}}{r_{aB}}+\frac{r_{aB}^i r_{aB}^j}{r_{aB}^3}\right)\nabla_{\rm el}^j$$

The spin-dependent terms are neglected because we specialize this correction to a ground ${}^1\Sigma_g^+$ state. The complete correction to the molecular energy level is then given by a vibrationally averaged electronic potential $\mathcal{E}^{(4,1)}(R)$ with the additional contribution from the relativistically perturbed vibrational wavefunction,

$$E^{(4,1)} = \langle\chi|\,\mathcal{E}^{(4,1)}(R)\,|\chi\rangle + 2\langle\chi|\delta\chi\rangle, \tag{V.28}$$
$$|\delta\chi\rangle = \mathcal{E}^{(4,0)}(R)\frac{1}{(E^{(2,0)}-H_n)'}\mathcal{E}^{(2,1)}(R)\,|\chi\rangle\,. \tag{V.29}$$

The $\frac{1}{(E^{(2,0)}-H_n)'}$ stands for the reduced resolvent operating on the vibrational eigenstates of H_n,

$$\frac{1}{(E^{(2,0)}-H_n)'} \equiv \sum_{\chi'\neq\chi}\frac{|\chi'\rangle\,\langle\chi'|}{E^{(2,0)}-E'^{(2,0)}}, \tag{V.30}$$

where $E'^{(2,0)}$ stands for the eigenvalue corresponding to $|\chi'\rangle$. Finally, the $|\delta\chi\rangle$ is obtained by solving the Eq. (V.29) numerically. In our DVR-based implementation it is done by directly diagonalizing H_N, thus solving the nuclear eigensystem for all eigenvectors and eigenvalues.

For thorough and detailed description of the details concerning calculations of $\mathcal{E}^{(4,1)}(R)$ we refer to P. Czachorowski's Ph. D. thesis [179] and Ref. [**?**], here we merely present its R-behavior on Fig. V.1.

Table V.2 unveils an excellent agreement, on the order of a few 10^{-6} cm^{-1}, between NAPT calculations (together with a simple estimate of higher order effects) with fully nonadiabatic naECG results in the case of ground rovibrational level (0,0).

4 Relativistic heteronuclear recoil correction

Although in the previous Section, an excellent agreement between NAPT predictions and fully nonadiabatic naECG results was observed in the ground rovibrational states of the lightest isotopologues, we conjecture that higher order recoil corrections might actually be bigger than simple $m/\mu_n E^{(4,1)}$ estimate in case of vibrationally excited states.

The following presents an unpublished results concerning calculations of leading terms of the purely heteronuclear relativistic recoil correction (part of $E^{(4,2)}$) to rovibrational levels. The motiviation behind the following derivation (performed jointly with the Su-

Table V.2: Convergence of $\langle\chi|\mathcal{E}^{(4,1)}(R)|\chi\rangle$ and $2\langle\chi|\delta\chi\rangle$ – two components comprising the NAPT-based value of $E^{(4)}$ (in cm^{-1}). The uncertainties of the final NAPT-based values of $E^{(4)}$ contain an estimate of the higher order nonadiabatic effects, given by $E^{(4,1)}/\mu_n$. Adapted from Ref. [178].

Component	H_2	HD	D_2
$\langle\chi|\mathcal{E}^{(4,1)}(R)|\chi\rangle$ (N=128)	0.002 376 07	0.001 794 00	0.001 205 590
$\langle\chi|\mathcal{E}^{(4,1)}(R)|\chi\rangle$ (N=256)	0.002 370 19	0.001 789 61	0.001 202 694
$\langle\chi|\mathcal{E}^{(4,1)}(R)|\chi\rangle$ (N=512)	0.002 368 67	0.001 788 48	0.001 201 951
$\langle\chi|\mathcal{E}^{(4,1)}(R)|\chi\rangle$ ($N\to\infty$)	0.002 368(1)	0.001 788(1)	0.001 201 7(4)
$2\langle\chi|\delta\chi\rangle$	−0.000 451 1	−0.000 342 0	−0.000 230 9
$E^{(4,1)}$	0.001 917(1)	0.001 446(1)	0.000 970 8(4)
$E^{(4,0)}$	−0.533 130(1)	−0.531 334(1)	−0.529 179(1)
$E^{(4)}$	−0.531 213(2)	−0.529 888(2)	−0.528 208(1)
naECG [?]	−0.531 215 6(5)	−0.529 887 5(2)	−0.528 206 1(1)
Difference	0.000 003(2)	−0.000 001(2)	−0.000 002(1)

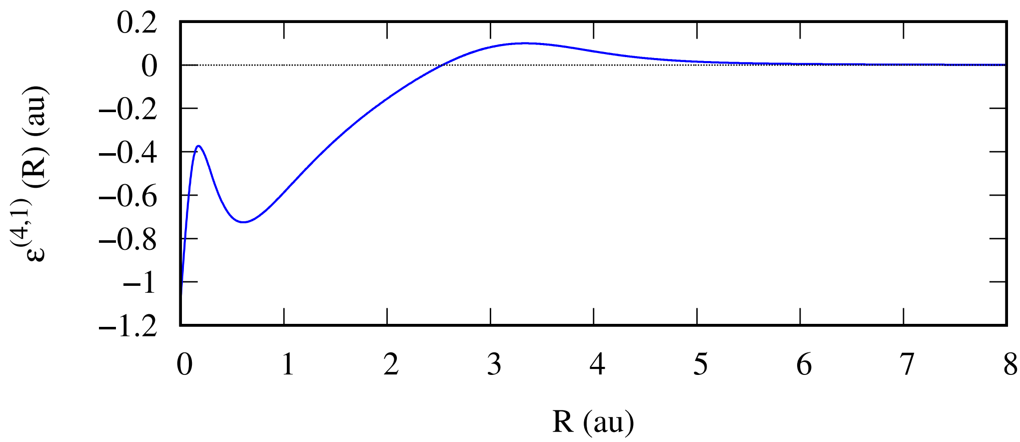

Figure V.1: The solid black line represents $\mathcal{E}^{(4,1)}(R)$ given by Eq. (V.25) with the asymptotic hydrogenic limit subtracted.

pervisor) and numerical calculations is due to the anticipated contribution to the rovibrational transitions of heteronuclear isotopologues (HD, HT, DT), which could explain the prevailing $\sim 2\sigma$ disagreement in HD between experimental values and those obtained from ab-initio theory.

We emphasize, that the result presented here is *not* a complete $E^{(4,2)}$ correction to the molecular level energy because we:

- completely disregard the purely homonuclear contribution to $E^{(4,2)}$,
- only leading terms contributing to nuclear kinetic energy are retained.

Nevertheless, it should serve as a rough estimate of heteronuclear relativistic recoil effects with $\pm 25\%$ accuracy, at least for relatively low-ν rovibrational states.

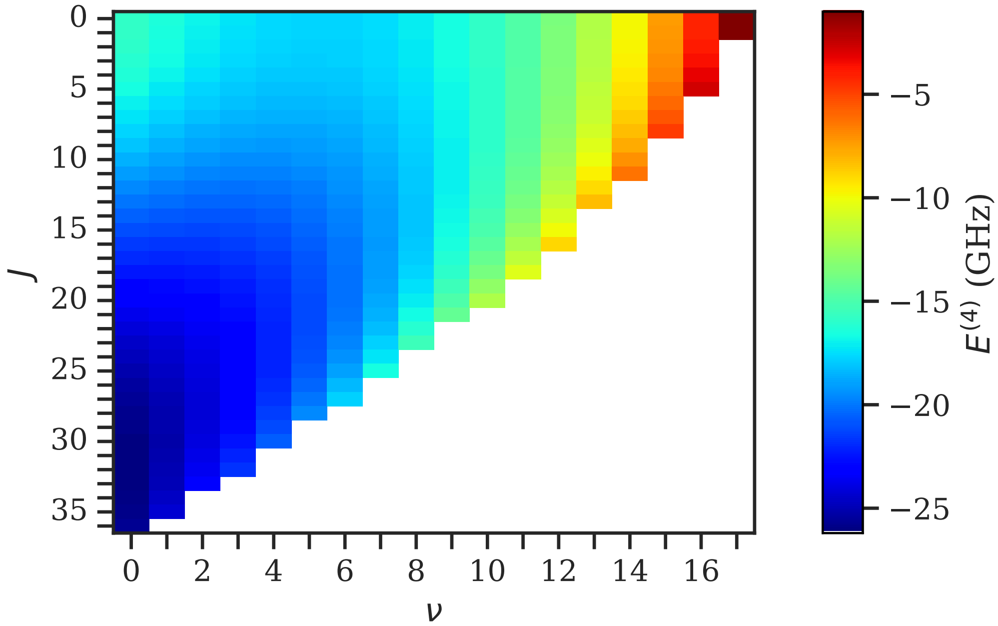

Figure V.2: Shift of the $D_0(\mathrm{HD})$ due to complete $E^{(4)}$.

4.1 Definitions

We consider a two-electron diatomic molecule in the reference frame attached to the geometrical center of the nuclei. The total wave function ψ is a solution of the stationary Schrödinger equation

$$H\,\psi = E\,\psi\,, \tag{V.31}$$

with the Hamiltonian

$$H = H_{\mathrm{el}} + H_{\mathrm{n}}\,, \tag{V.32}$$

split into the electronic and nuclear parts. In the electronic Hamiltonian

$$H_{\mathrm{el}} = -\sum_a \frac{\nabla_a^2}{2\,m_{\mathrm{e}}} + V\,, \tag{V.33}$$

where V is the Coulomb interaction

$$V = -\frac{1}{r_{1A}} - \frac{1}{r_{1B}} - \frac{1}{r_{2A}} - \frac{1}{r_{2B}} + \frac{1}{r_{12}} + \frac{1}{R}, \tag{V.34}$$

the nuclei have fixed positions $\vec{R}_A$ (proton) and $\vec{R}_B$ (deuteron), and $\vec{R} = \vec{R}_A - \vec{R}_B$. The nuclear Hamiltonian

$$H_{\mathrm{n}} = -\frac{\nabla_A^2}{2\,m_A} - \frac{\nabla_B^2}{2\,m_B}\,, \tag{V.35}$$

when the reference frame is fixed at the geometrical center, can be written down as a sum of two components

$$H'_{\rm n} = -\frac{\nabla_R^2}{2\,\mu_{\rm n}} - \frac{\nabla_{\rm el}^2}{8\,\mu_{\rm n}} \tag{V.36}$$

$$H''_{\rm n} = \frac{1}{2}\left(\frac{1}{M_A} - \frac{1}{M_B}\right)\vec{\nabla}_R \cdot \vec{\nabla}_{\rm el} \tag{V.37}$$

the first one being even and the second—odd with respect to the inversion. In the above $\vec{\nabla}_{\rm el} = \sum_a \vec{\nabla}_a$ and $\mu_{\rm n} = (1/M_A + 1/M_B)^{-1}$ is the reduced nuclear mass.

In the adiabatic approximation the total wave function ψ of the molecule is represented as a product of the electronic wave function ϕ and the nuclear wave function χ. The electronic wave function obeys the clamped nuclei electronic Schrödinger equation

$$\left[H_{\rm el} - \mathcal{E}_{\rm el}(R)\right]|\phi\rangle = 0, \tag{V.38}$$

while the wave function χ is a solution to the nuclear Schrödinger equation with the effective potential generated by electrons

$$(\mathcal{H} - E)\,|\chi\rangle = 0\,, \tag{V.39}$$

where

$$\mathcal{H} = -\frac{\vec{\nabla}_R^2}{2\,\mu_{\rm n}} + \mathcal{E}_{\rm a}(R) + \mathcal{E}_{\rm el}(R). \tag{V.40}$$

The function

$$\mathcal{E}_{\rm a}(R) = \langle\phi\,|H_{\rm n}|\,\phi\rangle_{\rm el} \tag{V.41}$$

is the so-called adiabatic correction. Due to the inversion symmetry of ϕ with respect to the geometrical center, $\langle\phi|H''_{\rm n}|\phi\rangle_{\rm el} = 0$ and

$$\begin{aligned}\mathcal{E}_{\rm a}(R) &= \left\langle\phi\,\middle|H'_{\rm n}\middle|\,\phi\right\rangle_{\rm el} \\ &= \frac{1}{2\,\mu_{\rm n}}\left\langle\phi\left|\overleftarrow{\nabla}_R \cdot \vec{\nabla}_R\right|\phi\right\rangle_{\rm el} - \frac{1}{8\,\mu_{\rm n}}\left\langle\phi\left|\vec{\nabla}_{\rm el}^2\right|\phi\right\rangle.\end{aligned} \tag{V.42}$$

4.2 Derivation

4.2.1 Relativistic recoil

Relativistic recoil correction

$$\delta H = -\sum_{a=1,2}\sum_{X=A,B}\frac{\alpha}{2\,m\,M_X}\,\nabla_a^i\,d_{aX}^{ij}\,\nabla_X^j, \tag{V.43}$$

with

$$d^{ij}_{aX} = \frac{\delta^{ij}}{r_{aX}} + \frac{r^i_{aX}\, r^j_{aX}}{r^3_{aX}}. \tag{V.44}$$

It can be written down as a sum of two components

$$\delta H' = -\sum_{a=1,2}\sum_{X=A,B} \frac{\alpha}{4\, m\, \mu_{\rm n}}\, \nabla^i_a\, d^{ij}_{aX}\, \nabla^j_X \tag{V.45}$$

$$\delta H'' = -\sum_{a=1,2} \frac{\alpha}{4\, m} \left(\frac{1}{M_A} - \frac{1}{M_B}\right) \nabla^i_a \times \left[d^{ij}_{aA}\, \nabla^j_A - d^{ij}_{aB}\, \nabla^j_B\right] \tag{V.46}$$

Using

$$\vec\nabla_A = \frac{\vec\nabla_A + \vec\nabla_B}{2} + \frac{\vec\nabla_A - \vec\nabla_B}{2} = -\frac{\vec\nabla_{\rm el}}{2} + \vec\nabla_R \tag{V.47}$$

$$\vec\nabla_B = \frac{\vec\nabla_A + \vec\nabla_B}{2} - \frac{\vec\nabla_A - \vec\nabla_B}{2} = -\frac{\vec\nabla_{\rm el}}{2} - \vec\nabla_R \tag{V.48}$$

and neglecting $\nabla_{\rm el}$ the second component can be written as

$$\delta H'' = 2\lambda\, \vec{Q}\, \vec\nabla_R \tag{V.49}$$

where

$$\lambda = \frac{1}{2}\left(\frac{1}{M_A} - \frac{1}{M_B}\right) \tag{V.50}$$

$$Q^j = -\sum_{a=1,2}\sum_{X=A,B} \frac{\alpha}{4\, m}\, \nabla^i_a\, d^{ij}_{aX} \tag{V.51}$$

4.2.2 Cross term

We now consider the second order correction

$$\delta E_A = \left\langle \phi \middle| H''_{\rm n}\, \frac{1}{\mathcal{E}_{\rm el} - H_{\rm el}}\, \delta H'' \middle| \phi \right\rangle + {\rm h.c.} \tag{V.52}$$

$$= 2\lambda^2 \left\langle \phi \middle| \vec\nabla_R \vec\nabla_{\rm el}\, \frac{1}{\mathcal{E}_{\rm el} - H_{\rm el}}\, \vec{Q}\, \vec\nabla_R \middle| \phi \right\rangle + {\rm h.c.}$$

$$\approx 2\lambda^2\, \nabla^i_R \left\langle \phi \middle| \nabla^i_{\rm el}\, \frac{1}{\mathcal{E}_{\rm el} - H_{\rm el}}\, Q^j + Q^i\, \frac{1}{\mathcal{E}_{\rm el} - H_{\rm el}}\, \nabla^j_{\rm el} \middle| \phi \right\rangle \nabla^j_R, \tag{V.53}$$

where in the last line we leave only the dominant term with ∇_R acting on the vibrational nuclear wave function, which constitute the correction to the nuclear kinetic energy. This is due to the fact of different effective mass-scaling of the $\nabla_R \phi$ versus $\nabla_R \chi$.

Using

$$\vec{\nabla}_{\rm el} = m\,[\mathcal{E}_{\rm el} - H_{\rm el}\,,\,\vec{x}_{\rm el}] \tag{V.54}$$

δE_A becomes

$$\delta E_A = 2\lambda^2\, m\, \nabla^i_R \,\big\langle\phi\big|Q^i\, x^j_{\rm el} - x^i_{\rm el}\, Q^j\big|\phi\big\rangle\, \nabla^j_R. \tag{V.55}$$

Since ϕ is the Σ^+ state, the expectation value has to be symmetric in i, j indices, thus

$$\delta E_A = 2\lambda^2\, m\, \nabla^i_R \,\big\langle\phi\big|[Q^i\,,\,x^j_{\rm el}]\big|\phi\big\rangle\, \nabla^j_R \tag{V.56}$$

$$= -\,\frac{1}{2}\lambda^2\,\alpha^2\,\nabla^i_R\, Q^{ij}_A\, \nabla^j_R \tag{V.57}$$

where

$$Q^{ij}_A = -\,\frac{1}{2}\sum_{a=1,2}\sum_{X=A,B}\langle\phi|d^{ij}_{aX}|\phi\rangle \tag{V.58}$$

$$= A_{\|}\, n^i\, n^j + A_\perp\,(\delta^{ij} - n^i\, n^j) \tag{V.59}$$

Term A contributes to $\mathcal{W}_\|$ and thus dominates and B contributes to $\mathcal{W}_\perp$,

$$\delta E_A = \lambda^2\,\alpha^2\,\Big(\nabla^i_R\, n^i\, A_\|\, n^j\, \nabla^j_R + \nabla^i_R\, A_\perp(\delta^{ij} - n^i\, n^j)\,\nabla^j_R\Big) \tag{V.60}$$

where

$$A_\| = -\,\frac{1}{2}\sum_{a=1,2}\sum_{X=A,B}\left\langle\phi\middle|\frac{1}{r_{aX}} + \frac{(\vec{n}\cdot\vec{r}_{aX})^2}{r^3_{aX}}\middle|\phi\right\rangle, \tag{V.61}$$

$$A_\perp = -\,\frac{1}{4}\sum_{a=1,2}\sum_{X=A,B}\left\langle\phi\middle|\frac{3}{r_{aX}} - \frac{(\vec{n}\cdot\vec{r}_{aX})^2}{r^3_{aX}}\middle|\phi\right\rangle. \tag{V.62}$$

Using the identity $\frac{r^i_{aX}}{r^3_{aX}} = -\nabla^i_a\left(\frac{1}{r_{aX}}\right)$ and integrating by parts,

$$A_\| = -\sum_{a=1,2}\sum_{X=A,B}\left\langle\phi\middle|\frac{1}{r_{aX}}\middle|\phi\right\rangle + n^i n^j\left\langle\nabla^j_a\phi\middle|\frac{r^i_{aX}}{r_{aX}}\middle|\phi\right\rangle, \tag{V.63}$$

$$A_\perp = -\frac{1}{2}\sum_{a=1,2}\sum_{X=A,B}\left\langle\phi\middle|\frac{1}{r_{aX}}\middle|\phi\right\rangle - n^i n^j\left\langle\nabla^j_a\phi\middle|\frac{r^i_{aX}}{r_{aX}}\middle|\phi\right\rangle, \tag{V.64}$$

4.2.3 Relativistic perturbation of $E^{(2,2)}$

We now consider corrections to $E^{(4,0)}$ arising as a second order perturbation by H''_{n},

$$\begin{aligned}\delta E_B &= \left\langle \phi \middle| H''_{\mathrm{n}} \frac{1}{\mathcal{E}-H} H''_{\mathrm{n}} \middle| \phi \right\rangle \\ &= \lambda^2 \left\langle \phi \middle| \nabla^i_R \nabla^i_{\mathrm{el}} \frac{1}{\mathcal{E}-H} \nabla^j_R \nabla^j_{\mathrm{el}} \middle| \phi \right\rangle \\ &= \lambda^2 \nabla^i_R \left\langle \phi \middle| \nabla^i_{\mathrm{el}} \frac{1}{\mathcal{E}-H} \nabla^j_{\mathrm{el}} \middle| \phi \right\rangle \nabla^j_R \\ &= \lambda^2 \nabla^i_R Q^{ij}_B \nabla^j_R\end{aligned} \tag{V.65}$$

and perturb Q^{ij}_B by a relativistic correction

$$\begin{aligned}Q^{ij}_B = &\left\langle \phi \middle| \delta H \frac{1}{(\mathcal{E}-H)'} \nabla^i_{\mathrm{el}} \frac{1}{\mathcal{E}-H} \nabla^j_{\mathrm{el}} \middle| \phi \right\rangle + \left\langle \phi \middle| \nabla^i_{\mathrm{el}} \frac{1}{\mathcal{E}-H} (\delta H - \delta E) \frac{1}{\mathcal{E}-H} \nabla^j_{\mathrm{el}} \middle| \phi \right\rangle \\ &+ \left\langle \phi \middle| \nabla^i_{\mathrm{el}} \frac{1}{\mathcal{E}-H} \nabla^j_{\mathrm{el}} \frac{1}{(\mathcal{E}-H)'} \delta H \middle| \phi \right\rangle\end{aligned} \tag{V.66}$$

Using the commutation relation with $m = 1$

$$\vec{\nabla}_{\mathrm{el}} = [\mathcal{E}-H \, , \, \vec{x}_{\mathrm{el}}] \tag{V.67}$$

$$\begin{aligned}Q^{ij}_B = &\left\langle \phi \middle| \delta H \frac{1}{(\mathcal{E}-H)'} [\mathcal{E}-H \, , \, x^i_{\mathrm{el}}] \frac{1}{\mathcal{E}-H} [\mathcal{E}-H \, , \, x^j_{\mathrm{el}}] \middle| \phi \right\rangle \\ &+ \left\langle \phi \middle| [\mathcal{E}-H \, , \, x^i_{\mathrm{el}}] \frac{1}{\mathcal{E}-H} (\delta H - \delta E) \frac{1}{\mathcal{E}-H} [\mathcal{E}-H \, , \, x^j_{\mathrm{el}}] \middle| \phi \right\rangle \\ &+ \left\langle \phi \middle| [\mathcal{E}-H \, , \, x^i_{\mathrm{el}}] \frac{1}{\mathcal{E}-H} [\mathcal{E}-H \, , \, x^j_{\mathrm{el}}] \frac{1}{(\mathcal{E}-H)'} \delta H \middle| \phi \right\rangle \\ = &\left\langle \phi \middle| (\delta H - \delta E) \, x^i_{\mathrm{el}} \, x^j_{\mathrm{el}} \middle| \phi \right\rangle - \left\langle \phi \middle| \delta H \frac{1}{(\mathcal{E}-H)'} x^i_{\mathrm{el}} (\mathcal{E}-H) \, x^j_{\mathrm{el}} \middle| \phi \right\rangle \\ &- \left\langle \phi \middle| x^i_{\mathrm{el}} (\delta H - \delta E) \, x^j_{\mathrm{el}} \middle| \phi \right\rangle \\ &- \left\langle \phi \middle| x^i_{\mathrm{el}} (\mathcal{E}-H) \, x^j_{\mathrm{el}} \frac{1}{(\mathcal{E}-H)'} \delta H \middle| \phi \right\rangle + \left\langle \phi \middle| x^i_{\mathrm{el}} \, x^j_{\mathrm{el}} (\delta H - \delta E) \middle| \phi \right\rangle\end{aligned} \tag{V.68}$$

Because ϕ is a Σ state, Q^{ij}_B has to be a symmetric tensor, thus

$$x^i_{\mathrm{el}} (\mathcal{E}-H) \, x^j_{\mathrm{el}} \approx \frac{1}{2} [x^i_{\mathrm{el}} [\mathcal{E}-H \, , \, x^j_{\mathrm{el}}]] + \frac{1}{2} x^i_{\mathrm{el}} \, x^j_{\mathrm{el}} (\mathcal{E}-H) + \frac{1}{2} (\mathcal{E}-H) \, x^i_{\mathrm{el}} \, x^j_{\mathrm{el}} \tag{V.69}$$

and Q_B^{ij} becomes

$$Q_B^{ij} = \frac{1}{2}\,\langle\phi|(\delta H - \delta E)\,x_{\rm el}^i\,x_{\rm el}^j|\phi\rangle - \langle\phi|\,x_{\rm el}^i\,(\delta H - \delta E)\,x_{\rm el}^j|\phi\rangle + \frac{1}{2}\,\langle\phi|\,x_{\rm el}^i\,x_{\rm el}^j\,(\delta H - \delta E)|\phi\rangle$$
$$= -\,\frac{1}{2}\,\langle\phi|[x_{\rm el}^i,[\delta H - \delta E\,,\;x_{\rm el}^j]]|\phi\rangle. \tag{V.70}$$

We are considering the relativistic correction to Q_B^{ij}, thus the perturbation operator is $\delta H = H^{(4,0)}$,

$$H^{(4,0)} = -\,\frac{p_1^4+p_2^4}{8} - \frac{1}{2}p_1^i d^{ij} p_2^j + \pi\left(\frac{1}{2}\delta^{(3)}(\vec r_{12}) + \delta^{(3)}(\vec r_{1A}) + \delta^{(3)}(\vec r_{2A}) + \delta^{(3)}(\vec r_{1B}) + \delta^{(3)}(\vec r_{2B})\right), \tag{V.71}$$

The only nonzero contribution to the commutator of Eq. (V.70) coming from δH is from $p_1^4+p_2^4$ and Breit terms.

Using the following commutation rules with $m=1$,

$$[x_{\rm el}^i,[p_1^4+p_2^4,x_{\rm el}^j] = 8\left(\delta^{ij}\frac{p_1^2+p_2^2}{2} + p_1^i\,p_1^j + p_2^i\,p_2^j\right), \tag{V.72}$$
$$[x_{\rm el}^i,[p_1^k\,d^{kl}\,p_2^l,x_{\rm el}^j] = 2\,d^{ij}, \tag{V.73}$$

$$Q_B^{ij} = \frac{1}{2}\langle\phi|d_{12}^{ij}|\phi\rangle + \frac{1}{2}\langle\phi|\,\delta^{ij}\frac{p_1^2+p_2^2}{2} + p_1^i\,p_1^j + p_2^i\,p_2^j|\phi\rangle \tag{V.74}$$

$$Q_B^{ij} = B_\parallel\,n^i\,n^j + B_\perp\,(\delta^{ij} - n^i\,n^j), \tag{V.75}$$
$$B_\parallel = \left\langle\frac{1}{r_{12}}\right\rangle + n^i n^j\left\langle\nabla_1^j\phi\middle|\frac{r_{12}^i}{r_{12}}\middle|\phi\right\rangle + \frac{1}{4}\langle p_1^2+p_2^2\rangle + \frac{1}{2}\sum_{a=1,2}\left\langle(\vec n\cdot\vec p_a)^2\right\rangle, \tag{V.76}$$
$$B_\perp = \frac{1}{2}\left\langle\frac{1}{r_{12}}\right\rangle - \frac{1}{2}n^i n^j\left\langle\nabla_1^j\phi\middle|\frac{r_{12}^i}{r_{12}}\middle|\phi\right\rangle + \frac{1}{2}\langle p_1^2+p_2^2\rangle - \frac{1}{4}\sum_{a=1,2}\left\langle(\vec n\cdot\vec p_a)^2\right\rangle, \tag{V.77}$$

4.2.4 Breit nucleus-nucleus contribution

Another, and final, contribution comes directly from the nucleus-nucleus Breit term of relativistic Hamiltonian

$$\delta E_C = -\frac{1}{2}\frac{1}{M_A M_B}p_A^i\left(\frac{\delta^{ij}}{R} + \frac{R^i R^j}{R^3}\right)p_B^j, \tag{V.78}$$

with p_A and p_B pertaining to the momenta of nucleus A and B, respectively. In view of simple identity,

$$\frac{1}{M_A M_B} = \frac{1}{4\mu_n^2} - \lambda^2, \tag{V.79}$$

the δE_C contributes to the λ^2 order correction,

$$Q_C^{ij} = C_\parallel n^i n^j + C_\perp \left(\delta^{ij} - n^i n^j\right), \tag{V.80}$$

$$C_\parallel = \frac{1}{R}, \tag{V.81}$$

$$C_\perp = \frac{1}{2R}, \tag{V.82}$$

Consequently, $A_{\parallel/\perp}$, $B_{\parallel/\perp}$, and $C_{\parallel/\perp}$ constitute a total contribution at order λ^2 to $\mathcal{W}_\parallel$ and $\mathcal{W}_\perp$, respectively, see Section **??** and Eq. (32) and (33) of Ref. [202],

$$\delta\mathcal{W}_{\parallel/\perp} = \lambda^2\, \alpha^2\, \left(A_{\parallel/\perp} + B_{\parallel/\perp} + C_{\parallel/\perp}\right), \tag{V.83}$$

(V.84)

We find it reassuring that with the parts A, B, and C summed together, the terms behaving like $1/R$ cancel out and asymptotic large-R behavior is $\sim 1/R^4$ – the same as in the case of BO relativistic corrections and leading order relativistic recoil correction – $E^{(4,1)}$.

4.3 Numerical calculations

The implementation of corrections $A_{\parallel/\perp}$ and $B_{\parallel/\perp}$ is straightforward in the ECG basis and part $C_{\parallel/\perp}$ is trivial. Numerical values obtained with up to 1024 ECG basis functions are presented in Table V.3 and the R-dependence is plotted on Fig. V.3. The correction is implemented as a modification to H2SPECTRE, see Chapter VI, which shifts the nonadiabatic potentials $\mathcal{W}_{\parallel/\perp}$ and resulting shift in the energy levels of HD is presented in Fig. V.4.

4.4 Discussion

We have shown that the heteronuclear part of $E^{(4,2)}$ appears to bigger than its overly conservative estimate by $\frac{m}{\mu_n}E^{(4,1)}$ by calculating the purely heteronuclear leading contribution. Ultimately, these effect are too small to explain prevailing experimental-theoretical discrepancies in the rovibrational transition energies.

Table V.3: Numerical values of $A_{\|}(R)$, $A_{\perp}(R)$, $B_{\|}(R)$, and $B_{\perp}(R)$, extrapolated from the results obtained with ECG bases of size N =64, 128, 256, 512, 1024. Uncertainties arise purely from extrapolation to complete basis set limit.

R/au	$A_{\|}/au$	$A_{\perp}/au$	$B_{\|}/au$	$B_{\perp}/au$
0.05	8.962 912 208 585(10)	8.952 437 362 19(2)	3.025 748 828 895(9)	3.028 638 978 761(8)
0.1	8.857 447 421 8(2)	8.821 610 117 04(9)	2.964 526 093 27(4)	2.974 413 424 05(3)
0.2	8.539 232 554 8(5)	8.433 235 755 0(4)	2.786 538 060 9(2)	2.815 519 525 1(3)
0.3	8.162 497 21(2)	7.982 438 641(2)	2.585 681 776(7)	2.634 173 483(6)
0.4	7.779 546 119 6(3)	7.532 518 080 94(7)	2.390 830 252 28(8)	2.456 143 869 84(7)
0.5	7.412 994 04(4)	7.109 009 53(4)	2.212 441 74(3)	2.291 185 36(3)
0.6	7.071 594 101 8(6)	6.720 542 665 41(8)	2.053 162 758 5(2)	2.142 120 284 6(2)
0.7	6.757 713 685 3(9)	6.368 356 552 0(6)	1.912 484 289 8(3)	2.008 878 829 7(5)
0.8	6.470 847 320 8(7)	6.050 607 225 07(5)	1.788 751 401 1(2)	1.890 275 279 3(3)
0.9	6.209 276 662 9(10)	5.764 318 741 2(2)	1.680 017 099 4(5)	1.784 782 194 4(5)
1.0	5.970 861 053 0(6)	5.506 262 902 587(7)	1.584 393 269 4(2)	1.690 861 591 4(3)
1.1	5.753 408 932 9(3)	5.273 341 399 8(2)	1.500 179 991 36(8)	1.607 096 561 4(2)
1.2	5.554 845 252 0(4)	5.062 735 942 48(5)	1.425 898 701 4(3)	1.532 233 682 8(3)
1.3	5.373 278 441 5(5)	4.871 950 397 16(4)	1.360 285 038 8(3)	1.465 186 239 4(3)
1.4	5.207 018 452 6(8)	4.698 804 337 72(6)	1.302 266 657 0(2)	1.405 021 454 6(3)
1.4011	5.205 268 965 2(7)	4.696 990 517 33(2)	1.301 667 171 3(2)	1.404 394 827 7(3)
1.5	5.054 571 582 1(5)	4.541 406 426 71(4)	1.250 937 153 74(8)	1.350 942 340 1(3)
1.6	4.914 625 095 7(4)	4.398 121 205 2(2)	1.205 530 848 52(4)	1.302 268 915 8(2)
1.7	4.786 028 169 6(3)	4.267 535 572 7(2)	1.165 400 174 10(5)	1.258 420 775 7(2)
1.8	4.667 772 345 62(3)	4.148 427 646 8(2)	1.129 996 103 2(2)	1.218 901 676 7(2)

Continued on next page

Table V.3 – *Continued from previous page*

R/au	$A_{\parallel}/au$	$A_{\perp}/au$	$B_{\parallel}/au$	$B_{\perp}/au$
1.9	4.558 972 959 73(9)	4.039 738 941 4(2)	1.098 851 460 4(3)	1.183 286 227 3(3)
2.0	4.458 852 124 3(2)	3.940 549 960 7(3)	1.071 566 748 8(3)	1.151 208 501 36(8)
2.1	4.366 723 394 5(4)	3.850 058 940 6(2)	1.047 798 076 2(2)	1.122 352 313 8(2)
2.2	4.281 978 035 4(9)	3.767 563 329 9(2)	1.027 246 787 2(3)	1.096 442 879 1(3)
2.3	4.204 072 731 1(5)	3.692 443 583 97(4)	1.009 650 469 7(2)	1.073 239 604 6(3)
2.4	4.132 518 563 6(5)	3.624 148 886 81(2)	0.994 775 068 0(4)	1.052 529 806 7(3)
2.5	4.066 871 105 5(7)	3.562 184 498 2(7)	0.982 407 928 6(8)	1.034 123 183 7(2)
2.6	4.006 721 545 0(5)	3.506 100 498 6(4)	0.972 351 662 4(4)	1.017 846 938 1(2)
2.7	3.951 688 801 7(2)	3.455 481 815 3(4)	0.964 418 800 2(3)	1.003 541 480 19(7)
2.8	3.901 412 672 7(2)	3.409 939 498 2(4)	0.958 427 273 9(2)	0.991 056 703 6(2)
2.9	3.855 548 088 8(6)	3.369 103 304 31(8)	0.954 196 820 1(2)	0.980 248 854 4(3)
3.0	3.813 760 607(3)	3.332 615 704 4(7)	0.951 546 423 1(10)	0.970 978 050 9(7)
3.2	3.741 114 820 4(10)	3.271 294 835 6(2)	0.950 250 809 0(4)	0.956 497 587 0(4)
3.4	3.680 928 435 0(4)	3.223 244 779 8(6)	0.953 054 681 1(3)	0.946 525 868 53(9)
3.6	3.630 768 714(3)	3.185 826 728 6(8)	0.958 493 483 2(10)	0.940 001 321 0(7)
3.8	3.588 394 184 5(8)	3.156 571 930 9(8)	0.965 223 544 4(8)	0.935 932 120 1(2)
4.0	3.551 854 461(3)	3.133 296 590(2)	0.972 129 740(2)	0.933 453 168 3(6)
4.2	3.519 564 980(4)	3.114 198 481(2)	0.978 397 222(2)	0.931 871 641 2(10)
4.4	3.490 328 198 8(4)	3.097 897 265 4(3)	0.983 524 694 89(8)	0.930 684 010 9(2)
4.6	3.463 301 194(3)	3.083 412 526(2)	0.987 284 917(2)	0.929 562 998 7(7)
4.8	3.437 929 336 1(8)	3.070 098 360 5(8)	0.989 655 612 1(8)	0.928 324 510 5(2)
5.0	3.413 869 821(3)	3.057 561 060(2)	0.990 745 478(2)	0.926 887 700 5(7)

Continued on next page

Table V.3 – *Continued from previous page*

R/au	$A_{\parallel}/au$	$A_{\perp}/au$	$B_{\parallel}/au$	$B_{\perp}/au$
5.2	3.390 922 311 1(5)	3.045 580 752 2(2)	0.990 731 521 73(9)	0.925 238 121 9(3)
5.4	3.368 974 664 3(5)	3.034 047 898 4(6)	0.989 813 937 3(6)	0.923 398 827 95(4)
5.6	3.347 964 769(2)	3.022 917 217(2)	0.988 187 872(2)	0.921 410 268 1(4)
5.8	3.327 855 905(3)	3.012 177 031(2)	0.986 028 341(3)	0.919 317 678 4(9)
6.0	3.308 622 047 9(4)	3.001 830 363 1(2)	0.983 484 058 0(4)	0.917 163 994 0(2)
6.5	3.264 209 099 2(2)	2.977 726 348 56(6)	0.976 177 347 09(3)	0.911 739 822 85(3)
7.0	3.224 697 887 8(5)	2.956 148 380 7(3)	0.968 443 203 19(4)	0.906 546 661 47(2)
7.5	3.189 586 379 1(6)	2.936 972 278 3(3)	0.960 921 515 00(10)	0.901 768 419 25(5)
8.0	3.158 340 169 6(3)	2.919 969 416 1(2)	0.953 885 142 2(2)	0.897 456 905 45(7)
8.5	3.130 447 351 3(3)	2.904 874 503 9(2)	0.947 419 351 38(5)	0.893 597 636 51(2)
9.0	3.105 447 893 90(10)	2.891 428 466 68(5)	0.941 521 523 44(9)	0.890 148 786 87(4)
9.5	3.082 943 007 9(2)	2.879 398 321 47(9)	0.936 152 335 8(2)	0.887 061 153 30(5)
10.0	3.062 593 494 4(3)	2.868 583 174 1(2)	0.931 260 500 2(2)	0.884 287 209 22(5)
∞	2.666 ...	2.666 ...	0.833 ...	0.833 ...

5 Finite nuclear size corrections

The leading order correction due to the finite size of the nucleus [2] is based on the hydrogenic theory with the adjustment of the electronic density at the nuclei,

$$H^{(4)}_{\text{fns}} = \frac{2\pi}{3}\left[\delta^3(r_{1A}) + \delta^3(r_{1B}) + \delta^3(r_{2A}) + \delta^3(r_{2B})\right]\frac{r_A^2 + r_B^2}{2}. \tag{V.85}$$

Physically it can be thought of as originating from the modification of the Coulomb potential by the finite charge distribution of the nuclei. Unlike the muonic systems, at the current level of electronic molecular hydrogen higher-order corrections due to nuclear size (higher multipole moments) and nuclear polarizability are negligible.

Although this corrections is very small (typically a few MHz, see Table V.4) it is required to explain observed experimental spectra, which nowadays reach unprecedented, sub MHz accuracy [203].

Table V.4: Shift (in MHz) due to the finite nuclear size correction with root mean nuclear charge radius for 2018 CODATA [25] recommended values, $r_p = 0.8414(19)$ fm, $r_d = 2.12799(74)$ fm, and $r_t =$ fm from Ref. [204]. Total uncertainty (in parentheses) is completely dominated by the uncertainty of the radii.

Isotopologue	$E^{(4)}_{\text{fns}}$
H_2	$-0.9322(43)$
D_2	$-6.0567(54)$
T_2	$-4.17(17)$
HD	$-3.4724(51)$
HT	$-2.528(85)$
DT	$-5.114(86)$

The necessity to include this correction introduces the mean square charge radius of the A/B nucleus in the context of spectroscopic data another parameter as an input to the ab-initio predictions,

$$E_{\text{tot}} = E_{\text{theo}} + C^{(4)}_{\text{fns}}\frac{r_A^2 + r_B^2}{2} \tag{V.86}$$

Because the uncertainty of $C^{(4)}_{\text{fns}}$ is much lower than that of either of the radii, one can invert the problem and use accurate values of E_{theo} and $C^{(4)}_{\text{fns}}$ and experimental values of E_{tot} to determine the radii.

[2] formally contributing to $E^{(4)}$, because it enters through the Dirac form factor

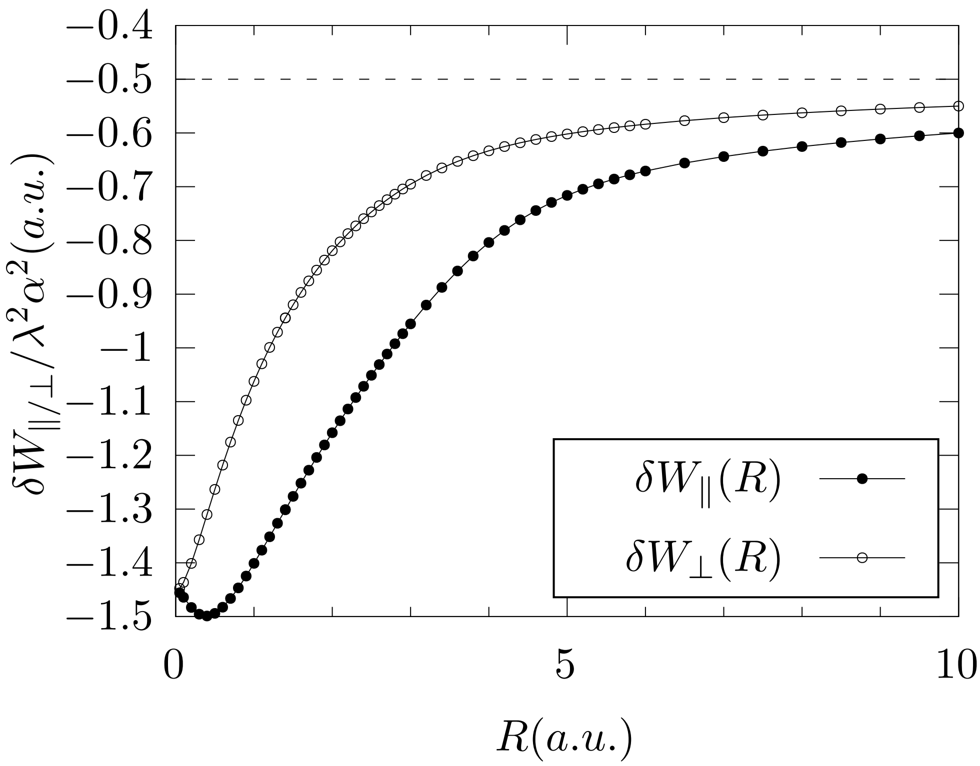

Figure V.3: R-dependence of the heteronuclear correction to the nuclear kinetic energy. Notice the coindicidence at united-atom due to the lift of the system's symmetry.

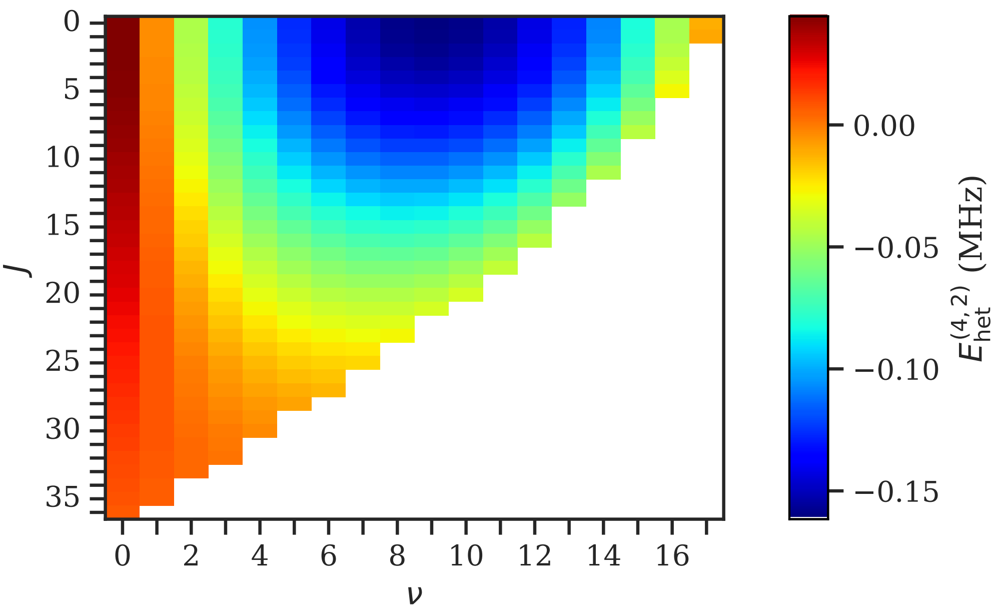

Figure V.4: Total contribution of heteronuclear relativistic recoil to rovibrational energy levels of HD.

6 Quantum electrodynamic corrections in Born-Oppenheimer approximation

This Section is based on work [A4] and addresses the application of the ECG method for the calculations of QED corrections to the molecular hydrogen levels. The calculations are restricted to the level of Born-Oppenheimer approximation with a particular emphasis on the most computationally intensive quantity called Bethe logarithm. By 2 to 3 orders of magnitude and eliminate the uncertainty of $E^{(5,0)}$ from the uncertainty budget.

The main motivation behind work [A4] is inherited from the considerations outlined in previous Sections concerning relativistic corrections. The aim is to explain the observed experimental-theoretical discrepancy with particular emphasis on the HD isotopologue, which is most accurately measured and hints at $\sim 2\sigma$ discrepancy. With this endeavour we follow a similar line of thought as in the case of $E^{(4)}$ (relativistic) contributions to the molecular energy levels: first we verify the accuracy of QED corrections at the level of Born-Oppenheimer approximation and then address the finite nuclear mass QED effects.

6.1 Introduction

Quantum electrodynamic effects (QED) in atomic and molecular spectra are very difficult to determine computationally, despite the fact that the exact formulas are well known [205]. For this reason, they are often only roughly estimated based on hydrogenic results [206]. However, to obtain transition energies for few-electron systems with accuracy comparable to modern spectroscopic measurements, a high-precision computational method that accounts for a complete leading-order QED has to be employed. So far, such calculations have been performed only for atoms with up to four electrons [207–216], and only for the simplest molecule, i.e., two-electron molecular hydrogen (H_2 and its deuterated and tritiated isotopologues) [198].

Recent measurements of several rovibrational P- and R-branch transitions in the fundamental and overtone bands of the HD molecule have reached unprecedented sub-MHz uncertainty [7–13, 217–219]. It exceeds by at least an order of magnitude the accuracy of theoretical predictions including relativistic and QED contributions [68, 144, 201, 220, 221]. Moreover, systematic discrepancies of 1.4-1.9σ are observed between calculated and experimental values, the origin of which is currently not clear. To improve theoretical predictions, at first, it is necessary to determine more precisely the leading $m\alpha^5$ QED correction [198]. Its numerical uncertainty is comparable to the estimate of unknown finite nuclear mass (nonadiabatic) QED effects. Therefore, the development of a computational method that significantly reduces such numerical inaccuracies is an indispensable step towards advancing the present theory of the hydrogen molecule to a higher level of accuracy.

In this Section we present high-precision calculations of leading $m\alpha^5$ QED correction in the ground electronic state of a hydrogen molecule, using the Born-Oppenheimer (BO) approximation, thus omitting the nonadiabatic effect. Our goal is to improve the accuracy of previous results [198] by at least two orders of magnitude, including the most computationally demanding Bethe logarithm term. To accomplish this, we employ explicitly correlated Gaussian (ECG) basis functions and perform extensive variational optimization over all nonlinear parameters. The decisive advantage of the ECG method is that the underlying integrations are manageable and very fast in numerical evaluation due to the compact formulas for matrix elements of the nonrelativistic Hamiltonian, and they involve only well-known error function and elementary ones. Even though Gaussian functions have the drawback of improper short-range form and fail to correctly describe the Kato cusp, it can be overcome with a sufficiently large and well-optimized ECG basis set together with dedicated regularization techniques that accelerate the convergence of singular operators. Furthermore, additional ECG integrals that arise as a consequence of the regularization can be efficiently evaluated by means of dedicated numerical quadrature. Increasing the accuracy of the Bethe logarithm requires also the development of efficient optimization algorithms, employing larger bases and a denser grid in the Schwartz integral method [209] evaluated for a wide range of internuclear distances. In addition, it is important to derive leading asymptotic terms, which are crucial for fitting the contours in numerical integration. All this considerable effort is vital in laying the foundation for the future determination of non-adiabatic QED effects, which are the bottleneck limiting the current accuracy of theoretical predictions for rovibrational energy levels of hydrogen molecule isotopologues.

6.2 Leading order QED correction

As a starting point we assume the adiabatic approximation (clamped nuclei), so that the total molecular wavefunction Ψ is a product of the electronic and nuclear parts,

$$\Psi = \chi(\vec{R})\,\phi(\vec{r}_1, \vec{r}_2; R). \tag{V.87}$$

The leading $m\alpha^5$ QED correction

$$E^{(5,0)} = \langle \chi | \mathcal{E}^{(5,0)}(R) | \chi \rangle \tag{V.88}$$

to the molecular level is obtained by averaging the potential $\mathcal{E}^{(5,0)}(R)$ of Eq. (V.89) with the nuclear wavefunction χ; see [221] for details. The QED potential $\mathcal{E}^{(5,0)}$ for a two-electron diatomic molecule can be compactly represented as [205],

$$\begin{aligned}\mathcal{E}^{(5,0)}(R) = \frac{4}{3}\Big(\frac{19}{30} - 2\ln\alpha - \ln k_0\Big)\sum_{i,X} Z_X \langle \delta^3(\vec{r}_{iX})\rangle \\ + \Big(\frac{164}{15} + \frac{14}{3}\ln\alpha\Big)\langle \delta^3(\vec{r}_{12})\rangle - \frac{14}{3}\frac{1}{4\pi}\Big\langle \frac{1}{r_{12}^3}\Big\rangle_\varepsilon\end{aligned} \tag{V.89}$$

where R is the internuclear distance, Z_X is the charge of nucleus X, the expectation value $\langle \ldots \rangle$ stands for integration over electronic degrees of freedom with the nonrelativistic wave function ϕ, $\ln k_0$ is the Bethe logarithm [222] (see Eq. (V.91) below), and the last term is the Araki-Sucher correction [223, 224] with $\langle r_{ij}^{-3}\rangle_\varepsilon$ denoting the following limit:

$$\left\langle \frac{1}{r_{ij}^3} \right\rangle_\varepsilon \equiv \lim_{\varepsilon\to 0}\left[\left\langle \frac{\Theta(r_{ij}-\varepsilon)}{r_{ij}^3}\right\rangle + (\gamma_E + \ln\varepsilon)\big\langle 4\pi\delta(\vec{r}_{ij})\big\rangle\right]. \tag{V.90}$$

The symbol γ_E denotes the Euler-Mascheroni constant, and $\Theta(x)$ is the Heaviside step function.

6.3 Bethe logarithm

At the level of Born-Oppenheimer approximation, Bethe logarithm enters as the R-dependent electronic quantity, defined as the following ratio of matrix elements [222],

$$\ln k_0 \equiv \frac{\langle\vec{\nabla}(\mathcal{H}-\mathcal{E})\ln(2(\mathcal{H}-\mathcal{E}))\vec{\nabla}\rangle}{\langle\vec{\nabla}(\mathcal{H}-\mathcal{E})\vec{\nabla}\rangle}, \tag{V.91}$$

with the electronic Hamiltonian,

$$\mathcal{H} \equiv -\frac{1}{2}\sum_i \nabla_i^2 - \sum_{i,X}\frac{Z_X}{r_{iX}} + \frac{1}{r_{12}} + \frac{Z_A Z_B}{R}, \tag{V.92}$$

and $\mathcal{E}$ its lowest energy eigenvalue,

$$\mathcal{H}\phi(\vec{r}_1,\vec{r}_2;R) = \mathcal{E}(R)\phi(\vec{r}_1,\vec{r}_2;R). \tag{V.93}$$

It can be represented in terms of the integral [215, 216],

$$\ln k_0 = \frac{1}{\mathcal{D}}\int_0^1 dt\,\frac{f(t)-f_0-f_2\,t^2}{t^3} \tag{V.94}$$

with

$$f(t) = -\left\langle\vec{\nabla}\,\frac{k}{k+\mathcal{H}-\mathcal{E}}\,\vec{\nabla}\right\rangle, \qquad t = \frac{1}{\sqrt{1+2\,k}}. \tag{V.95}$$

In the BO approximation, the current operator is purely electronic,

$$\vec{\nabla} = \vec{\nabla}_1 + \vec{\nabla}_2\,, \tag{V.96}$$

and the denominator

$$\mathcal{D} = 2\,\pi\sum_{i,X}\langle\delta^3(\vec{r}_{iX})\rangle, \tag{V.97}$$

where the index i runs over electrons and X over nuclei. The function $f(t)$ in Eq. (V.94) has the following expansion around $t=0$,

$$f(t) = f_0 + f_2\,t^2 + f_3\,t^3 + (f_4^l \ln t + f_4)\,t^4 + \mathcal{O}(t^5)\,, \tag{V.98}$$

with the coefficients

$$
\begin{aligned}
f_0 &= -\langle\vec{\nabla}^2\rangle, \quad f_2 = -2\,\mathcal{D}\,, \quad f_3 = 8\,\mathcal{D}, \quad f_4^l = 16\,\mathcal{D}, \\
f_4 &= 4\left[\sum_{i,X}\left\langle\frac{1}{r_{iX}^4}\right\rangle_\varepsilon + \sum_{\substack{(i,X),(j,Y)\\(i,X)\neq(j,Y)}}\left\langle\frac{\vec{r}_{iX}\vec{r}_{jY}}{r_{iX}^3 r_{jY}^3}\right\rangle\right] \\
&- 2\,\mathcal{D}\Big(1-4(1+\ln 4)\Big),
\end{aligned}
\tag{V.99}
$$

where

$$
\begin{aligned}
\left\langle\frac{1}{r_{ij}^4}\right\rangle_\varepsilon \equiv \lim_{\varepsilon\to 0}\Bigg[\left\langle\frac{\Theta(r_{ij}-\varepsilon)}{r_{ij}^4}\right\rangle - \frac{\langle 4\pi\delta(\vec{r}_{ij})\rangle}{\varepsilon} \\
+ 2\left\langle 4\pi\delta(\vec{r}_{ij})\frac{\partial}{\partial r_{ij}}\right\rangle(\gamma_E + \ln\varepsilon)\Bigg].
\end{aligned}
\tag{V.100}
$$

In the early days of quantum electrodynamics the calculation of the Bethe logarithm for systems beyond hydrogen-like atoms, even with a few percent accuracy, emerged as a challenging task [225–227]. In the approach presented by Schwartz [209, 228, 229] the evaluation of $f(t)$ was reformulated into the second-order problem of finding $\vec{\phi}_1$ satisfying the following inhomogeneous differential equation:

$$
(\mathcal{E}-\mathcal{H}-k)\vec{\phi}_1 = \vec{\nabla}\phi,
\tag{V.101}
$$

so that the sum over states $f(t)$ is simply given by $\vec{\phi}_1$ as

$$
f(t) = k\langle\vec{\phi}_1|\vec{\nabla}|\phi\rangle.
\tag{V.102}
$$

This is equivalent to finding a stationary value of the following Ritz functional

$$
w(k) = 2\langle\phi|\vec{\nabla}|\vec{\phi}_1\rangle + \langle\vec{\phi}_1|\mathcal{E}-\mathcal{H}-k|\vec{\phi}_1\rangle,
\tag{V.103}
$$

which with the stationarity condition

$$
\delta w(k) \equiv 2\langle\phi|\vec{\nabla}|\delta\vec{\phi}_1\rangle + 2\langle\vec{\phi}_1|\mathcal{E}-\mathcal{H}-k|\delta\vec{\phi}_1\rangle = 0
\tag{V.104}
$$

recovers (V.101) due to the arbitrariness of variation $\delta\vec{\phi}_1$. Such a formulation allows for variational computation of $w(k)$. For the sake of evaluating the integral (V.94), the matrix element (V.102) has to be minimized on a grid of values of k, bearing in mind the manifest dependence of $\vec{\phi}_1$ on k.

6.4 Method

For the purpose of variational calculations of the resolvent, we follow with the decomposition of $f(t)$, into $f_{\|}(t)$ and $f_{\perp}(t)$, which emerges from the decomposition of $\vec{\nabla}$,

$$\vec{\nabla} = \vec{n}\,(\vec{n}\cdot\vec{\nabla}) - \vec{n}\times(\vec{n}\times\vec{\nabla}). \tag{V.105}$$

Namely,

$$f(t) = f_{\|}(t) + f_{\perp}(t), \tag{V.106}$$

$$f_{\|}(t) = -\left\langle Q_{\|}\,\frac{k}{k+\mathcal{H}-\mathcal{E}}\,Q_{\|}\right\rangle,$$

$$f_{\perp}(t) = -\left\langle \vec{Q}_{\perp}\,\frac{k}{k+\mathcal{H}-\mathcal{E}}\,\vec{Q}_{\perp}\right\rangle, \tag{V.107}$$

where

$$Q_{\|} = \vec{n}\cdot\vec{\nabla}, \tag{V.108}$$

$$\vec{Q}_{\perp} = \vec{n}\times(\vec{n}\times\vec{\nabla}). \tag{V.109}$$

Because the ground state is of Σ_g^+ symmetry, this entails dipole connected intermediate states of Σ_u^+ and Π_u^- symmetry in the resolvents in $f_{\|}$ and $f_{\perp}$, respectively.

The external wavefunction ϕ is expanded in ECG basis functions; see Eq. (V.113) below. For a series of basis sizes $N \in \{64, 128, 256, 512, 768, 1024\}$ and for 55 values of internuclear distance R in the range $0.05-10$ au, we have minimized $f_{\|}(t)$ and $f_{\perp}(t)$ on a uniform grid ($\Delta t = 0.01$). We followed the heuristic approach of Refs. [67, 69] and set the size of intermediate state basis as $N' = 2N$ for $t \leq 0.1$ and $N' = \frac{3}{2}N$ otherwise.

To efficiently evaluate the integral (V.94) we split the integration domain into two regions: $t \in \langle 0, t_{\rm crit}\rangle$ and $t \in (t_{\rm crit}, 1\rangle$. The high-$t$ region is free of singularities, and $f(t)$ can be efficiently integrated numerically. For this purpose we have optimized $f(t > t_{\rm crit})$ on a uniform t-grid with the spacing of 0.01. Because $f(1)$ satisfies the generalized Thomas-Reiche-Kuhn (TRK) sum rule [230],

$$\langle\vec{\nabla}(\mathcal{H}-\mathcal{E})^{-1}\vec{\nabla}\rangle = -3, \tag{V.110}$$

we have utilized it in practical computations to deduce the completeness of the intermediate state basis and estimate the numerical uncertainty of $f(t)$. Then, the integral is evaluated by means of interpolating the numerical data with a high-order polynomial (typically of order 18). With the largest bases considered, the uncertainty resulting from numerical integration in the high-t region is of order 10^{-11}, which is a few orders of magnitude less than the uncertainty coming from the integration of the low-t region, the latter being of critical importance for high accuracy of the final value of $\ln k_0$.

Primarily, in low-t region a strong numerical cancellation between $f(t)$ and leading asymptotic terms f_0 and f_2t^2 occurs. We emphasize that for high photon momenta ($t \to 0$)

the integrand in the integral definition of $\ln k_0$, see Eq. (V.94), is dominated by $\sim t^{-3}$, so that two leading terms of Taylor expansion have to be subtracted from $f(t)$ to render it integrable. For that reason, $f(t < t_{\rm crit})$ cannot be evaluated with high-accuracy in the same way as in high-t region, and we resort to elementary, term-by-term, analytical integration of the asymptotic expansion (V.98). Nonetheless, to achieve a highly precise final value of $\ln k_0$, inclusion only of known terms (up to $\sim t^4$) is insufficient and higher-order coefficients of low-t asymptotics of $f(t)$ have to be added. They are determined by fitting them from the numerical data from the range $(t_{\rm cut}, t_{\rm crit})$ as,

$$\delta f(t) \equiv f(t) - \big(f_0 + f_2\, t^2 + f_3\, t^3 + (f_4^l \ln t + f_4)\, t^4\big), \tag{V.111}$$

with the functional form of fitted expansion deduced from the known behavior of $f(t)$ for the hydrogen atom [231, 232],

$$\frac{\delta f(t)}{t^5} = \sum_{m=0}^{M} t^m (f_m + f_m^l \ln t), \tag{V.112}$$

with fixed $f_m^l = 0$ for m even. For very low values of t a $t_{\rm cut}$ cutoff discards numerical points $f(t < t_{\rm cut})$, which are of insufficient numerical accuracy, due to the presence of t^{-3} acting as a weighting factor greatly enhancing the demand on the numerical accuracy of $f(t)$ as $t \to 0$. Resultantly, values of $f(t < t_{\rm cut})$ have to be discarded completely and cannot be used even for the purpose of fitting higher order terms of low-t asymptotics.

Ultimately, $t_{\rm cut}$, $t_{\rm crit}$, and M are adjustable parameters, which are tuned with the purpose of reaching the final value of $\ln k_0$, such that it presents weak sensitivity to their change. Fluctuations of $\ln k_0$ due the change of those parameters around their optimal values serve as an uncertainty estimation. Typically, optimal values lie in the range $t_{\rm cut} \in (0.02, 0.06)$, $t_{\rm crit} \in (0.12, 0.23)$, and $M \in (2, 6)$, with pronounced tendency of preffered larger $t_{\rm crit}$ whenever higher fit order M is demanded.

6.5 ECG method

In our calculations we utilize an explicitly correlated Gaussian (ECG) basis,

$$\begin{aligned} \phi &= \sum_i c_i \phi_i(\vec{r}_1, \vec{r}_2), \\ \phi_i &= (1 \pm \mathcal{P}_{A\leftrightarrow B})(1 \pm \mathcal{P}_{1\leftrightarrow 2}) \\ &\quad \times e^{-a_{12} r_{12}^2 - a_{1A} r_{1A}^2 - a_{1B} r_{1B}^2 - a_{2A} r_{2A}^2 - a_{2B} r_{2B}^2}. \end{aligned} \tag{V.113}$$

Direct inclusion of the interelectronic distance r_{12} in the exponent of trial wavefunction renders it a two-particle, two-center geminal, *explicitly correlated* basis. The primary virtue of the ECG basis is that all the requisite integrals for calculations of nonrelativistic energy and $f(t)$ can be evaluated very efficiently.

According to (V.89), the $\mathcal{E}^{(5,0)}$ correction appears as a deceivingly simple sum of expectation values. Those expectation values, however, are of operators that are rather nontrivial.

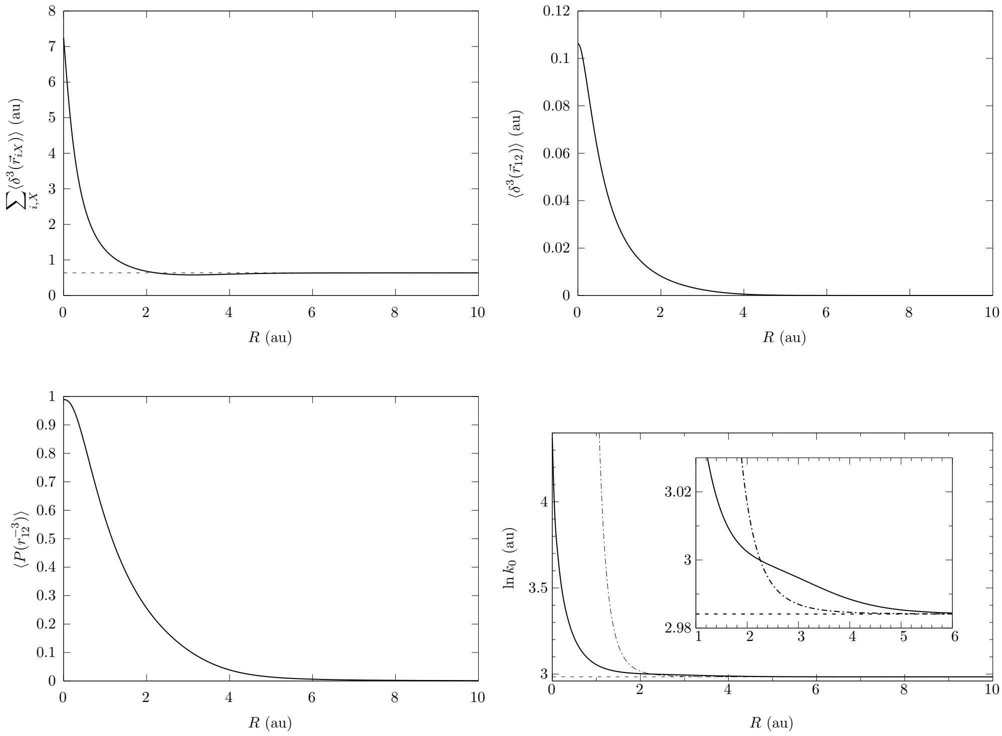

Figure V.5: The R-dependence of components contributing to electronic QED potential $\mathcal{E}^{(5,0)}$. From upper left to lower right: sum of nucleus-electron Dirac delta, electron-electron Dirac delta, Araki-Sucher correction, electronic Bethe logarithm. All of those change most significantly in the low-R region where the electronic density changes most rapidly from that of a ground state helium atom.

They probe the wavefunction in the vicinity of Coulombic singularities, as in the case of Araki-Sucher correction or even exactly pointwise at those singularities in the case of Dirac delta functions.

For detailed description of both ECG integrals and regularization of singular operators we refer to the earlier Section II.**??**. The regularization procedure is pivotal for achieving well-converged, high-accuracy expectation values of singular operators with ECG functions [68, 69].

Table V.5: Convergence of the electronic BO energy ($\mathcal{E}$) and terms contributing to $\mathcal{E}^{(5,0)}$ with increasing basis size N at $R = 1.4$ au. For fixed N, the uncertainty of $\ln k_0$ originates from uncertainties of the $f_{i>4}$. Here, as well as for all other values of R, this uncertainty dominates over the uncertainty resulting from extrapolation to the complete basis set limit. All presented digits of Dirac delta expectation values and $\langle r_{12}^{-3}\rangle_\varepsilon$ are accurate.

N	$\mathcal{E}$	$\sum_{i,X}\langle\delta^3(\vec{r}_{iX})\rangle$	$\langle\delta^3(\vec{r}_{12})\rangle$	$\langle r_{12}^{-3}\rangle_\varepsilon$	$\ln k_0$
64	−1.174 474 384 972 363	0.919 300 2223	0.016 739 9980	0.414 497 7238	3.018 421(77)
128	−1.174 475 663 522 751	0.919 333 4195	0.016 742 9651	0.414 364 3945	3.018 549 0(37)
256	−1.174 475 712 366 731	0.919 335 9183	0.016 743 2525	0.414 346 7147	3.018 561 00(43)
512	−1.174 475 714 135 081	0.919 336 1813	0.016 743 2745	0.414 345 0950	3.018 563 264(40)
768	−1.174 475 714 210 245	0.919 336 2021	0.016 743 2769	0.414 344 8871	3.018 563 400(20)
1024	−1.174 475 714 218 617	0.919 336 2099	0.016 743 2776	0.414 344 8224	3.018 563 453(28)
∞	−1.174 475 714 221(1)	0.919 336 214(3)	0.016 743 2780(4)	0.414 344 79(3)	3.018 563 480(38)
Ref. [198]	–	0.919 34(1)	0.016 74(1)	0.414 30(1)	3.018 55(1)
Ref. [233]	−1.174 475 714(1)	–	–	–	3.018 55(3)
Ref. [68][3]	−1.174 475 714 203	0.919 336 206(7)	0.016 743 2783(5)	–	–
Ref. [38, 68][4]	−1.174 475 714 220 443 4(5)	0.919 336 211(2)	0.016 743 2783(3)	–	–

6.6 Hydrogenic asymptotic coefficients

The hydrogen molecule in its ground state dissociates into H($1s$)+H($1s$). Therefore, in our calculations we benefit from the fact that the analytical form of $f(t)$, the essential part of the integrand of the integral representation of $\ln k_0$, is known exactly for the hydrogen-like atom [231, 232]:

$$f^{\mathrm{H}}(t) \equiv -384\frac{t^5}{(1+t)^8(2-t)}\,{}_2F_1(4, 2-t, 3-t; \xi), \tag{V.114}$$

where ${}_2F_1$ is the hypergeometric function in standard notation [234] and

$$\xi = [(1-t)/(1+t)]^2, \qquad t = Z/\sqrt{-2(\mathcal{E}-k)}. \tag{V.115}$$

Resultantly, the numerical value of the Bethe logarithm for the ground state of the hydrogen atom ($Z = 1$, $\mathcal{E} = -1/2$) is known with many-digit accuracy [235],

$$\ln k_0(\mathrm{H}) = 2.984\,128\,555\,765\,498\,\ldots \tag{V.116}$$

and it admits a low-t expansion,

$$\begin{aligned} f^{\mathrm{H}}(t) &= 2 - 8t^2 + 32t^3 + 8t^4(8\ln t - 5 + 16\ln 2) - \frac{32}{3}t^5\left(6+\pi^2\right) \\ &\quad - 8t^6(16\ln t + 8\zeta(3) - 31 + 32\ln 2) - \frac{32}{45}t^7\left(-75 - 30\pi^2 + \pi^4\right) \\ &\quad + \frac{8}{9}t^8(120\ln t - 72\zeta(5) + 144\zeta(3) - 289 + 240\ln 2) + O(t^9), \end{aligned} \tag{V.117}$$

where $\zeta(x)$ is the Riemann zeta function and $\zeta(3)$ is also known as the Apéry constant. The dominating contribution to the Bethe logarithm comes from the high momenta of photon excitation [236], thus involving highly excited continuum states[237]. Therefore, its value is very insensitive to the details of perturbation of electronic structure as induced by the presence of another hydrogen atom. As a result, we expect that not only $f(t)$ but also individual terms of its Taylor expansions should be relatively close to those of $f^{\mathrm{H}}(t)$ for all but very small values of R.

In Figure V.6 we have plotted the ratio f_4^l/f_4 divided by $f_4^{\mathrm{H}l}/f_4^{\mathrm{H}}$, where the latter one is the same ratio but extracted from $f^{\mathrm{H}}(t)$ – an analytical formula for $f(t)$ for hydrogen-like atom [231, 232]. This ratio shows very weak dependence on R and departs significantly from hydrogenic values only for small internuclear distances. Consequently, we found it beneficial to fix the f_n^l/f_n ratio to the hydrogenic ratio for the purpose of stabilizing the numerical fit. Otherwise the f_n and f_n^l coefficients are mutually strongly correlated and sensitive to the fit parameters due to near degeneracy between terms t^n and $t^n \ln t$ for given value of n. We call such a fit expansion with fixed f_n^l/f_n ratio *log-contracted* (l-c). Indeed, we observe that for $R > 1$ au there is virtually no difference in final values of $\ln k_0$, yet, l-c fit exhibits slightly smaller variance with respect to variation of fit order and values of t_{cut} and t_{crit}. Clearly, for sufficiently small values of R, log-contraction is not reliable because it makes the fit expansion too stiff, as $f(t)$ starts to resemble that of

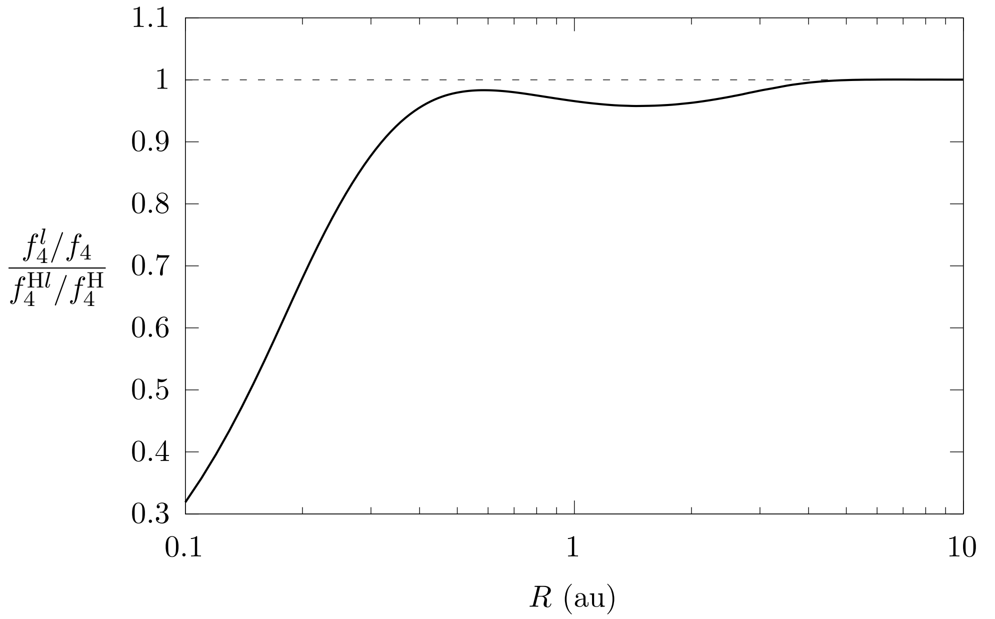

Figure V.6: Solid black line is the ratio between f_4^l/f_4, with both coefficients calculated by Eq. (V.99) divided by the same ratio of Taylor coefficients taken from hydrogenic $f^{\mathrm{H}}(t)$. Dashed line is drawn to guide the eye to the asymptotic hydrogenic limit.

the ground state of helium atom, rather than hydrogen atom.

Table V.6: Convergence of $\ln k_0$ with the basis size N at $R = 1.4$ au with and without log-contraction.

N	$\ln k_0$	$\ln k_0$ (l-c)[5]
64	3.018 444(79)	3.018 444(78)
128	3.018 548 9(22)	3.018 548 7(23)
256	3.018 561 43(28)	3.018 561 39(29)
512	3.018 563 296(31)	3.018 563 278(17)
768	3.018 563 451(36)	3.018 563 429(16)
1024	3.018 563 500(53)	3.018 563 482(23)
∞	3.018 563 525(64)	3.018 563 508(27)

We have observed that $\ln k_0$ calculated with log-contraction tends to consistently yield slightly lower values than the uncontracted fit expansion for all values of R, though the difference is minuscule and decreases to values much lower than the critical region fit uncertainty for bigger values of R. As depicted by Figure V.6 such a coefficient contraction is not justified only for very small values of $R < 0.4$ au, for which the configuration resembles $(1s)^2$ configuration of helium atom.

Ultimately though, we have concluded that there is no physical grounds justifying the use of log-contraction and we used an unconstrained fit at the expense of higher uncertainty.

6.7 Evaluation of f_4 through integration by parts

In the evaluation of f_4 term,

$$f_4 = 4\left[\sum_{i,X}\left\langle\frac{1}{r_{iX}^4}\right\rangle_\varepsilon + \sum_{\substack{(i,X),(j,Y)\\(i,X)\neq(j,Y)}}\left\langle\frac{\vec{r}_{iX}\vec{r}_{jY}}{r_{iX}^3 r_{jY}^3}\right\rangle\right] - 2\,\mathcal{D}\Big(1-4(1+\ln 4)\Big),$$

the part with $(a,b)=(c,d)$, proportional to r_{ab}^{-4} is separated and we focus on the $(a,b)\neq(c,d)$ term,

$$f_4^{(abcd)} \equiv \left\langle \Psi_k \frac{\vec{r}_{ab}}{r_{ab}^3}\frac{\vec{r}_{cd}}{r_{cd}^3}\Psi_l\right\rangle = \langle\Psi_k \nabla_a^i\left(\frac{1}{r_{ab}}\right)\nabla_c^i\left(\frac{1}{r_{cd}}\right)\Psi_l\rangle \tag{V.118}$$

first we integrate by parts with respect to ∇_a^i

$$f_4^{(abcd)} = -\langle\nabla_a^i(\Psi_k)\left[\frac{1}{r_{ab}}\nabla_c^i\left(\frac{1}{r_{cd}}\right)\right]\Psi_l\rangle + \frac{\delta_{ac}+\delta_{ad}}{2}\langle\Psi_k\frac{1}{r_{ab}}4\pi\delta^{(3)}(\vec{r}_{cd})\,\Psi_l\rangle + (k\leftrightarrow l), \tag{V.119}$$

and now integrate first term by parts with respect to ∇_c^i,

$$\begin{aligned} f_4^{(abcd)} = {} & \langle\nabla_a^i\nabla_c^i\Psi_k\frac{1}{r_{ab}r_{cd}}\Psi_l\rangle + \langle\nabla_a^i(\Psi_k)\frac{1}{r_{ab}r_{cd}}\nabla_c^i(\Psi_l)\rangle + \langle\nabla_a^i(\Psi_k)\left[\frac{1}{r_{cd}}\nabla_c^i\left(\frac{1}{r_{ab}}\right)\right]\Psi_l\rangle \\ & + \frac{\delta_{ac}+\delta_{ad}}{2}\langle\Psi_k\frac{1}{r_{ab}}4\pi\delta^{(3)}(\vec{r}_{cd})\,\Psi_l\rangle + (k\leftrightarrow l), \end{aligned} \tag{V.120}$$

where $(k\leftrightarrow l)$ stands for all the terms in the expression repeated, but with labels k and l interchanged. It is clear that whenever $a\neq c$ and $b\neq c$ only first two terms survive. Nevertheless, in the general case since both Eq. (V.119) and Eq. (V.120) are identities for the expectation value we started with, we consider analogous set of equations with action of ∇_c^i by parts first, and by ∇_a^i subsequently and add all four equations together. This completely removes the action of ∇ from both $\frac{1}{r_{ab}}$ and $\frac{1}{r_{cd}}$ and we obtain working formula,

$$\begin{aligned} f_4^{(abcd)} = \left\langle\Psi_k\frac{\vec{r}_{ab}}{r_{ab}^3}\frac{\vec{r}_{cd}}{r_{cd}^3}\Psi_l\right\rangle = {} & \frac{1}{2}\langle\nabla_a^i\nabla_c^i\Psi_k\frac{1}{r_{ab}r_{cd}}\Psi_l\rangle + \frac{1}{2}\langle\Psi_k\frac{1}{r_{ab}r_{cd}}\nabla_a^i\nabla_c^i\Psi_l\rangle + \langle\nabla_a^i(\Psi_k)\frac{1}{r_{ab}r_{cd}}\nabla_c^i(\Psi_l)\rangle \\ & + \frac{1}{2}\langle\Psi_k\left[\frac{(\delta_{ac}+\delta_{ad})}{r_{ab}}4\pi\delta^{(3)}(\vec{r}_{cd}) + \frac{(\delta_{ca}+\delta_{cb})}{r_{cd}}4\pi\delta^{(3)}(\vec{r}_{ab})\right]\Psi_l\rangle \end{aligned} \tag{V.121}$$

which can be readily implemented in terms of single index-lowering transform $\frac{1}{r} = \frac{2}{\sqrt{\pi}}\int_0^\infty dt\, e^{-t^2r^2}$ acting on *Coulomb* ECG integrals. Note that in the BO approximation, the last terms containing $\delta^{(3)}(\vec{r})$ vanishes when case (a,X,b,X) is considered and in the case (a,X,a,Y) those terms simplify to,

$$\frac{1}{R}\langle\Psi_k\left[4\pi\delta^{(3)}(\vec{r}_{aX}) + 4\pi\delta^{(3)}(\vec{r}_{aY})\right]\Psi_l\rangle, \tag{V.122}$$

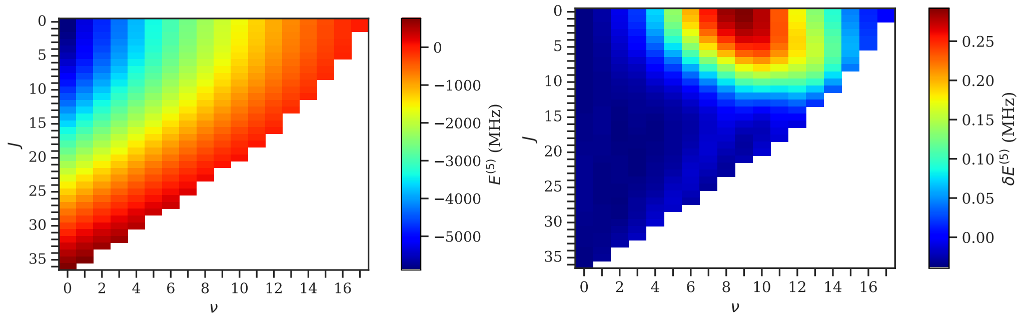

Figure V.7: Total contribution (left panel) to the shift in the energy of rovibrational levels of HD due to leading-order QED effects and the shift (right panel) due to present recalculation with respect to Ref. [198].

Inconspicuously, in a more general cases when positions of X and Y are not fixed (e.g. with fully nonadiabatic wavefunction for H_2), indices a and c, over which differentiation is taken, can always be chosen such that $a \neq c$, such that problematic, more singular, terms of the form,

$$\left\langle \Psi_k \frac{1}{r_{cd}} 4\pi\delta^{(3)}\left(\vec{r}_{ab}\right) \Psi_l \right\rangle, \tag{V.123}$$

are not present.

6.8 Results and Convergence

The greater accuracy of $\ln k_0$ near the equilibrium is a consequence of purposeful computational focus on optimization of $f(t)$ by employing larger basis sets (N=768,1024). Moreover, $\ln k_0(R)$ changes rather slowly for $R > 5$ au, and this region is much less important in view of averaging $\mathcal{E}^{(5,0)}$ with nuclear wavefunction; therefore, the largest size of external basis used there was only $N = 512$. Deterioration of $\ln k_0$ uncertainty as $R \to 0$ is the consequence of large uncertainty of fitted expansion in the low-t region, due to its high sensitivity to the fitting parameters.

Although $\ln k_0$ as a function of R changes rapidly from its united-atom helium value to the hydrogenic one in a manner resembling exponential decay, it exhibits nontrivial behavior in the region around equilibrium internuclear distance[6], see Figs. V.9 and V.8. Consequently, commonly used one-parameter approximation to the R-behavior of the Bethe logarithm,

$$\ln k_0(\mathrm{H}) + \left[\ln k_0(\mathrm{He}) \; - \; \ln k_0(\mathrm{H})\right] e^{-aR}, \tag{V.124}$$

when both united-atom and dissociation limits are usually known much more accurately (as is the case with H_2), is far from sufficient for high-precision theoretical predictions.

[6]The evolution of $\ln k_0(R)$ as the function of R could be vaguely attributed to the nontrivial evolution of electron density, but to our knowledge there are no comprehensive framework in which this behaviour can be explained quantitatively, just like for any other more complicated higher order correction.

Convergence with the basis size and comparison to the literature of Dirac delta, Araki-Sucher and Bethe logarithm at $R = 1.4$ au is presented in Table V.5. Final values of $\mathcal{E}^{(5,0)}$ and its essential components are presented in Table V.7, whereas its R-behavior is plotted in Fig. V.10.

Ultimately, we regard obtained absolute Bethe logarithm accuracy of 3×10^{-8} with $N \sim 1000$ to be satisfactory, especially in view of its proximity to the absolute accuracy of the Araki-Sucher term which is of similar magnitude (about 10^{-8}).

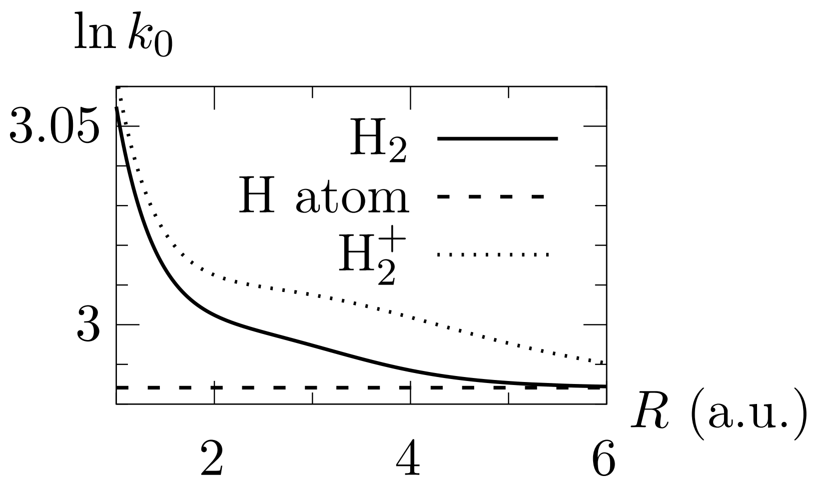

Figure V.8: Electronic Bethe logarithm $\ln k_0(R)$, for H_2 (solid) and H_2^+ (dotted) with atomic hydrogen value (dashed).

6.9 Long-range asymptotics

At the dissociation limit only the first term of Eq. (V.89) persists, so that

$$\mathcal{E}^{(5,0)}(\infty) = \frac{4}{3}\left(\frac{19}{30} - 2\ln\alpha - \ln k_0(\mathrm{H})\right)\frac{2}{\pi} \tag{V.125}$$

$$= 6.357\,448\,103\,05(2), \tag{V.126}$$

with $1/\alpha = 137.035\,999\,206(11)$ [**?**] and the value of $\ln k_0(\mathrm{H})$ given by Eq. (V.116).

We have found that $\langle r_{12}^{-3}\rangle_\varepsilon$, as evaluated according to Eq. (II.66) using a single quadrature utilizing transform Eq. (II.58), exhibits very clear $\sim m^{-6}$ convergence, with m being the number of quadrature nodes, Eq. (II.55). Therefore, a very accurate Richardson extrapolation is possible, which allows for effortless improvement of the accuracy by roughly two orders of magnitude. Although the accuracy of those operators is usually good enough even with $m = 40$, we have found such an acceleration of convergence very useful and necessary for the sake of as accurate as possible comparison to analytical long-range asymptotic expansion of $\langle r_{12}^{-3}\rangle_\varepsilon$, which reads [238],

$$\left\langle \frac{1}{r_{12}^3} \right\rangle_\varepsilon = \frac{1}{R^3} + \frac{6}{R^5} + \frac{75}{R^7} - C_6\,\frac{10}{R^8} + \frac{1575}{R^9} + \mathcal{O}(R^{-10}), \tag{V.127}$$

where $C_6 = 6.499026705405\ldots$ is the leading order coefficient (dipole-dipole) of the long-range asymptotics of dispersion energy.

Due to the high accuracy of our data, we have attempted to fit higher-order terms by subtracting the asymptotics up to order R^{-9} and fitting a series in powers of $1/R$. We have found such fits to be sensitive to both the expansion order and the number of points used. We noticed that the leading coefficient of the fit is oscillating around a value given by (V.128) as the expansion order is incremented by one. This observation strongly suggests the presence of higher order terms with large coefficients, and we estimate the next term to be $-3400/R^{10}$ with 50% uncertainty. A meaningful comparison with even higher-order terms would require data at $R > 20$ au or higher accuracy (better than 10^{-12}) of our large-R results, which entails costly optimization of even larger basis sets and is of little practical significance.

[araki chi2 test of power behaviour with number of quadrature nodes]

$$\left\langle \frac{1}{r_{12}^3} \right\rangle_\varepsilon = \frac{1}{R^3} + \frac{6}{R^5} + \frac{75}{R^7} - C_6\,\frac{10}{R^8} + \frac{1575}{R^9} + \mathcal{O}(R^{-10}), \tag{V.128}$$

The Bethe logarithm in H_2 is known to behave asymptotically as

$$\ln k_0(R) = \ln k_0(\mathrm{H}) + \frac{L_6}{R^6} + \mathcal{O}(R^{-8}) \quad \text{as} \quad R \to \infty, \tag{V.129}$$

with [198, 238] $L_6 = 2.082\,773\,197$. Comparison with our data suggests that this asymptotic expansion is not sufficient to accurately describe the behavior of $\ln k_0(R)$ for R as large as 6-10 au, in spite of its numerical value rapidly approaching that of the hydrogen atom. In particular, this two-term asymptotic expansion diverges from numerical data by as much as 27, 157, and 568% at $R = 10, 8$, and 6 au, respectively. This suggests the significance of higher order terms. Large magnitude of their coefficients is tentatively confirmed by our fitting attempts.

6.10 Conclusions

We have performed highly accurate calculations of QED effects in the ground state of molecular hydrogen. Due to the accuracy of order of 10^{-8}, which is 2 to 3 orders better than previous calculations [198], major numerical uncertainty of the QED effects on the molecular levels has been eliminated. Nevertheless, the shift of about 0.03 MHz with respect to Ref. [198] is below the level of existing discrepancies with measured transition energies (1.4-1.9 $\sigma \approx 2$ MHz) in the HD molecule. Fully nonadiabatic QED calculations [67, 69] performed for the lowest levels of H_2 ($\nu = 0$, $J = 0$) reduce the uncertainty of the QED contribution to the level of 5 kHz. Together with the results obtained in present work, this indicates the significance of nonadiabatic QED effects in hydrogen molecule and its isotopologues. These effects can be calculated with the help of nonadiabatic perturbation theory (NAPT) [190], which is planned in the near future, and present work can be regarded as a first step toward this goal.

The results obtained here are included as R-dependent potentials in the updated version (v7.4) of the publicly available computer code H2SPECTRE [221].

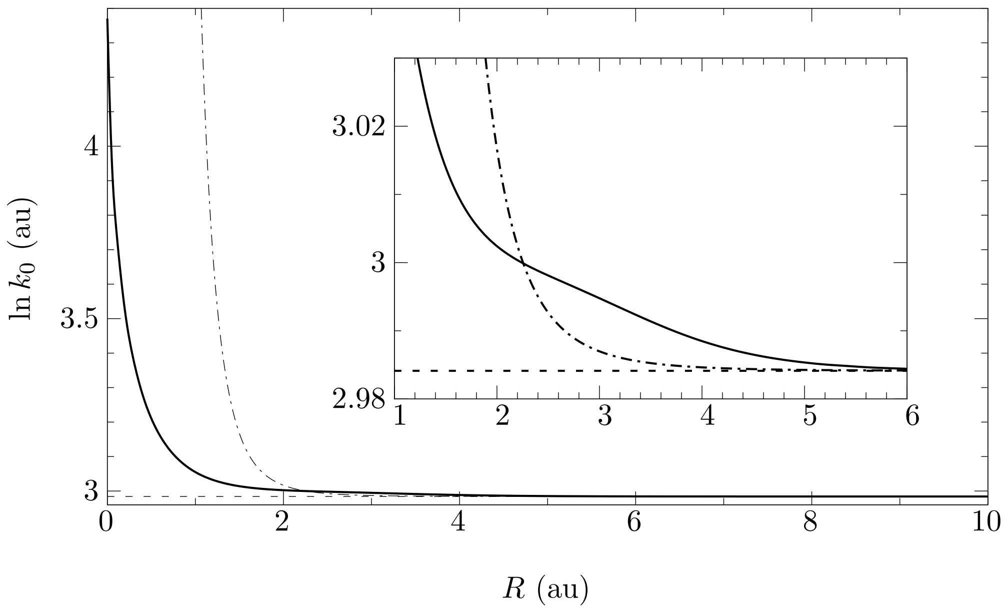

Figure V.9: The solid black line represents $\ln k_0(R)$, Eq. (V.94). A very rapid drop from the united-atom (helium) limit can be observed. The inset displays nontrivial dependence of $\ln k_0$ as a function of R in the region $R = 1 - 6$ au, which prevents the use of a simple exponential decay fit. The dash-dotted line presents the only known leading order long-range asymptotics, Eq. (V.129). The dashed line corresponds to the asymptotic hydrogenic limit.

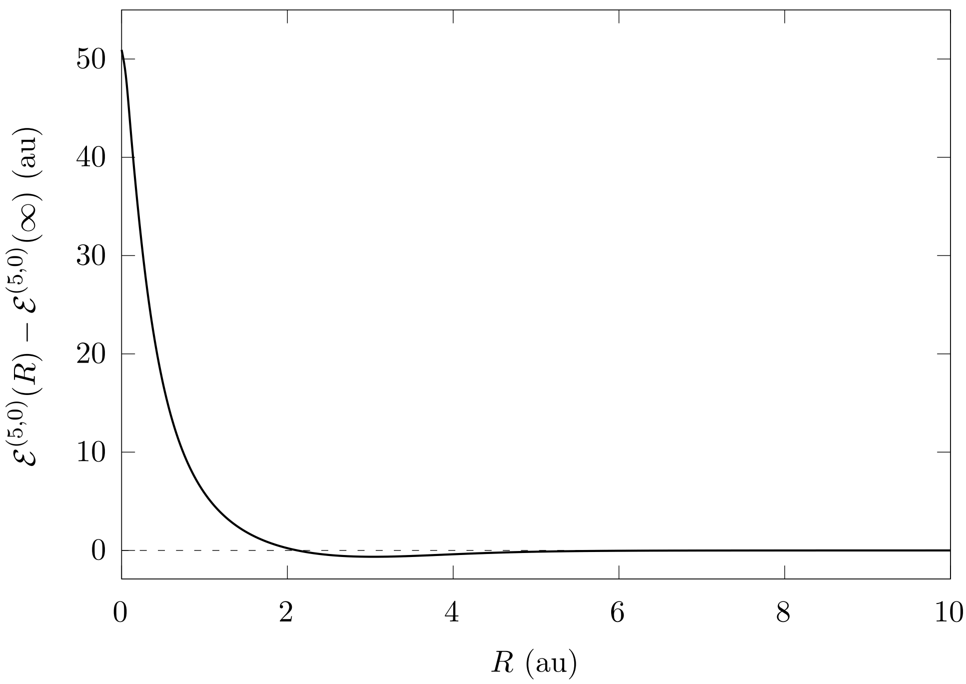

Figure V.10: The solid black line represents $\mathcal{E}^{(5,0)}$ of Eq. (V.89) as a function of R with the asymptotic hydrogenic limit subtracted.

Table V.7: Terms contributing to $\mathcal{E}^{(5,0)}$ as a function of R. Uncertainties originate from extrapolation to the complete basis set. All quantities in au, $\ln k_0$ is dimensionless.

R	$\sum_{i,X}\langle\delta^3(\vec{r}_{iX})\rangle$	$\langle\delta^3(\vec{r}_{12})\rangle$	$\langle r_{12}^{-3}\rangle_\varepsilon$	$\ln k_0$	$\mathcal{E}^{(5,0)}(R)-\mathcal{E}^{(5,0)}(\infty)$
0.0	7.24171727400(4)[7]	0.106345370635(1)??	0.989273545024(1)??	4.3701602230703(3)[8]	50.930716724136(3)
0.05	6.4890437210(4)	0.105003821909(7)	0.9881318794(5)	3.9610(2)	48.362(2)
0.1	5.770597278(3)	0.10157055016(10)	0.98432455(2)	3.7616(2)	43.700(2)
0.2	4.568931914(3)	0.09136818987(9)	0.96590419(2)	3.52291(5)	34.5292(3)
0.3	3.671598383(2)	0.0798419070(2)	0.93232441(2)	3.37749(2)	27.07582(5)
0.4	3.007974280(3)	0.0688732774(1)	0.88704623(2)	3.279584(5)	21.33818(2)
0.5	2.512087713(3)	0.0591374522(2)	0.83484011(4)	3.210230(2)	16.950265(6)
0.6	2.135554242(4)	0.0507632372(2)	0.77971886(2)	3.1595728(9)	13.569055(3)
0.7	1.844767256(4)	0.0436605313(2)	0.72449332(2)	3.1218242(4)	10.9319924(9)
0.8	1.616559028(4)	0.0376678752(4)	0.67093263(4)	3.0933129(2)	8.8483668(4)
0.9	1.434821980(8)	0.0326147204(4)	0.62004755(4)	3.07157925(5)	7.18120486(9)
1.0	1.288195834(4)	0.0283452755(4)	0.57234019(4)	3.05490864(6)	5.8317574(1)
1.1	1.168538455(4)	0.0247256344(4)	0.52798840(4)	3.04206959(5)	4.72813145(7)
1.2	1.069918931(4)	0.0216439932(3)	0.48697212(3)	3.03215694(6)	3.81734866(9)
1.3	0.987949457(3)	0.0190083084(3)	0.44915639(3)	3.02449314(6)	3.05986972(9)
1.4	0.919336214(3)	0.0167432780(4)	0.41434479(3)	3.01856348(4)	2.42581252(4)
1.4011	0.918645801(5)	0.0167201832(4)	0.41397774(4)	3.01850633(3)	2.41943366(4)
1.5	0.861572961(6)	0.0147874126(5)	0.38231287(4)	3.01397237(6)	1.89232027(8)
1.6	0.812728773(5)	0.0130904713(5)	0.35282881(5)	3.01041312(6)	1.44170996(7)
1.7	0.771298712(4)	0.0116113186(4)	0.32566573(3)	3.00764631(6)	1.06015438(6)

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Table V.7 – *Continued from previous page*

R	$\sum_{i,X}\langle\delta^3(\vec{r}_{iX})\rangle$	$\langle\delta^3(\vec{r}_{12})\rangle$	$\langle r_{12}^{-3}\rangle_\varepsilon$	$\ln k_0$	$\mathcal{E}^{(5,0)}(R)-\mathcal{E}^{(5,0)}(\infty)$
1.8	0.736097174(4)	0.0103161797(3)	0.30060873(3)	3.00548408(5)	0.73673165(5)
1.9	0.706180622(4)	0.0091772346(2)	0.27745861(2)	3.00377871(6)	0.46273095(6)
2.0	0.680790767(4)	0.0081714960(4)	0.25603365(4)	3.00241335(9)	0.23113917(9)
2.1	0.659312208(4)	0.0072799102(4)	0.23617006(3)	3.00129678(5)	0.03625438(5)
2.2	0.641240392(4)	0.0064866435(2)	0.21772165(3)	3.0003573(2)	−0.1266062(1)
2.3	0.626157038(4)	0.0057785088(3)	0.20055918(3)	2.9995393(3)	−0.2613324(2)
2.4	0.613711019(4)	0.0051445018(2)	0.18456954(2)	2.99880014(8)	−0.37119725(7)
2.5	0.603603308(5)	0.0045754299(3)	0.16965457(3)	2.9981078(3)	−0.4589970(2)
2.6	0.595575025(6)	0.0040636043(3)	0.15573008(2)	2.9974395(2)	−0.5271620(2)
2.7	0.589397878(6)	0.0036025887(9)	0.14272450(8)	2.99677927(9)	−0.57784529(8)
2.8	0.584866587(6)	0.0031869850(9)	0.13057766(9)	2.99611714(9)	−0.61299348(7)
2.9	0.581792978(6)	0.0028122509(3)	0.11923957(3)	2.9954475(3)	−0.6344010(2)
3.0	0.580001468(5)	0.0024745485(2)	0.10866836(2)	2.9947706(3)	−0.6437534(2)
3.2	0.579608561(5)	0.0018975786(7)	0.08969278(6)	2.9933998(2)	−0.6326256(1)
3.4	0.582448355(5)	0.0014346013(5)	0.07342502(5)	2.9920403(2)	−0.5916362(1)
3.6	0.587399916(3)	0.0010683465(2)	0.05967099(2)	2.9907405(2)	−0.5317100(2)
3.8	0.593491441(3)	0.0007837408(3)	0.04822793(3)	2.9895459(4)	−0.4623141(4)
4.0	0.599942218(4)	0.0005669019(3)	0.03886333(2)	2.9884879(1)	−0.3910095(7)
4.2	0.606187475(4)	0.0004049339(2)	0.03131461(2)	2.9875819(9)	−0.3231954(8)
4.4	0.611872454(2)	0.0002861635(2)	0.025304362(9)	2.9868296(3)	−0.2621756(8)
4.6	0.616819342(2)	0.00020046794(8)	0.020560798(7)	2.9862180(4)	−0.2094973(3)
4.8	0.620980474(2)	0.00013946740(5)	0.016835178(4)	2.9857306(2)	−0.1654339(2)

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Table V.7 – *Continued from previous page*

R	$\sum_{i,X}\langle\delta^3(\vec{r}_{iX})\rangle$	$\langle\delta^3(\vec{r}_{12})\rangle$	$\langle r_{12}^{-3}\rangle_\varepsilon$	$\ln k_0$	$\mathcal{E}^{(5,0)}(R)-\mathcal{E}^{(5,0)}(\infty)$
5.0	0.624391499(3)	0.00009651477(4)	0.013912356(3)	2.9853497(3)	−0.1294587(3)
5.2	0.627132992(2)	0.00006652495(4)	0.011614267(3)	2.9850545(5)	−0.1006249(4)
5.4	0.629303303(2)	0.00004571971(2)	0.009798327(2)	2.9848280(5)	−0.0778397(4)
5.6	0.631001614(2)	0.00003135473(3)	0.008353048(2)	2.9846557(3)	−0.0600270(3)
5.8	0.632318799(2)	0.00002147077(1)	0.007192666(1)	2.9845254(3)	−0.0462145(2)
6.0	0.633333462(2)	0.00001468696(3)	0.006251868(2)	2.9844270(3)	−0.0355683(3)
6.5	0.634946115(2)	0.000005668122(8)	0.0045649148(5)	2.9842755(4)	−0.0186014(4)
7.0	0.635760799(2)	0.000002183104(3)	0.0034749552(2)	2.9842020(5)	−0.0099569(4)
7.5	0.636169868(2)	0.000000840032(2)	0.00272930901(9)	2.9841664(4)	−0.0055487(5)
8.0	0.636376357(2)	0.0000003230160(9)	0.00219493423(5)	2.9841490(4)	−0.0032671(6)
8.5	0.636482278(2)	0.0000001241243(5)	0.00179784702(2)	2.9841401(4)	−0.0020520(6)
9.0	0.636538096(2)	0.0000000476605(5)	0.001494408972(5)	2.9841350(3)	−0.0013766(3)
9.5	0.636568630(2)	0.0000000182846(2)	0.001257399493(6)	2.9841331(4)	−0.0009818(6)
10.0	0.636586108(2)	0.0000000070084(2)	0.001068988784(2)	2.9841314(4)	−0.0007357(6)
11.0	0.636603270(2)	0.00000000102659(2)	0.000792906742(2)		
12.0	0.636610686(2)	0.00000000014980(1)	0.000605092990(2)		
13.0	0.636614385(2)	0.00000000002177(1)	0.000472597263(2)		
14.0	0.636616412(2)	0.00000000000315(1)	0.000376332776(2)		
15.0	0.636617594(2)	0.00000000000045(2)	0.000304652082(2)		
16.0	0.636618315(2)	0.00000000000006(1)	0.000250149428(2)		
17.0	0.636618771(2)	0.00000000000001(1)	0.000207953638(2)		
18.0	0.636619068(2)	0.00000000000000(1)	0.000174767149(2)		

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Table V.7 – *Continued from previous page*

R	$\sum_{i,X}\langle\delta^3(\vec{r}_{iX})\rangle$	$\langle\delta^3(\vec{r}_{12})\rangle$	$\langle r_{12}^{-3}\rangle_\varepsilon$	$\ln k_0$	$\mathcal{E}^{(5,0)}(R)-\mathcal{E}^{(5,0)}(\infty)$
19.0	0.636619267(2)	0.00000000000000(1)	0.000148301511(2)		
20.0	0.636619402(2)	0.00000000000000(1)	0.000126933698(2)		
∞	0.63661977236	0.0	0.0	2.984128555765	0.0

7 Finite nuclear mass quantum electrodynamic corrections

As we have presented in the previous Section, the shift of about 0.03 MHz with respect to Ref. [198] is below the level of existing discrepancies with measured transition energies (1.4-1.9 $\sigma \approx 2$ MHz) in the HD molecule. Fully nonadiabatic QED calculations [67, 69] performed for the lowest levels of H_2 ($\nu = 0$, $J = 0$) reduce the uncertainty of the QED contribution to the level of 5 kHz. Together with the results obtained in present work, this indicates the significance of nonadiabatic QED effects in hydrogen molecule and its isotopologues. Current BO-level results are the first, necessary step towards evaluation of leading order nonadiabatic QED corrections using the NAPT methodology and this work consitutes the fundamental significance of our results for the application of current results to a discrepancy in HD.

Before calculations were finalized, we have speculated that the improvement of numerical uncertainty of the BO QED effects alone might explain the discrepancy, similarly as was the case with the highly accurate recalculation of relativistic correction in Ref. [68], which revealed the significance of nonadiabatic relativistic effects, evaluated soon after in Ref. [201].

Here, the resulting shift in rovibrational energies due to our improvement of numerical accuracy of QED effects at the BO level has proven to be too small to explain the discrepancy. All of this, together with recent measurements reaching few tens of kHz accuracy and purely heteronuclear relativistic recoil effects being too small to explain the discrepancy, point towards significance of nonadiabatic QED effects at the level of a few MHz.

Owing to present work, these effects can now be calculated with the help of nonadiabatic perturbation theory (NAPT) [190]. The actual calculations of the QED-NAPT corrections for the hydrogen molecule isotopologues, unfortunetely, did not fit into the timeframe of this thesis, but are planned to be pursued in the near future.

In the context of dissociation energies, fully nonadiabatic (naECG) QED calculations for the ground rovibrational state for each isotopologue were reported [69, 240].

8 Higher-order QED corrections

In order to explain observed transitions in the rovibrational spectra, even higher order QED effects have to be accounted for. Their effect on the molecular levels in based on a recent accurate calculations of $\alpha^6 m$ correction [241] and an estimation of $\alpha^7 m$ based on the dominating term from hydrogenic theory.

The $\alpha^6 m$ correction enters as a correction to the effective potential,

$$\mathcal{E}^{(6,0)}(R) \equiv \langle\Psi| H^{(6,0)} |\Psi\rangle + \langle\Psi| H^{(4,0)} \frac{1}{(\mathcal{E}^{(2,0)} - H^{(2,0)})'} H^{(4,0)} |\Psi\rangle \,, \tag{V.130}$$

with the second term originating from the second order of perturbation theory with relativistic BO Hamiltonian, $H^{(4,0)}$, acting as the perturbation operator. The complete contribution to the molecular level energy is then given by,

$$E^{(6,0)} \equiv \langle\chi|\, \mathcal{E}^{(6,0)}(R)\, |\chi\rangle + \langle\chi|\, \mathcal{E}^{(4,0)}(R) \frac{1}{(\mathcal{E}^{(2,0)} - H_N)'} \mathcal{E}^{(4,0)}(R)\, |\chi\rangle\,, \tag{V.131}$$

where we explicitly write the R-dependence of electronic potentials $\mathcal{E}^{(6,0)}(R)$ and $\mathcal{E}^{(4,0)}(R)$ to emphasize its vibrational averaging.

The effective Hamiltonian, $H^{(6,0)}$ at the $m\alpha^6$ order is constructed by means of dimensionally regularized NRQED in complete analogy to the case of singlet states of He atom [242], with straightforward adjustments to two Coulombic centers. The effort to obtain final working formulas in the coordinate space is considerable due to the necessity of careful regularization of singular operators. Total contribution can be divided into,

$$H^{(6,0)} = H_Q + H_H + H_{\rm rad}. \tag{V.132}$$

The low-energy scale contribution H_Q, resulting from one- and two- photon exchange ($k \sim \alpha m$) is too lenghty to be presented here, see Ref. [241]. For the high-energy part H_H we leave out only regular terms[9]

$$H'_H \equiv \left(-\frac{39\,\zeta(3)}{\pi^2} + \frac{32}{\pi^2} - 6\,\ln(2) + \frac{7}{3}\right) \frac{\pi\,\alpha^3}{4\,m^2}\,\delta^3(r_{12}). \tag{V.133}$$

The last contribution comes from one- and two-loop radiative corrections known from the hydrogenic theory with the obvious modification of the pointwise electronic density on the coalescence points.

$$\begin{aligned}
H_{\rm rad} &= H_{R1} + H_{R2}, \\
H_{R1} &= \frac{\alpha^3\pi}{m^2}\left[\frac{427}{96} - 2\,\ln(2)\right]\left[Z_A^2\delta^3(r_{1A}) + Z_A^2\delta^3(r_{2A}) + Z_B^2\delta^3(r_{1B}) + Z_B^2\delta^3(r_{2B})\right] \\
&\quad + \frac{\alpha^3\pi}{m^2}\left[\frac{6\,\zeta(3)}{\pi^2} - \frac{697}{27\,\pi^2} - 8\,\ln(2) + \frac{1099}{72}\right]\delta^3(r_{12}) \qquad \text{(V.134)} \\
H_{R2} &= \frac{\alpha^3\pi}{m^2}\left[-\frac{9\,\zeta(3)}{4\,\pi^2} - \frac{2179}{648\,\pi^2} + \frac{3\,\ln(2)}{2} - \frac{10}{27}\right] \\
&\times \left[Z_A\delta^3(r_{1A}) + Z_A\delta^3(r_{2A}) + Z_B\delta^3(r_{1B}) + Z_B\delta^3(r_{2B})\right] \\
&\quad + \frac{\alpha^3\pi}{m^2}\left[\frac{15\,\zeta(3)}{2\,\pi^2} + \frac{631}{54\,\pi^2} - 5\,\ln(2) + \frac{29}{27}\right]\delta^3(r_{12}), \qquad \text{(V.135)}
\end{aligned}$$

Intriguingly, the one-loop radiative correction accounts for, by far the largest (> 95%) contribution to the complete $m\alpha^6$ correction for $D_0(H_2)$ (and other isotopologues). This correction alone was previously used [198] as an estimate of the $m\alpha^6$ effects, thus complete evaluation of $m\alpha^6$ confirms the accuracy of former estimate to within a few percent.

All of the higher order QED corrections are estimated based only on the leading $\ln^2\left[(Z_X\alpha)^{-2}\right]$

[9] the cancellation between this hard three-photon contribution, second-order contribution and low-energy part is detailed in Ref. [241]

term from the hydrogenic theory [243] contributing at the $m\alpha^7$,

$$H^{(7,0)} \approx -\frac{\alpha^4}{m} \sum_{X=A,B} Z_X^3 \, \ln^2\left[(Z_X\alpha)^{-2}\right] \sum_{a=1,2} \delta^3(r_{aX}). \tag{V.136}$$

Finally we note, that in case of dissociation energy, one is interested in the energy difference with respect to the dissociation products. Accordingly the higher-order effect is the difference between energy shifts in bound and dissociated state. Typically QED corrections are sensitive to the electronic density in the vicinity of nucleus-electron coalescence points and insensitive to valence effects induced by the bonding. Therefore, the energy shift in the dissociation energy is much smaller than the shift to either bound or dissociated configuration. Such a cancellation is even more significant in case of asymmetric diatomic systems such as HeH^+ [244].

CHAPTER VI

NUMERICAL SOLUTION OF NUCLEAR EQUATION

1 Numerical solution of the nuclear equation – H2spectre

The radial equation reads

$$H_n \chi(R) = E^{(2,0)}\,\chi(R), \tag{VI.1}$$

with J the rotational quantum number. At the BO level,

$$H_n = -\frac{1}{2\mu_n}\frac{d^2}{dR^2} + \mathcal{Y}_{\mathrm{BO}}(R), \tag{VI.2}$$

where

$$\mathcal{Y}_{\mathrm{BO}}(R) = \mathcal{E}(R) + \frac{J(J+1)}{2\mu_n R^2} \tag{VI.3}$$

The necessity for the numerical solvers for the nuclear wavefuction can be simply motivated by the fact that the effective electronic potential is typically known only numerically. Even if the electronic potential would be known analytically its known numerical form suggests that its analytical form is usually very complicated.

On top of that, as introduced in Chapter IV, when higher order corrections are included the H_n in the Eq. (VI.1) admits modifications not only not only to the potential $\mathcal{Y}(R)$, but also the nuclear kinetic operator becomes R-dependent as the effect of nonadiabatic corrections, which results in a very complicated differential equation, too complex to be solved using analytical methods.[1]

[1]The only region where analytic methods seem to be possible to apply with success are the the limiting

1.1 Discrete Variable Representation (DVR)

For the purpose of solving Eq. VI.1 we follow the already well-tested scheme based on the DVR method DVR method. This method is a pseudo-spectral method which can be reminiscent of the Gaussian quadrature methods, because by design this method is constructed to have rapid decay of errors with the number of discretization points. Namely, with the total of N mesh points, one aims to achieve a power law behaviour of the errors $\sim A^{-N}$ or even exponential, $\sim 1/N!$, rather than polynomial, $\sim N^{-\alpha}$, which is typical of straightforward methods.

Use of the DVR is advantageous because the Hamiltonian matrix is easy to evaluate and it is sparse, requiring only matrix-vector operations and no integral evaluations. In particular, the potential operator is simply a product operator and the kinetic energy operator is a second-order differential operator.

The radial function ansatz relies of the Fourier-basis variant by Colbert and Miller[245].

$$\chi(R) = \sum_{n=1}^{N} f_n \phi_n(R), \tag{VI.4}$$

with N being the number of grid points and $\phi_n(R)$ being the particle-in-a-box eigenfunctions

$$\phi_n(R) = \left(\frac{2}{b-a}\right)^{1/2} \sin\left[\frac{n\pi(R-a)}{b-a}\right], \tag{VI.5}$$

with the domain of radial coordinate R restricted to the section $[a, b]$.

Then, by virtue of orthonormality and completeness[2], the coefficients f_n are given in terms of the numerical quadrature,

$$f_n = \sum_{m=1}^{N} w_n \phi_n(R_m)\, \chi(R_m), \tag{VI.6}$$

where the radial position R is discretize on a uniform grid of N points,

$$\begin{aligned} R_m &\equiv a + \frac{m(b-a)}{N+1}, \\ \Delta R &\equiv \frac{b-a}{N+1}. \end{aligned} \tag{VI.7}$$

Note that the above definition entails, that both endpoints a and b are absent in the discretized grid R_m, where $m = 1, \ldots, N$. In the case of radial nuclear equation, Eq. (VI.1) the domain is $(0, \infty)$.

cases of dissociation and united-atom, which might provide an insight into the asymptotic analytical form of the solutions in those regions.

[2]Completeness in the limit $N \to \infty$

1.2 H2spectre

The implementation of the DVR method adapted to the hydrogen molecule isotopologues has been released as H2SPECTRE program, which is presented in the Ph. D. thesis of P. Czachorowski [179**?**] and for more detailed description we refer to the Chapter 6 therein. Here, we utilize the same approach by simply including additional contributions to the $\mathcal{Y}(R)$ and effective nuclear masses.

The potential matrix is diagonal and the dense structure of the kinetic energy matrix can be seen as originating from the infinite-order finite difference,

$$f''(0) = \frac{1}{(\Delta x)^2}\left[f_0\frac{\pi^2}{3} + \sum_{k=1}^{\infty}(f_k + f_{-k})\frac{2(-1)^k}{k^2}\right], \tag{VI.8}$$

whereas in the finite order one would have a multidiagonal matrix, which might otherwise constitute a considerable simplification with large matrix sizes. Ultimately, the DVR Hamiltonian matrix is of the form,

$$\begin{aligned} H_{ii} =& \frac{1}{\mu_{\|}(R)\Delta R^2}\left(\frac{\pi^2}{3} - \frac{1}{2i^2}\right) + \mathcal{W}'_{\|}(R_i) + \frac{\mathcal{W}''_{\|}(R_i)}{2} \\ &+ \frac{1}{\mu_{\perp}(R)\Delta R^2}\frac{J(J+1)}{2\mu_a R_i^2} + \mathcal{Y}(R_i), \end{aligned} \tag{VI.9}$$

$$H_{ij} = \frac{(-1)^{i-j}}{2}\left(\frac{1}{\mu_a} + \mathcal{W}_{\|}(R_i) + \mathcal{W}_{\|}(R_j)\right)\left(\frac{2}{(i-j)^2} - \frac{2}{(i+j)^2}\right) \tag{VI.10}$$

where the offdiagonal elements originate only from the kinetic energy operator and all the corrections to the potential enter $\mathcal{Y}(R)$. Asymptotic hydrogenic values have to be subtracted from both the $\mathcal{W}_{\|/\perp}$ nonadiabatic potentials, as well as all the corrections contributing to the potential $\mathcal{Y}(R)$, because energy levels are calculated with respect to the dissociation limit. Effective reduced mass approches that of two separated hydrogen atoms,

$$\frac{1}{\mu_a} = \frac{1}{m_A + 1} + \frac{1}{m_B + 1} \tag{VI.11}$$

CHAPTER VII

CONCLUSIONS AND OUTLOOK

Prevailing discrepancies in the rovibrational spectra toghether with the most recent measurements in the (2-0) overtone band of homonuclear isotopologues[14, 246], seem to disfavor the conjecture that the discrepancy results from effects arising purely from the heteronuclear effects. Both the spectroscopy and the inability to explain the discrepancy with theory including other effects hint toward the significance of the finite nuclear mass QED effects on the order of a few MHz. The new evaluation of leading QED corrections can now serve as the zeroth-order starting point for the NAPT calculations of leading-order QED recoil corrections.

With the suitability of Kolos-Wolniewicz basis not only to BO energy but also nonadiabatic couplings, opportunities to account for the vibronic interactions in the manifold involving excited states become now feasible.

REFERENCES

[1] M. Puchalski, J. Komasa, P. Czachorowski, and K. Pachucki, Phys. Rev. Lett. **122**, 103003 (2019), URL https://doi.org/10.1103%2Fphysrevlett.122.103003.

[2] J. Liu, E. J. Salumbides, U. Hollenstein, J. C. J. Koelemeij, K. S. E. Eikema, W. Ubachs, and F. Merkt, J. Chem. Phys. **130**, 174306 (2009), URL https://doi.org/10.1063%2F1.3120443.

[3] D. E. Jennings, A. Weber, and J. W. Brault, Appl. Opt. **25**, 284 (1986), URL https://doi.org/10.1364%2Fao.25.000284.

[4] C.-F. Cheng, J. Hussels, M. Niu, H. Bethlem, K. Eikema, E. Salumbides, W. Ubachs, M. Beyer, N. Hölsch, J. Agner, et al., Phys. Rev. Lett. **121**, 013001 (2018), URL https://doi.org/10.1103%2Fphysrevlett.121.013001.

[5] R. Altmann, L. Dreissen, E. Salumbides, W. Ubachs, and K. Eikema, Phys. Rev. Lett. **120**, 043204 (2018), URL https://doi.org/10.1103%2Fphysrevlett.120.043204.

[6] N. Hölsch, M. Beyer, E. J. Salumbides, K. S. Eikema, W. Ubachs, C. Jungen, and F. Merkt, Phys. Rev. Lett. **122**, 103002 (2019), URL https://doi.org/10.1103%2Fphysrevlett.122.103002.

[7] M. L. Diouf, F. M. J. Cozijn, K.-F. Lai, E. J. Salumbides, and W. Ubachs, Phys. Rev. Res. **2**, 023209 (2020), URL https://link.aps.org/doi/10.1103/PhysRevResearch.2.023209.

[8] A. Fast and S. A. Meek, Phys. Rev. Lett. **125**, 023001 (2020), URL https://link.aps.org/doi/10.1103/PhysRevLett.125.023001.

[9] M. L. Diouf, F. M. J. Cozijn, B. Darquié, E. J. Salumbides, and W. Ubachs, Opt. Lett. **44**, 4733 (2019), URL https://opg.optica.org/ol/abstract.cfm?URI=ol-44-19-4733.

[10] F. M. J. Cozijn, M. L. Diouf, V. Hermann, E. J. Salumbides, M. Schlösser, and W. Ubachs, Phys. Rev. A **105**, 062823 (2022), URL https://link.aps.org/doi/10.1103/PhysRevA.105.062823.

[11] S. Kassi, C. Lauzin, J. Chaillot, and A. Campargue, Phys. Chem. Chem. Phys. **24**, 23164 (2022), URL https://doi.org/10.1039%2Fd2cp02151j.

[12] T.-P. Hua, Y. R. Sun, and S.-M. Hu, Opt. Lett. **45**, 4863 (2020), URL https://doi.org/10.1364%2Fol.401879.

[13] M.-Y. Yu, Q.-H. Liu, C.-F. Cheng, and S.-M. Hu, Mol. Phys. p. e2127382 (2022), URL https://doi.org/10.1080%2F00268976.2022.2127382.

[14] S. Wójtewicz, R. Gotti, D. Gatti, M. Lamperti, P. Laporta, H. Jóźwiak, F. Thibault, P. Wcisło, and M. Marangoni, Physical Review A **101** (2020), URL https://doi.org/10.1103%2Fphysreva.101.052504.

[15] A. Fast and S. A. Meek, Molecular Physics **120** (2021), URL https://doi.org/10.1080%2F00268976.2021.1999520.

[16] P. Wcisło, F. Thibault, M. Zaborowski, S. Wójtewicz, A. Cygan, G. Kowzan, P. Masłowski, J. Komasa, M. Puchalski, K. Pachucki, et al., Journal of Quantitative Spectroscopy and Radiative Transfer **213**, 41 (2018), URL https://doi.org/10.1016%2Fj.jqsrt.2018.04.011.

[17] U. D. Jentschura and G. S. Adkins, *Quantum Electrodynamics: Atoms, Lasers and Gravity* (WORLD SCIENTIFIC, 2021), URL https://doi.org/10.1142%2F12722.

[18] G. Corongiu and E. Clementi, The Journal of Chemical Physics **131**, 034301 (2009).

[19] G. Corongiu and E. Clementi, The Journal of Physical Chemistry A **113**, 14791 (2009).

[20] G. Corongiu and E. Clementi, Int. J. Quantum Chem. **111**, 3517 (2010), URL https://doi.org/10.1002%2Fqua.22831.

[21] K. Pachucki, Physical Review A **76** (2007), URL https://doi.org/10.1103%2Fphysreva.76.022106.

[22] A. Wienczek, M. Puchalski, and K. Pachucki, Physical Review A **90** (2014), URL https://doi.org/10.1103%2Fphysreva.90.022508.

[23] K. Pachucki and V. A. Yerokhin, Physical Review A **100** (2019), URL https://doi.org/10.1103%2Fphysreva.100.062510.

[24] R. S. Mulliken, Journal of the American Chemical Society **86**, 3183 (1964), URL https://doi.org/10.1021%2Fja01070a001.

[25] E. Tiesinga, P. J. Mohr, D. B. Newell, and B. N. Taylor, Rev. Mod. Phys. **93**, 025010 (2021), URL https://link.aps.org/doi/10.1103/RevModPhys.93.025010.

[26] J. Rychlewski and J. Komasa, in *Explicitly Correlated Wave Functions in Chemistry and Physics* (Springer Netherlands, 2003), pp. 91–147, URL https://doi.org/10.1007%2F978-94-017-0313-0_2.

[27] L. Kong, F. A. Bischoff, and E. F. Valeev, Chemical Reviews **112**, 75 (2011), URL https://doi.org/10.1021%2Fcr200204r.

[28] R. T. Pack and W. B. Brown, The Journal of Chemical Physics **45**, 556 (1966), URL https://doi.org/10.1063%2F1.1727605.

[29] D. P. Tew, The Journal of Chemical Physics **129**, 014104 (2008), URL https://doi.org/10.1063%2F1.2945900.

[30] S. Fournais, M. Hoffmann-Ostenhof, T. Hoffmann-Ostenhof, and T. Østergaard Sørensen, Communications in Mathematical Physics **255**, 183 (2005), URL https://doi.org/10.1007%2Fs00220-004-1257-6.

[31] W. Kolos and C. C. J. Roothaan, Reviews of Modern Physics **32**, 205 (1960), URL https://doi.org/10.1103%2Frevmodphys.32.205.

[32] W. Kolos and C. C. J. Roothaan, Reviews of Modern Physics **32**, 219 (1960), URL https://doi.org/10.1103%2Frevmodphys.32.219.

[33] C. C. J. Roothaan, The Journal of Chemical Physics **19**, 1445 (1951), URL https://doi.org/10.1063%2F1.1748100.

[34] K. Rüdenberg, The Journal of Chemical Physics **19**, 1459 (1951), URL https://doi.org/10.1063%2F1.1748101.

[35] C. C. J. Roothaan, The Journal of Chemical Physics **28**, 982 (1958), URL https://doi.org/10.1063%2F1.1744313.

[36] K. Pachucki, Phys. Rev. A **88**, 022507 (2013), URL https://doi.org/10.1103%2Fphysreva.88.022507.

[37] W. Kołos and L. Wolniewicz, J. Chem. Phys. **45**, 509 (1966), URL https://doi.org/10.1063%2F1.1727598.

[38] K. Pachucki, Phys. Rev. A **82**, 032509 (2010), URL https://link.aps.org/doi/10.1103/PhysRevA.82.032509.

[39] K. Pachucki and J. Komasa, Physical Review A **83**, 042510 (2011).

[40] G. Corongiu and E. Clementi, The Journal of Chemical Physics **131**, 184306 (2009).

[41] R. S. Mulliken, Journal of the American Chemical Society **88**, 1849 (1966).

[42] G. Staszewska and L. Wolniewicz, Journal of Molecular Spectroscopy **212**, 208 (2002).

[43] W. Kołos and L. Wolniewicz, The Journal of Chemical Physics **45**, 509 (1966).

[44] J. S. Sims and S. A. Hagstrom, The Journal of Chemical Physics **124**, 094101 (2006).

[45] G. W. F. Drake, Physica Scripta **T83**, 83 (1999).

[46] J. Rychlewski, ed., *Explicitly Correlated Wave Functions in Chemistry and Physics* (Springer Netherlands, 2003).

[47] W. Kołos and J. Rychlewski, J. Mol. Spectrosc. **62**, 109 (1976), ISSN 0022-2852, URL https://www.sciencedirect.com/science/article/pii/002228527690268X.

[48] L. Wolniewicz, Chem. Phys. Lett. **233**, 644 (1995), URL https://doi.org/10.1016%2F0009-2614%2894%2901498-k.

[49] L. Wolniewicz, J. Mol. Spectrosc. **169**, 329 (1995), URL https://doi.org/10.1006%2Fjmsp.1995.1027.

[50] H. M. James and A. S. Coolidge, J. Chem. Phys. **1**, 825 (1933), URL https://doi.org/10.1063%2F1.1749252.

[51] J. S. Sims and S. A. Hagstrom, J. Chem. Phys. **124**, 094101 (2006), URL https://doi.org/10.1063%2F1.2173250.

[52] M. Siłkowski and K. Pachucki, J. Chem. Phys. **152**, 174308 (2020), URL https://doi.org/10.1063%2F5.0008086.

[53] K. Pachucki, Phys. Rev. A **80**, 032520 (2009), URL https://doi.org/10.1103%2Fphysreva.80.032520.

[54] M. Lesiuk and R. Moszynski, Physical Review A **86** (2012), URL https://doi.org/10.1103%2Fphysreva.86.052513.

[55] K. Pachucki, Physical Review A **86**, 052514 (2012).

[56] M. Lesiuk, Ph.D. thesis, University of Warsaw (2017).

[57] C. M. Bender and S. A. Orszag, *Advanced Mathematical Methods for Scientists and Engineers I* (Springer New York, 1999), URL https://doi.org/10.1007%2F978-1-4757-3069-2.

[58] R. Bukowski, B. Jeziorski, and K. Szalewicz, The Journal of Chemical Physics **100**, 1366 (1994), URL https://doi.org/10.1063%2F1.466614.

[59] Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences **258**, 421 (1960), URL https://doi.org/10.1098%2Frspa.1960.0197.

[60] Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences **258**, 402 (1960), URL https://doi.org/10.1098%2Frspa.1960.0195.

[61] Proceedings of the Royal Society of London. Series A. Mathematical and Physical Sciences **258**, 412 (1960), URL https://doi.org/10.1098%2Frspa.1960.0196.

[62] J. Mitroy, S. Bubin, W. Horiuchi, Y. Suzuki, L. Adamowicz, W. Cencek, K. Szalewicz, J. Komasa, D. Blume, and K. Varga, Reviews of Modern Physics **85**, 693 (2013), URL https://doi.org/10.1103%2Frevmodphys.85.693.

[63] K. Pachucki, M. Puchalski, and V. Yerokhin, Computer Physics Communications **185**, 2913 (2014), URL https://doi.org/10.1016%2Fj.cpc.2014.06.018.

[64] R. J. Drachman, J. Phys. B: At. Mol. Phys. **14**, 2733 (1981), URL https://doi.org/10.1088%2F0022-3700%2F14%2F16%2F003.

[65] K. Pachucki, W. Cencek, and J. Komasa, J. Chem. Phys. **122**, 184101 (2005), URL https://doi.org/10.1063%2F1.1888572.

[66] M. Puchalski, J. Komasa, P. Czachorowski, and K. Pachucki, Phys. Rev. Lett. **122**, 103003 (2019), URL https://link.aps.org/doi/10.1103/PhysRevLett.122.103003.

[67] M. Puchalski, J. Komasa, A. Spyszkiewicz, and K. Pachucki, Phys. Rev. A **100**, 020503(R) (2019), URL https://link.aps.org/doi/10.1103/PhysRevA.100.020503.

[68] M. Puchalski, J. Komasa, and K. Pachucki, Phys. Rev. A **95**, 052506 (2017), URL https://link.aps.org/doi/10.1103/PhysRevA.95.052506.

[69] M. Puchalski, J. Komasa, P. Czachorowski, and K. Pachucki, Phys. Rev. Lett. **122**, 103003 (2019), URL https://link.aps.org/doi/10.1103/PhysRevLett.122.103003.

[70] W. Cencek and J. Rychlewski, The Journal of Chemical Physics **98**, 1252 (1993), URL https://doi.org/10.1063%2F1.464293.

[71] W. Cencek and J. Rychlewski, The Journal of Chemical Physics **102**, 2533 (1995), URL https://doi.org/10.1063%2F1.468682.

[72] J. Komasa, W. Cencek, and J. Rychlewski, Physical Review A **52**, 4500 (1995), URL https://doi.org/10.1103%2Fphysreva.52.4500.

[73] J. Komasa and J. Rychlewski, Chemical Physics Letters **249**, 253 (1996), URL https://doi.org/10.1016%2F0009-2614%2895%2901392-x.

[74] J. Rychlewski, W. Cencek, and J. Komasa, Chemical Physics Letters **229**, 657 (1994), URL https://doi.org/10.1016%2F0009-2614%2894%2901108-7.

[75] W. Cencek and K. Szalewicz, International Journal of Quantum Chemistry **108**, 2191 (2008), URL https://doi.org/10.1002%2Fqua.21740.

[76] W. Kolos and C. C. J. Roothaan, Reviews of Modern Physics **32**, 205 (1960), URL https://doi.org/10.1103%2Frevmodphys.32.205.

[77] J. Podolanski, Ann. Phys. **402**, 868 (1931).

[78] K. Rüdenberg, The Journal of Chemical Physics **19**, 1459 (1951), URL https://doi.org/10.1063%2F1.1748101.

[79] W. Kolos and L. Wolniewicz, Chemical Physics Letters **24**, 457 (1974), URL https://doi.org/10.1016%2F0009-2614%2874%2980155-7.

[80] W. Kolos and L. Wolniewicz, Chemical Physics Letters **24**, 457 (1974), URL https://doi.org/10.1016%2F0009-2614%2874%2980155-7.

[81] W. Heitler and F. London, Zeitschrift für Physik **44**, 455 (1927), URL https://doi.org/10.1007%2Fbf01397394.

[82] C. Herring, Reviews of Modern Physics **34**, 631 (1962), URL https://doi.org/10.1103%2Frevmodphys.34.631.

[83] J. D. Hogg, Ph.D. thesis, University of Edinburgh (2010).

[84] K. Szalewicz, K. Patkowski, and B. Jeziorski, in *Intermolecular Forces and Clusters II* (Springer Berlin Heidelberg, 2005), pp. 43–117, URL https://doi.org/10.1007%2F430_004.

[85] T. Ćwiok, B. Jeziorski, W. Kołos, R. Moszynski, J. Rychlewski, and K. Szalewicz, Chemical Physics Letters **195**, 67 (1992), URL https://doi.org/10.1016%2F0009-2614%2892%2985912-t.

[86] T. Ćwiok, B. Jeziorski, W. Kol/os, R. Moszynski, and K. Szalewicz, The Journal of Chemical Physics **97**, 7555 (1992), URL https://doi.org/10.1063%2F1.463475.

[87] J. H. V. Vleck and A. Sherman, Reviews of Modern Physics **7**, 167 (1935), URL https://doi.org/10.1103%2Frevmodphys.7.167.

[88] Y. Sugiura, Zeitschrift für Physik **45**, 484 (1927), URL https://doi.org/10.1007%2Fbf01329207.

[89] K. T. Tang, J. P. Toennies, and C. L. Yiu, The Journal of Chemical Physics **99**, 377 (1993), URL https://doi.org/10.1063%2F1.465760.

[90] K. Tang, J. P. Toennies, and C. L. Yiu, International Reviews in Physical Chemistry **17**, 363 (1998), URL https://doi.org/10.1080%2F014423598230090.

[91] B. L. Burrows, A. Dalgarno, and M. Cohen, Physical Review A **86** (2012), URL https://doi.org/10.1103%2Fphysreva.86.052525.

[92] B. L. Burrows, A. Dalgarno, and M. Cohen, Physical Review A **81** (2010), URL https://doi.org/10.1103%2Fphysreva.81.042508.

[93] L. P. Gor'kov and L. P. Pitaevskii, Dokl. Akad. Nauk SSSR **151**, 822 (1963).

[94] C. Herring and M. Flicker, Physical Review **134**, A362 (1964), URL https://doi.org/10.1103%2Fphysrev.134.a362.

[95] R. J. Damburg, R. K. Propin, S. Graffi, V. Grecchi, E. M. Harrell, J. Čížek, J. Paldus, and H. J. Silverstone, Physical Review Letters **52**, 1112 (1984), URL https://doi.org/10.1103%2Fphysrevlett.52.1112.

[96] J. Cížek, R. J. Damburg, S. Graffi, V. Grecchi, E. M. Harrell, J. G. Harris, S. Nakai, J. Paldus, R. K. Propin, and H. J. Silverstone, Physical Review A **33**, 12 (1986), URL https://doi.org/10.1103%2Fphysreva.33.12.

[97] P. Gniewek and B. Jeziorski, Physical Review A **90** (2014), URL https://doi.org/10.1103%2Fphysreva.90.022506.

[98] P. Gniewek and B. Jeziorski, Physical Review A **94** (2016), URL https://doi.org/10.1103%2Fphysreva.94.042708.

[99] E. A. Andreev, Theor. Chim. Acta **28**, 235 (1973).

[100] T. Scott, M. Aubert-Frécon, D. Andrae, J. Grotendorst, J. M. III, and M. Glasser, Applicable Algebra in Engineering, Communication and Computing **15** (2004), URL https://doi.org/10.1007%2Fs00200-004-0156-6.

[101] T. Holstein, The Journal of Physical Chemistry **56**, 832 (1952), URL https://doi.org/10.1021%2Fj150499a004.

[102] S. J. Umanski and A. I. Voronin, Theor. Chim. Acta **12**, 166 (1968).

[103] T. Kato, Communications on Pure and Applied Mathematics **10**, 151 (1957), URL https://doi.org/10.1002%2Fcpa.3160100201.

[104] P. Gniewek and B. Jeziorski, Physical Review A **94** (2016), URL https://doi.org/10.1103%2Fphysreva.94.042708.

[105] Sprecher, Daniel, Ph.D. thesis (2013), URL http://hdl.handle.net/20.500.11850/74157.

[106] D. Sprecher, C. Jungen, and F. Merkt, The Journal of Chemical Physics **140**, 104303 (2014), URL https://doi.org/10.1063%2F1.4866809.

[107] E. Mátyus and D. Ferenc, Molecular Physics **120** (2022), URL https://doi.org/10.1080%2F00268976.2022.2074905.

[108] G. Herzberg and C. Jungen, J. Mol. Spectrosc. **41**, 425 (1972), URL https://doi.org/10.1016%2F0022-2852%2872%2990064-1.

[109] D. Sprecher, C. Jungen, and F. Merkt, J. Chem. Phys. **140**, 104303 (2014), URL https://doi.org/10.1063%2F1.4866809.

[110] D. Sprecher and F. Merkt, J. Chem. Phys. **140**, 124313 (2014), URL https://doi.org/10.1063%2F1.4868024.

[111] M. Beyer, N. Hölsch, J. A. Agner, J. Deiglmayr, H. Schmutz, and F. Merkt, Phys. Rev. A **97**, 012501 (2018), URL https://doi.org/10.1103%2Fphysreva.97.012501.

[112] N. Hölsch, M. Beyer, and F. Merkt, Phys. Chem. Chem. Phys. **20**, 26837 (2018), URL https://doi.org/10.1039%2Fc8cp05233f.

[113] M. Beyer, N. Hölsch, J. Hussels, C.-F. Cheng, E. Salumbides, K. Eikema, W. Ubachs, C. Jungen, and F. Merkt, Phys. Rev. Lett. **123**, 163002 (2019), URL https://doi.org/10.1103%2Fphysrevlett.123.163002.

[114] W. Ubachs, J. Koelemeij, K. Eikema, and E. Salumbides, Journal of Molecular Spectroscopy **320**, 1 (2016), ISSN 0022-2852.

[115] M. Niu, E. Salumbides, G. Dickenson, K. Eikema, and W. Ubachs, Journal of Molecular Spectroscopy **300**, 44 (2014), ISSN 0022-2852, spectroscopic Tests of Fundamental Physics.

[116] K.-F. Lai, P. Czachorowski, M. Schlösser, M. Puchalski, J. Komasa, K. Pachucki, W. Ubachs, and E. J. Salumbides, Phys. Rev. Research **1**, 033124 (2019).

[117] P. Czachorowski, M. Puchalski, J. Komasa, and K. Pachucki, Phys. Rev. A **98**, 052506 (2018).

[118] T. Detmer, P. Schmelcher, and L. S. Cederbaum, The Journal of Chemical Physics **109**, 9694 (1998).

[119] W. Cencek, J. Komasa, and J. Rychlewski, Chemical Physics Letters **246**, 417 (1995).

[120] J. Komasa and W. Cencek, Computational Methods in Science and Technology **9**, 79 (2003).

[121] H. Nakashima and H. Nakatsuji, The Journal of Chemical Physics **149**, 244116 (2018).

[122] L. Wolniewicz and K. Dressler, The Journal of Chemical Physics **100**, 444 (1994).

[123] T. Orlikowski, G. Staszewska, and L. Wolniewicz, Molecular Physics **96**, 1445 (1999).

[124] G. Staszewska and L. Wolniewicz, Journal of Molecular Spectroscopy **198**, 416 (1999).

[125] L. Wolniewicz and G. Staszewska, Journal of Molecular Spectroscopy **220**, 45 (2003).

[126] K.-F. Lai, M. Beyer, E. J. Salumbides, and W. Ubachs, The Journal of Physical Chemistry A **125**, 1221 (2021).

[127] D. Sprecher, M. Beyer, and F. Merkt, Molecular Physics **111**, 2100 (2013).

[128] N. Kouchi, M. Ukai, and Y. Hatano, Journal of Physics B: Atomic, Molecular and Optical Physics **30**, 2319 (1997).

[129] M. Glass-Maujean, C. Jungen, A. Vasserot, H. Schmoranzer, A. Knie, S. Kübler, A. Ehresmann, and W. Ubachs, Journal of Molecular Spectroscopy **338**, 22 (2017).

[130] M. Beyer, N. Hölsch, J. Hussels, C.-F. Cheng, E. J. Salumbides, K. S. E. Eikema, W. Ubachs, C. Jungen, and F. Merkt, Phys. Rev. Lett. **123**, 163002 (2019).

[131] D. Sprecher and F. Merkt, The Journal of Chemical Physics **140**, 124313 (2014).

[132] K. Takahashi, Y. Sakata, Y. Hino, and Y. Sakai, The European Physical Journal D **68**, 83 (2014).

[133] M. Glass-Maujean, The Journal of Chemical Physics **85**, 4830 (1986).

[134] A. K. Edwards and Q. Zheng, Journal of Physics B: Atomic, Molecular and Optical Physics **34**, 1539 (2001).

[135] J. O. Aasen, BIT **11**, 233 (1971).

[136] G. Ballard, D. Becker, J. Demmel, J. Dongarra, A. Druinsky, I. Peled, O. Schwartz, S. Toledo, and I. Yamazaki, in *2013 IEEE 27th International Symposium on Parallel and Distributed Processing* (IEEE, 2013).

[137] J. Dongarra, M. Gates, A. Haidar, J. Kurzak, P. Luszczek, P. Wu, I. Yamazaki, A. Yarkhan, M. Abalenkovs, N. Bagherpour, et al., ACM Transactions on Mathematical Software **45**, 1 (2019).

[138] Y. Hida, X. Li, and D. Bailey, in *Proceedings 15th IEEE Symposium on Computer Arithmetic. ARITH-15 2001* (IEEE Comput. Soc, 2001).

[139] K. Pachucki, Physical Review A **85**, 042511 (2012).

[140] G. Drake, in *Springer Handbook of Atomic, Molecular, and Optical Physics* (Springer New York, 2006), pp. 199–219.

[141] W. Kołos and J. Rychlewski, Journal of Molecular Spectroscopy **177**, 146 (1996).

[142] J. Hörnquist, P. Hedvall, Å. Larson, and A. E. Orel, Physical Review A **106** (2022), URL https://doi.org/10.1103%2Fphysreva.106.062821.

[143] H. Nakatsuji and H. Nakashima, The Journal of Chemical Physics **142**, 084117 (2015).

[144] K. Pachucki and J. Komasa, J. Chem. Phys. **141**, 224103 (2014), URL https://doi.org/10.1063%2F1.4902981.

[145] W. Kołos and J. Rychlewski, J. Mol. Spectrosc. **66**, 428 (1977), URL https://doi.org/10.1016%2F0022-2852%2877%2990301-0.

[146] W. Kołos and J. Rychlewski, J. Mol. Spectrosc. **91**, 128 (1982), URL https://doi.org/10.1016%2F0022-2852%2882%2990036-4.

[147] L. Wolniewicz and K. Dressler, J. Chem. Phys. **88**, 3861 (1988), URL https://doi.org/10.1063%2F1.453888.

[148] J. Rychlewski, J. Mol. Spectrosc. **149**, 125 (1991), URL https://doi.org/10.1016%2F0022-2852%2891%2990147-3.

[149] B. Jeziorski, R. Bukowski, and K. Szalewicz, Int. J. Quantum Chem. **61**, 769 (1997), URL https://doi.org/10.1002%2F%28sici%291097-461x%281997%2961%3A5%3C769%3A%3Aaid-qua4%3E3.0.co%3B2-u.

[150] L. Wolniewicz, J. Mol. Spectrosc. **174**, 132 (1995), URL https://doi.org/10.1006%2Fjmsp.1995.1275.

[151] J. Komasa and A. J. Thakkar, Chem. Phys. Lett. **222**, 65 (1994), URL https://doi.org/10.1016%2F0009-2614%2894%2900308-4.

[152] W. Cencek, J. Komasa, and J. Rychlewski, Chem. Phys. Lett. **246**, 417 (1995), URL https://doi.org/10.1016%2F0009-2614%2895%2901146-8.

[153] H. Nakatsuji, Phys. Rev. Lett. **93**, 030403 (2004), URL https://doi.org/10.1103%2Fphysrevlett.93.030403.

[154] H. Nakatsuji and H. Nakashima, J. Chem. Phys. **142**, 084117 (2015), URL https://doi.org/10.1063%2F1.4909520.

[155] Y. I. Kurokawa, H. Nakashima, and H. Nakatsuji, Phys. Chem. Chem. Phys. **21**, 6327 (2019), URL https://doi.org/10.1039%2Fc8cp05949g.

[156] H. Nakashima and H. Nakatsuji, J. Chem. Phys. **149**, 244116 (2018), URL https://doi.org/10.1063%2F1.5060659.

[157] Y. I. Kurokawa, H. Nakashima, and H. Nakatsuji, Phys. Chem. Chem. Phys. **22**, 13489 (2020), URL https://doi.org/10.1039%2Fd0cp01492c.

[158] K. Pachucki, M. Zientkiewicz, and V. Yerokhin, Comput. Phys. Commun. **208**, 162 (2016), URL https://doi.org/10.1016%2Fj.cpc.2016.07.024.

[159] W. R. Inc., *Mathematica, Version 13.2*, champaign, IL, 2022, URL https://www.wolfram.com/mathematica.

[160] S. Yu and K. Dressler, J. Chem. Phys. **101**, 7692 (1994), URL https://doi.org/10.1063%2F1.468263.

[161] C. Jungen, I. Dabrowski, G. Herzberg, and M. Vervloet, J. Chem. Phys. **93**, 2289 (1990), URL https://doi.org/10.1063%2F1.459008.

[162] C. Jungen, I. Dabrowski, G. Herzberg, and M. Vervloet, J. Mol. Spectrosc. **153**, 11 (1992), URL https://doi.org/10.1016%2F0022-2852%2892%2990452-t.

[163] G. Drake, *High Precision Calculations for Helium* (Springer New York, New York, NY, 2006), pp. 199–219, ISBN 978-0-387-26308-3, URL https://doi.org/10.1007/978-0-387-26308-3_11.

[164] R. S. Mulliken, Phys. Rev. **32**, 186 (1928), URL https://doi.org/10.1103%2Fphysrev.32.186.

[165] R. S. Mulliken, Rev. Mod. Phys. **4**, 1 (1932), URL https://doi.org/10.1103%2Frevmodphys.4.1.

[166] R. S. Mulliken, J. Chem. Phys. **23**, 1833 (1955), URL https://doi.org/10.1063%2F1.1740588.

[167] T. Sharp, At. Data Nucl. Data Tables **2**, 119 (1970), URL https://doi.org/10.1016%2Fs0092-640x%2870%2980007-9.

[168] S. Datta, S. A. Alexander, and R. L. Coldwell, Int. J. Quantum Chem. **111**, 4106 (2010), URL https://doi.org/10.1002%2Fqua.22959.

[169] S. Rothenberg and E. R. Davidson, J. Chem. Phys. **44**, 730 (1966), URL https://doi.org/10.1063%2F1.1726753.

[170] L. Wolniewicz and G. Staszewska, J. Mol. Spectrosc. **220**, 45 (2003), URL https://doi.org/10.1016%2Fs0022-2852%2803%2900121-8.

[171] I. Drira, J. Mol. Spectrosc. **198**, 52 (1999), URL https://doi.org/10.1006%2Fjmsp.1999.7934.

[172] A. Spielfiedel, J. Mol. Spectrosc. **217**, 162 (2003), URL https://doi.org/10.1016%2Fs0022-2852%2802%2900043-7.

[173] G. Staszewska, J. Phys. Chem. A **105**, 2308 (2001), URL https://doi.org/10.1021%2Fjp003781z.

[174] J. Rychlewski, W. Cencek, and J. Komasa, Chem. Phys. Lett. **229**, 657 (1994), URL https://doi.org/10.1016%2F0009-2614%2894%2901108-7.

[175] M. Puchalski, A. Spyszkiewicz, J. Komasa, and K. Pachucki, Phys. Rev. Lett. **121**, 073001 (2018), URL https://doi.org/10.1103%2Fphysrevlett.121.073001.

[176] J. Komasa, M. Puchalski, P. Czachorowski, G. Łach, and K. Pachucki, Phys. Rev. A **100**, 032519 (2019), URL https://doi.org/10.1103%2Fphysreva.100.032519.

[177] M. Puchalski, J. Komasa, and K. Pachucki, Phys. Rev. A **95**, 052506 (2017), URL https://doi.org/10.1103%2Fphysreva.95.052506.

[178] P. Czachorowski, M. Puchalski, J. Komasa, and K. Pachucki, Phys. Rev. A **98**, 052506 (2018), URL https://doi.org/10.1103%2Fphysreva.98.052506.

[179] P. Czachorowski, Ph.D. thesis, University of Warsaw (2019).

[180] K. Piszczatowski, G. Łach, M. Przybytek, J. Komasa, K. Pachucki, and B. Jeziorski, J. Chem. Theory Comput. **5**, 3039 (2009), URL https://doi.org/10.1021%2Fct900391p.

[181] M. Puchalski, J. Komasa, P. Czachorowski, and K. Pachucki, Phys. Rev. Lett. **117** (2016), URL https://doi.org/10.1103%2Fphysrevlett.117.263002.

[182] M. Siłkowski, M. Zientkiewicz, and K. Pachucki, Adv. Quant. Chem. **83**, 255 (2021), URL https://www.sciencedirect.com/science/article/pii/S0065327621000149.

[183] K. Pachucki and J. Komasa, Physical Chemistry Chemical Physics **20**, 247 (2018), URL https://doi.org/10.1039%2Fc7cp06516g.

[184] K. Pachucki and J. Komasa, Physical Chemistry Chemical Physics **20**, 26297 (2018), URL https://doi.org/10.1039%2Fc8cp05493b.

[185] K. Pachucki and J. Komasa, Physical Chemistry Chemical Physics **21**, 10272 (2019), URL https://doi.org/10.1039%2Fc9cp01308c.

[186] K. Pachucki and J. Komasa, Molecular Physics **120** (2022), URL https://doi.org/10.1080%2F00268976.2022.2040627.

[187] K. Pachucki and J. Komasa, The Journal of Chemical Physics **129**, 034102 (2008), URL https://doi.org/10.1063%2F1.2952517.

[188] K. Pachucki and J. Komasa, J. Chem. Phys. **130**, 164113 (2009), URL https://doi.org/10.1063%2F1.3114680.

[189] K.-F. Lai, E. J. Salumbides, M. Beyer, and W. Ubachs, Molecular Physics **120** (2021), URL https://doi.org/10.1080%2F00268976.2021.2018063.

[190] K. Pachucki and J. Komasa, J. Chem. Phys. **129**, 034102 (2008), URL https://doi.org/10.1063%2F1.2952517.

[191] N. Brambilla, G. Krein, J. T. Castellà, and A. Vairo, Physical Review D **97** (2018), URL https://doi.org/10.1103%2Fphysrevd.97.016016.

[192] K. Pachucki and J. Komasa, The Journal of Chemical Physics **143**, 034111 (2015), URL https://doi.org/10.1063%2F1.4927079.

[193] W. Kołsos, in *Advances in Quantum Chemistry Volume 5* (Elsevier, 1970), pp. 99–133, URL https://doi.org/10.1016%2Fs0065-3276%2808%2960337-8.

[194] S. L. Guberman, The Journal of Chemical Physics **78**, 1404 (1983), URL https://doi.org/10.1063%2F1.444882.

[195] J. D. Bjorken and S. D. Drell, *Relativistic quantum mechanics*, International series in pure and applied physics (McGraw-Hill, New York, NY, 1964), URL https://cds.cern.ch/record/100769.

[196] J. Zatorski, Ph.D. thesis, University of Warsaw (2009).

[197] K. G. Dyall, The Journal of Chemical Physics **100**, 2118 (1994), URL https://doi.org/10.1063%2F1.466508.

[198] K. Piszczatowski, G. Łach, M. Przybytek, J. Komasa, K. Pachucki, and B. Jeziorski, J. Chem. Theory Comput. **5**, 3039 (2009), URL https://doi.org/10.1021%2Fct900391p.

[199] L. Wolniewicz, The Journal of Chemical Physics **99**, 1851 (1993), URL https://doi.org/10.1063%2F1.465303.

[200] L. Wolniewicz, Acta Phys. Polon. **22**, 3 (1962).

[201] P. Czachorowski, M. Puchalski, J. Komasa, and K. Pachucki, Phys. Rev. A **98**, 052506 (2018), URL https://link.aps.org/doi/10.1103/PhysRevA.98.052506.

[202] K. Pachucki and J. Komasa, The Journal of Chemical Physics **130**, 164113 (2009), URL https://doi.org/10.1063%2F1.3114680.

[203] N. Hoelsch, Ph.D. thesis, Eidgenossische Technische Hochschule Zurich (2022).

[204] I. Angeli and K. Marinova, Atomic Data and Nuclear Data Tables **99**, 69 (2013), URL https://doi.org/10.1016%2Fj.adt.2011.12.006.

[205] H. A. Bethe and E. E. Salpeter, *Quantum Mechanics of One- and Two-Electron Atoms* (Springer Berlin Heidelberg, 1957), URL https://doi.org/10.1007%2F978-3-662-12869-5.

[206] M. I. Eides, H. Grotch, and V. A. Shelyuto, Phys. Rep. **342**, 63 (2001), URL https://doi.org/10.1016%2Fs0370-1573%2800%2900077-6.

[207] S. P. Goldman and G. W. F. Drake, Phys. Rev. Lett. **68**, 1683 (1992), URL https://doi.org/10.1103%2Fphysrevlett.68.1683.

[208] G. Drake and S. P. Goldman, Can. J. Phys. **77**, 835 (2000), URL https://doi.org/10.1139%2Fp00-010.

[209] C. Schwartz, Phys. Rev. **123**, 1700 (1961), URL https://doi.org/10.1103%2Fphysrev.123.1700.

[210] V. I. Korobov and S. V. Korobov, Phys. Rev. A **59**, 3394 (1999), URL https://link.aps.org/doi/10.1103/PhysRevA.59.3394.

[211] V. I. Korobov, Phys. Rev. A **85**, 042514 (2012), URL https://link.aps.org/doi/10.1103/PhysRevA.85.042514.

[212] V. I. Korobov, Phys. Rev. A **100**, 012517 (2019), URL https://link.aps.org/doi/10.1103/PhysRevA.100.012517.

[213] V. A. Yerokhin and K. Pachucki, Phys. Rev. A **81**, 022507 (2010), URL https://link.aps.org/doi/10.1103/PhysRevA.81.022507.

[214] Z.-C. Yan and G. W. F. Drake, Phys. Rev. Lett. **91**, 113004 (2003), URL https://link.aps.org/doi/10.1103/PhysRevLett.91.113004.

[215] K. Pachucki and J. Komasa, Phys. Rev. A **68**, 042507 (2003), URL https://link.aps.org/doi/10.1103/PhysRevA.68.042507.

[216] K. Pachucki and J. Komasa, Phys. Rev. Lett. **92**, 213001 (2004), URL https://link.aps.org/doi/10.1103/PhysRevLett.92.213001.

[217] F. M. J. Cozijn, P. Dupré, E. J. Salumbides, K. S. E. Eikema, and W. Ubachs, Phys. Rev. Lett. **120**, 153002 (2018), URL https://link.aps.org/doi/10.1103/PhysRevLett.120.153002.

[218] A. Castrillo, E. Fasci, and L. Gianfrani, Phys. Rev. A **103**, 022828 (2021), URL https://doi.org/10.1103%2Fphysreva.103.022828.

[219] S. Kassi, C. Lauzin, J. Chaillot, and A. Campargue, Phys. Chem. Chem. Phys. **24**, 23164 (2022), URL https://doi.org/10.1039%2Fd2cp02151j.

[220] K. Pachucki and J. Komasa, J. Chem. Phys. **143**, 034111 (2015), URL https://doi.org/10.1063%2F1.4927079.

[221] J. Komasa, M. Puchalski, P. Czachorowski, G. Łach, and K. Pachucki, Phys. Rev. A **100**, 032519 (2019), URL https://link.aps.org/doi/10.1103/PhysRevA.100.032519.

[222] H. A. Bethe, Phys. Rev. **72**, 339 (1947), URL https://doi.org/10.1103%2Fphysrev.72.339.

[223] H. Araki, Prog. Theor. Phys. **17**, 619 (1957), URL https://doi.org/10.1143%2Fptp.17.619.

[224] J. Sucher, Phys. Rev. **109**, 1010 (1958), URL https://doi.org/10.1103%2Fphysrev.109.1010.

[225] C. L. Pekeris, Phys. Rev. **115**, 1216 (1959), URL https://link.aps.org/doi/10.1103/PhysRev.115.1216.

[226] P. K. Kabir and E. E. Salpeter, Phys. Rev. **108**, 1256 (1957), URL https://doi.org/10.1103%2Fphysrev.108.1256.

[227] E. E. Salpeter and M. H. Zaidi, Phys. Rev. **125**, 248 (1962), URL https://doi.org/10.1103%2Fphysrev.125.248.

[228] C. Schwartz, Ann. Phys. (NY) **6**, 156 (1959), URL https://doi.org/10.1016%2F0003-4916%2859%2990032-6.

[229] C. Schwartz and J. Tiemann, Ann. Phys. (NY) **6**, 178 (1959), URL https://doi.org/10.1016%2F0003-4916%2859%2990034-x.

[230] B.-L. Zhou, J.-M. Zhu, and Z.-C. Yan, Phys. Rev. A **73**, 014501 (2006), URL https://doi.org/10.1103%2Fphysreva.73.014501.

[231] K. Pachucki, Ann. Phys. (NY) **226**, 1 (1993), URL https://doi.org/10.1006%2Faphy.1993.1063.

[232] M. Gavrila and A. Costescu, Phys. Rev. A **2**, 1752 (1970), URL https://doi.org/10.1103%2Fphysreva.2.1752.

[233] D. Ferenc and E. Mátyus, J. Phys. Chem. A **127**, 627 (2023), URL https://doi.org/10.1021/acs.jpca.2c05790.

[234] M. Abramowitz, I. A. Stegun, and R. H. Romer, Am. J. Phys. **56**, 958 (1988), URL https://doi.org/10.1119%2F1.15378.

[235] G. W. F. Drake and R. A. Swainson, Phys. Rev. A **41**, 1243 (1990), URL https://doi.org/10.1103%2Fphysreva.41.1243.

[236] H. A. Bethe, L. M. Brown, and J. R. Stehn, Phys. Rev. **77**, 370 (1950), URL https://doi.org/10.1103%2Fphysrev.77.370.

[237] U. D. Jentschura and P. J. Mohr, Physical Review A **72** (2005), URL https://doi.org/10.1103%2Fphysreva.72.012110.

[238] G. Łach, Ph.D. thesis, University of Warsaw (2007).

[239] A. M. Frolov, J. Chem. Phys. **126**, 104302 (2007), URL https://doi.org/10.1063/1.2709880.

[240] M. Puchalski, J. Komasa, A. Spyszkiewicz, and K. Pachucki, Physical Review A **100** (2019), URL https://doi.org/10.1103%2Fphysreva.100.020503.

[241] M. Puchalski, J. Komasa, P. Czachorowski, and K. Pachucki, Phys. Rev. Lett. **122**, 103003 (2019), URL https://link.aps.org/doi/10.1103/PhysRevLett.122.103003.

[242] K. Pachucki, Physical Review A **74** (2006), URL https://doi.org/10.1103%2Fphysreva.74.022512.

[243] M. I. Eides, H. Grotch, and V. A. Shelyuto, Physics Reports **342**, 63 (2001), URL https://doi.org/10.1016%2Fs0370-1573%2800%2900077-6.

[244] K. Pachucki and J. Komasa, The Journal of Chemical Physics **137**, 204314 (2012), URL https://doi.org/10.1063%2F1.4768169.

[245] D. T. Colbert and W. H. Miller, The Journal of Chemical Physics **96**, 1982 (1992), URL https://doi.org/10.1063%2F1.462100.

[246] H. Fleurbaey, A. O. Koroleva, S. Kassi, and A. Campargue, Physical Chemistry Chemical Physics **25**, 14749 (2023), URL https://doi.org/10.1039%2Fd3cp01136d.

APPENDIX

The following Appendix contains numerical data obtained as a result of variational calculations in Kolos-Wolniewicz basis. The data is presented in a form of 102 tables:

Σ^+ states with $n = 1 - 7$ are the subject of work [A2].

$1 - 4\ \Pi$, $1 - 3\Delta$, $1 - 2\Phi$, and $3\Phi_u$ states are the subject of work [A3].

All the other states presented here are as of yet, unpublished.

The data for two lowest states was obtained using silimar methods elsewhere, the ground $\mathrm{X}^1\Sigma_g^+$ state is available in Ref. [38] and lowest excited $\mathrm{b}^3\Sigma_u^+$ state in Ref. [39].

Table A1: R-dependence of Born-Oppenheimer energy, expecatation value of potential, mass polarization rescaled by a factor of 10^6 and $\mathrm{d}E/\mathrm{d}R$ (all in au) for the $2\,^1\Sigma_g^+$ (EF state). All uncertainties result from the extrapolation to the complete basis set limit.

$2\,^1\Sigma_g^+$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.3165157686164(5)	−1.63802080388(3)	−9295.059960(2)	−1.43569895234(3)
0.8	−0.4364255931314(3)	−1.66841423161(7)	−9254.886276(4)	−0.99445380668(6)
0.9	−0.5203504685443(3)	−1.67352488114(10)	−9217.520015(10)	−0.70313771562(9)
1.0	−0.5800855823898(3)	−1.66375763756(8)	−9184.555515(8)	−0.50358647278(7)
1.1	−0.62301687481874(9)	−1.64525410024(6)	−9157.634987(7)	−0.36292759146(5)
1.2	−0.653971526522602(4)	−1.62176338091(4)	−9138.5172075(2)	−0.261516939890(3)
1.3	−0.67621470498528(4)	−1.59563140971(6)	−9129.150272(7)	−0.18707846133(4)
1.4	−0.6920181809959(6)	−1.56835221899(6)	−9131.751666(8)	−0.13165418357(4)
1.5	−0.703000247100(2)	−1.54088846984(5)	−9148.899539(9)	−0.089925317093(3)
1.6	−0.7103369826577(3)	−1.51386454921(5)	−9183.639305(10)	−0.058244114934(3)
1.7	−0.7148979553059(4)	−1.48768656829(5)	−9239.609399(10)	−0.034053328042(3)
1.8	−0.7173358943405(8)	−1.46261917181(4)	−9321.188458(2)	−0.015526323961(2)
1.9	−0.71814744582335(7)	−1.43883635187(4)	−9433.661363(2)	−0.001337610646(2)
2.0	−0.71771527914871(4)	−1.41645665027(4)	−9583.389183(2)	0.009486954016(2)
2.1	−0.71633791367415(4)	−1.395569515233(4)	−9777.937644(2)	0.017669672435(2)
2.2	−0.71425134849499(7)	−1.376257902544(3)	−10026.045498(2)	0.023747633839(10)
2.3	−0.711645225229490(9)	−1.358622061876(3)	−10337.136951(2)	0.028116690688(7)
2.4	−0.708675480663436(6)	−1.342811121614(2)	−10719.644974(2)	0.031058266547(5)
2.5	−0.70547509665570(3)	−1.329073919572(6)	−11176.302459(2)	0.0327505094958(7)
2.6	−0.70216462869769(3)	−1.317851983412(6)	−11691.650169(2)	0.033260489994(4)
2.7	−0.69886488816962(8)	−1.309963413597(3)	−12199.198422(2)	0.032506060275(10)
2.8	−0.695715952317034(9)	−1.30697944220(5)	−12494.894657(10)	0.030161593729(2)
2.9	−0.692910056096402(5)	−1.311960043835(2)	−12015.535193(4)	0.025468989089(5)
3.0	−0.69074705639304(4)	−1.33045634500(2)	−9363.794557(6)	0.01701258926(7)
3.1	−0.68968737742023(6)	−1.36927041683(3)	−1977.835792(6)	0.00325946387(9)
3.2	−0.6902232606749(3)	−1.42552132408(4)	11363.6029483(3)	−0.01408587586(10)
3.3	−0.6923874588115(3)	−1.47735021907(3)	25656.074682(4)	−0.02805312165(8)
3.4	−0.6955734231882(3)	−1.50825051333(2)	34837.924744(6)	−0.03444225499(6)
3.5	−0.69907970370733(10)	−1.52050348920(2)	38396.64494(5)	−0.03495545194(4)
3.6	−0.70246066799592(8)	−1.52124790791(2)	38291.29749(10)	−0.03231293664(4)
3.7	−0.70549530375075(6)	−1.51545600835(2)	36175.74716(2)	−0.028233892122(3)
3.8	−0.70809017098561(4)	−1.50594634340(10)	33042.73043(3)	−0.023622631954(3)
3.9	−0.71021777747176(3)	−1.49431213543(9)	29447.48164(3)	−0.018942712947(2)
4.0	−0.71188450925360(3)	−1.48150080632(9)	25700.3073(4)	−0.014432946954(2)
4.1	−0.71311415278937(3)	−1.46810864021(8)	21977.0727(4)	−0.010214715763(2)
4.2	−0.71393911884368(3)	−1.45452853557(8)	18378.17722(3)	−0.006345309021(2)
4.3	−0.71439556008951(3)	−1.44102711744(8)	14960.17289(3)	−0.002845580759(2)
4.4	−0.71452055625195(8)	−1.42778748429(2)	11753.2227(4)	0.000284915502(3)
4.5	−0.71435045911994(10)	−1.41493459837(2)	8771.1199(4)	0.003059182193(3)
4.6	−0.71391992318097(8)	−1.40255146772(2)	6017.28330(3)	0.005497473617(3)
4.7	−0.71326136003309(8)	−1.39069014964(2)	3488.49442(3)	0.007623951154(3)
4.8	−0.71240466360150(10)	−1.37937964052(2)	1177.31621(3)	0.009464518058(3)
4.9	−0.71137711182375(10)	−1.36863175574(2)	−926.29287(2)	0.011045401613(3)
5.0	−0.71020338378787(10)	−1.35844562028(2)	−2833.87705(2)	0.012392229459(3)
5.1	−0.70890565134338(10)	−1.34881114308(2)	−4557.72130(2)	0.013529443059(3)

5.2	−0.70750371694388(10)	−1.33971171647(2)	−6110.32275(2)	0.014479945657(3)
5.3	−0.70601517799518(10)	−1.33112630920(2)	−7504.02695(10)	0.015264914490(3)
5.4	−0.70445560390474(10)	−1.32303107890(2)	−8750.78234(8)	0.015903727574(3)
5.5	−0.70283871626241(10)	−1.31540060179(2)	−9861.98065(6)	0.016413969223(3)
5.6	−0.70117656565623(10)	−1.30820879783(2)	−10848.35976(4)	0.016811488122(3)
5.7	−0.69947970087181(10)	−1.30142961510(2)	−11719.951741(3)	0.017110488884(2)
5.8	−0.6977573278576(3)	−1.29503752497(2)	−12486.063298(3)	0.017323643233(3)
5.9	−0.6960174570171(3)	−1.28900786971(2)	−13155.27894(4)	0.017462210903(3)
6.0	−0.6942670382246(7)	−1.28331709649(2)	−13735.479700(5)	0.017536163325(2)
6.5	−0.68554021616006(9)	−1.25921309170(2)	−15531.930008(8)	0.017210360094(2)
7.0	−0.6771656536490(3)	−1.24080286376(4)	−15941.42632(2)	0.01621834908(4)
7.5	−0.66936563139196(9)	−1.22655242781(2)	−15370.65529(5)	0.014957177996(2)
8.0	−0.662221029584(3)	−1.21550415448(4)	−14034.357514(3)	0.01361723808(4)
8.5	−0.655747598735(3)	−1.2071131220(5)	−12014.46729(10)	0.01228024417(5)
9.0	−0.649936081568(3)	−1.2011377725(7)	−9296.2244(5)	0.01097048785(6)
9.5	−0.644773573844(3)	−1.1975733475(6)	−5796.4030(6)	0.00968145265(5)
10.0	−0.640254776824(3)	−1.1965947170(5)	−1405.4879(6)	0.00839148366(4)
11.0	−0.633180755609(2)	−1.20321590006(6)	10011.1598(9)	0.005740510105(2)
12.0	−0.6287421262293(6)	−1.218974858915(3)	21713.717936(2)	0.003209116128(5)
13.0	−0.6264988169803(5)	−1.23424821145(2)	26487.5403(4)	0.001442263270(2)
14.0	−0.6255560932401(3)	−1.24323606006(8)	21518.0319(6)	0.000562580459(6)
15.0	−0.62520301412899(10)	−1.24739607062(7)	11333.8569(8)	0.000200663843(6)
16.0	−0.62507915479958(6)	−1.24903529632(4)	4106.1921(6)	0.0000701883301(3)
17.0	−0.62503467481894(4)	−1.249618654446(3)	1295.97322(3)	0.0000265114818(2)
18.0	−0.62501709693463(3)	−1.249833628400(10)	422.6948(5)	0.0000111425261(6)
19.0	−0.62500937671631(3)	−1.2499204240806(3)	153.00205(2)	0.00000517522905(2)
20.0	−0.625005640453183(5)	−1.2499585559039(6)	63.15281(2)	0.000002636250123(4)

Table A2: Same as for Table A1, but for $3\,^1\Sigma_g^+$ (GK state).

		$3\,^1\Sigma_g$		
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.24052172967(4)	−1.495942764(2)	−2700.9798(4)	−1.449856149(2)
0.8	−0.36181860110(7)	−1.53005814(3)	−2712.464(8)	−1.00802618(3)
0.9	−0.44706935588(3)	−1.538609026(7)	−2724.67173(2)	−0.716078127(6)
1.0	−0.508066130356(9)	−1.532010496(5)	−2738.0600(4)	−0.515878236(4)
1.1	−0.552582069001(3)	−1.5236710060(3)	1392.1803(3)	−0.3804607891(2)
1.2	−0.58525300050392(9)	−1.50448186039(2)	1661.06961(2)	−0.27831321616(2)
1.3	−0.60914005904039(8)	−1.48239441057(8)	1982.22099(4)	−0.20316484037(5)
1.4	−0.62651802275726(5)	−1.45892476067(5)	2367.536448(4)	−0.147063367963(3)
1.5	−0.63900865958776(6)	−1.435058229564(3)	2832.652059(4)	−0.104693940259(2)
1.6	−0.64779188669531(3)	−1.411443506172(2)	3398.425787(7)	−0.072412332988(5)
1.7	−0.653741492555054(3)	−1.388514589313(8)	4093.215054(5)	−0.047665649531(4)
1.8	−0.657514963179179(5)	−1.366570958702(9)	4956.4281926(2)	−0.028633906858(5)
1.9	−0.659614566278383(6)	−1.345834285484(2)	6044.231113(7)	−0.014002712067(6)
2.0	−0.660430067353057(8)	−1.326494350943(2)	7439.032887(2)	−0.002817108119(7)
2.1	−0.660269664591789(8)	−1.308755754229(3)	9265.850077(3)	0.005611226169(10)
2.2	−0.659383681634108(9)	−1.29290108246(4)	11721.67670(4)	0.011757400363(2)
2.3	−0.65798473081622(3)	−1.27939978758(5)	15130.27921(4)	0.015899858284(2)
2.4	−0.65626850228725(3)	−1.26912703798(7)	20047.40353(5)	0.018087486083(3)
2.5	−0.65444179894161(3)	−1.26383892951(2)	27460.71150(8)	0.01801786735(5)
2.6	−0.65277024225941(5)	−1.26718461289(2)	39112.49069(2)	0.01475225832(8)
2.7	−0.6516623968696(3)	−1.2862369384(4)	57581.73462(2)	0.00632883532(2)
2.8	−0.6517496000582(6)	−1.3294085009(2)	83769.3627(6)	−0.0092533217(6)
2.9	−0.6536264097214(5)	−1.3879259611(3)	109162.7225(6)	−0.0278183247(8)
3.0	−0.656985952465(5)	−1.4246210763(5)	119463.01552(2)	−0.03688305710(2)
3.1	−0.660470206304(5)	−1.4150086097(4)	112008.029228(2)	−0.03034457972(2)
3.2	−0.6626924221194(10)	−1.36749100741(6)	92317.713041(4)	−0.013158175991(2)
3.3	−0.663103508233(2)	−1.31244962802(5)	69683.03876(2)	0.0041689055894(3)
3.4	−0.6620703285659(3)	−1.271735506522(2)	51933.56833(8)	0.0154132795904(3)
3.5	−0.66020194102855(7)	−1.246024546865(3)	40215.59991(8)	0.02125123862592(3)
3.6	−0.6579257629168(5)	−1.22986049155(4)	32770.16849(7)	0.023886398411(4)
3.7	−0.6554820821082(6)	−1.21929217166(4)	27983.71597(6)	0.024776214205(7)
3.8	−0.653002475032(2)	−1.21216114410(5)	24846.73244(6)	0.024695738411(8)
3.9	−0.6505615272162(3)	−1.20732127366(5)	22768.52291(5)	0.024051738661(9)
4.0	−0.6482033570025(6)	−1.20413496019(5)	21398.69754(6)	0.023067938452(9)
4.1	−0.6459548376865(2)	−1.20221951086(5)	20521.44975(5)	0.021875649882(8)
4.2	−0.64383239417064(10)	−1.20132334871(5)	19997.85872(5)	0.020557485627(8)
4.3	−0.64184566547178(10)	−1.20126434485(4)	19734.36058(4)	0.019169066532(7)
4.4	−0.6399995848647(2)	−1.20189825008(5)	19665.09805(6)	0.017750209010(8)
4.5	−0.6382956324281(7)	−1.20310233574(4)	19741.75956(6)	0.016330873138(7)
4.6	−0.63673264328828(9)	−1.20476710975(4)	19927.58620(5)	0.014934386267(5)
4.7	−0.63530737413400(8)	−1.206792499672(3)	20193.77185(5)	0.013579201829(5)
4.8	−0.63401493771346(10)	−1.209086537217(4)	20517.27139(5)	0.012279862127(5)
4.9	−0.63284916440033(9)	−1.211565377600(3)	20879.44676(5)	0.011047541061(4)
5.0	−0.63180292088766(8)	−1.214153909085(3)	21265.20770(5)	0.0098903865380(3)
5.1	−0.63086839902846(8)	−1.216786464449(2)	21662.43646(5)	0.0088137909032(2)
5.2	−0.63003737814154(7)	−1.219407329245(2)	22061.56689(5)	0.0078206590458(2)
5.3	−0.62930145924297(6)	−1.221970885897(2)	22455.24183(5)	0.0069117042620(2)
5.4	−0.62865226805824(7)	−1.224441346458(2)	22838.00755(10)	0.0060857758625(2)

5.5	−0.62808162412265(6)	−1.226792109210(2)	23206.02748(10)	0.0053402070972(9)
5.6	−0.62758167482480(6)	−1.229004824979(2)	23556.81039(10)	0.0046711651197(7)
5.7	−0.62714499514593(5)	−1.231068280544(9)	23888.95593(2)	0.0040739841662(6)
5.8	−0.62676465558350(7)	−1.232977205276(2)	24201.92217(10)	0.0035434665328(5)
5.9	−0.62643426203426(7)	−1.234731091093(2)	24495.81965(9)	0.0030741411821(4)
6.0	−0.62614797215188(6)	−1.236333092598(9)	24771.23473(9)	0.00266047528425(4)
6.5	−0.62521086084365(5)	−1.242320657457(9)	25908.70002(2)	0.0012463175739(4)
7.0	−0.62478465339407(4)	−1.245776110138(8)	26759.48332(2)	0.0005418852356(6)
7.5	−0.62460914319878(4)	−1.247704674716(8)	27451.76146(2)	0.0002018148908(7)
8.0	−0.62455327090182(3)	−1.248769828698(8)	28069.50059(2)	0.0000420891382(8)
8.5	−0.62455262132199(3)	−1.249356501491(9)	28666.45825(3)	−0.0000295598644(8)
9.0	−0.624575830346187(10)	−1.249677981920(8)	29282.2100(4)	−0.0000584801364(7)
9.5	−0.624607741026967(10)	−1.249850865785(8)	29953.5030(4)	−0.0000668824980(7)
10.0	−0.624641136009254(10)	−1.249938760234(10)	30722.4642(6)	−0.0000656488216(8)
11.0	−0.624700931500543(8)	−1.249981947573(7)	32792.4527(5)	−0.0000527349610(6)
12.0	−0.624745654032564(9)	−1.249930423166(10)	36229.0151(7)	−0.0000365929250(7)
13.0	−0.624774071241936(9)	−1.249811738100(2)	42367.2273(9)	−0.0000202765858(9)
14.0	−0.62478671814281(3)	−1.249654161255(2)	52675.90915(2)	−0.0000057660692(9)
15.0	−0.62478894708267(3)	−1.249596038998(6)	65062.72693(3)	−0.00000120965549(3)
16.0	−0.62479368197811(3)	−1.24973857135(10)	73177.4589(3)	−0.000009450462(6)
17.0	−0.624807739272856(2)	−1.249918609(4)	76356.505(3)	−0.00001783122(3)
18.0	−0.62482745074638(3)	−1.2500286836793(5)	77391.700023(2)	−0.000020765677029(2)
19.0	−0.6248480715382(10)	−1.25007780291(4)	77737.846924(3)	−0.0000200873598(2)
20.0	−0.624867158264172(4)	−1.250093693927(9)	77867.33305(3)	−0.0000179688700(5)

Table A3: Same as for Table A1, but for $4\,^1\Sigma_g^+$ (H$\bar{H}$ state).

		$4\,^1\Sigma_g$		
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.2384696875123(8)	−1.496240703(6)	681.6828966(3)	−1.456144754(6)
0.8	−0.3603915563265(3)	−1.5321693233(2)	816.112839(2)	−1.0142327633(2)
0.9	−0.4462579793084(4)	−1.5424805412(7)	976.100103(10)	−0.7221828695(7)
1.0	−0.50785981526101(8)	−1.53759404866(3)	1166.11913(10)	−0.52187441815(3)
1.1	−0.5521941410403(7)	−1.5164166774(8)	−2753.550388(3)	−0.3745712685(6)
1.2	−0.5842811459688(10)	−1.4955892628(4)	−2771.433793(3)	−0.27252247571(3)
1.3	−0.6075935632469(5)	−1.4718855197(5)	−2792.78197(5)	−0.19746030254(3)
1.4	−0.6244046998458(4)	−1.44680887830(3)	−2818.613637(3)	−0.14142819901(2)
1.5	−0.6363344187520(3)	−1.42132899138(2)	−2850.206083(2)	−0.09910676926(7)
1.6	−0.6445602340445(3)	−1.39607443664(3)	−2889.167569(3)	−0.06684623035(2)
1.7	−0.6499528868034(3)	−1.37145227323(2)	−2937.561347(3)	−0.04208617625(10)
1.8	−0.6531659130439(6)	−1.34772426580(3)	−2998.090637(2)	−0.02299579985(2)
1.9	−0.6546962953392(3)	−1.32505686931(2)	−3074.37987(4)	−0.00824435717(8)
2.0	−0.6549264525221(3)	−1.30355524535(2)	−3171.41597(4)	0.00314882985(6)
2.1	−0.6541539216603(4)	−1.28328795793(2)	−3296.26646(4)	0.01191423114(5)
2.2	−0.6526128024307(3)	−1.26430738378(9)	−3459.29908(4)	0.018599191401(4)
2.3	−0.65048968891373(10)	−1.24667105425(7)	−3676.35836(5)	0.023612314595(3)
2.4	−0.64793607391020(10)	−1.230472040863(3)	−3972.87930(5)	0.027250044565(5)
2.5	−0.64507897451813(9)	−1.215895328524(3)	−4392.19194(6)	0.029705048204(2)
2.6	−0.6420319421269(3)	−1.20333979035(2)	−5013.50264(9)	0.03104772843(6)
2.7	−0.6389100778082(5)	−1.19368586439(2)	−5992.86398(5)	0.03116084860(7)
2.8	−0.6358535975992(2)	−1.18866860746(2)	−7648.12077(5)	0.02965663848(6)
2.9	−0.6330402363905(3)	−1.1895085484(2)	−10476.23375(3)	0.0264041119(4)
3.0	−0.6305541387855(3)	−1.1898718138(2)	−14243.0367(4)	0.0237454879(5)
3.1	−0.6281888937499(10)	−1.1821548374(9)	−17072.28107(3)	0.02394288711(3)
3.2	−0.6257322205584(4)	−1.1708440655(6)	−18179.96641(2)	0.02519386739(2)
3.3	−0.6231635846249(4)	−1.1602582484(5)	−18225.86703(7)	0.02608149117(2)
3.4	−0.6205353054470(3)	−1.1513262173(4)	−17821.377728(3)	0.02639540985(10)
3.5	−0.6178998751028(4)	−1.1439318849(4)	−17269.661854(8)	0.02624796150(9)
3.6	−0.6152967282451(4)	−1.1378255601(4)	−16697.509277(6)	0.02576886010(9)
3.7	−0.6127538693567(3)	−1.1328012594(4)	−16152.729663(2)	0.02505580523(10)
3.8	−0.6102910460896(7)	−1.1287067071(4)	−15650.077690(2)	0.02417773292(9)
3.9	−0.6079221733125(7)	−1.1254278466(4)	−15191.154752(3)	0.02318371795(9)
4.0	−0.6056569582833(4)	−1.1228749364(4)	−14772.920117(3)	0.02210974504(9)
4.1	−0.6035019745001(4)	−1.1209733679(5)	−14391.292694(3)	0.02098306856(10)
4.2	−0.6014613899225(4)	−1.1196582606(5)	−14042.58408(4)	0.01982488553(10)
4.3	−0.5995374858424(5)	−1.1188716598(5)	−13723.92770(4)	0.01865193298(2)
4.4	−0.5977310521263(4)	−1.1185614685(4)	−13433.212921(3)	0.01747741720(8)
4.5	−0.5960417114371(4)	−1.1186814890(4)	−13168.760951(3)	0.01631154084(8)
4.6	−0.5944682030351(5)	−1.1191920826(5)	−12928.868983(3)	0.01516180944(9)
4.7	−0.5930086414144(5)	−1.1200610255(5)	−12711.305882(3)	0.01403324625(9)
4.8	−0.5916607541314(4)	−1.1212642007(4)	−12512.823963(2)	0.01292860574(7)
4.9	−0.5904220958379(4)	−1.1227858419(4)	−12328.739052(3)	0.01184864281(7)
5.0	−0.5892902314439(7)	−1.1246181489(4)	−12152.617974(3)	0.01079246279(7)
5.1	−0.5882628801931(4)	−1.1267602111(4)	−11976.099054(3)	0.00975795085(8)
5.2	−0.5873380137133(4)	−1.1292162840(5)	−11788.859738(3)	0.00874225834(8)
5.3	−0.5865139039387(5)	−1.1319935504(5)	−11578.73887(4)	0.00774231272(8)
5.4	−0.5857891204283(4)	−1.1350995469(5)	−11332.019472(3)	0.00675531369(8)

5.5	−0.5851624802207(4)	−1.1385394660(5)	−11033.87841(4)	0.00577918080(8)
5.6	−0.5846329566579(5)	−1.1423135510(5)	−10669.00729(5)	0.00481292184(8)
5.7	−0.5841995563990(5)	−1.1464148011(5)	−10222.39864(6)	0.00385689679(8)
5.8	−0.5838611761462(4)	−1.1508272036(4)	−9680.27014(6)	0.00291295667(6)
5.9	−0.5836164523590(4)	−1.1555246898(4)	−9031.06840(8)	0.00198444322(6)
6.0	−0.5834636182075(4)	−1.1604709682(4)	−8266.45935(9)	0.00107604470(6)
6.5	−0.5839754830012(6)	−1.1871165857(5)	−2729.0483(2)	−0.00294855688(6)
7.0	−0.586185060781(4)	−1.2118054858(4)	4504.9753(3)	−0.00563362346(5)
7.5	−0.589360449965(3)	−1.2300537079(4)	11170.0920(3)	−0.00684437440(5)
8.0	−0.5928435588523(4)	−1.2412147840(5)	15842.1711(3)	−0.00694095828(5)
8.5	−0.5961889350444(4)	−1.2464217187(5)	18186.1148(3)	−0.00635809984(5)
9.0	−0.5991419650373(6)	−1.2469970250(6)	18360.2017(10)	−0.00541256610(5)
9.5	−0.6015725053126(3)	−1.2438992670(6)	16599.6753(6)	−0.00428992172(5)
10.0	−0.6034178991682(9)	−1.2376519768(2)	13076.6849(2)	−0.00308161784(10)
11.0	−0.6052418053477(10)	−1.2165864236(2)	1464.778(4)	−0.00055480117(2)
12.0	−0.604584452519(3)	−1.1877896058(3)	−12753.0032(4)	0.00178160826(3)
13.0	−0.601971058000(3)	−1.161453104(4)	−23148.262096(3)	0.00326838556(3)
14.0	−0.59836696457(3)	−1.1433253562(3)	−28149.5720(2)	0.00381489807(2)
15.0	−0.59451599673(3)	−1.1315674770(2)	−30108.1192(3)	0.00383096776(10)
16.0	−0.590775653672(8)	−1.1234807511(2)	−30815.7431(4)	0.00362940976(9)
17.0	−0.5872799639973(4)	−1.1174940194(2)	−31060.03132(4)	0.00335681815(9)
18.0	−0.584065109045(6)	−1.1128012291(2)	−31147.24941(3)	0.00307383272(9)
19.0	−0.581127641784(8)	−1.1089726541(2)	−31193.48965(3)	0.00280434892(8)
20.0	−0.578449007347(10)	−1.1057604593(2)	−31240.75347(3)	0.00255687776(6)

Table A4: Same as for Table A1, but for $5\,^1\Sigma_g^+$ (P state).

$5\,^1\Sigma_g$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.214825011937(6)	−1.446868730(5)	−1128.069013(2)	−1.453169580(5)
0.8	−0.336447866470(6)	−1.4818791811(3)	−1137.44945(7)	−1.0112293102(3)
0.9	−0.422012812363(6)	−1.4912671165(2)	−1147.15088(6)	−0.7191572131(2)
1.0	−0.483310990124(5)	−1.4854484798(2)	−1157.460417(3)	−0.5188264996(2)
1.1	−0.5279319108694(8)	−1.473741229(4)	710.0943(9)	−0.3798885520(3)
1.2	−0.5605424007861(6)	−1.4542957136(2)	848.4118(7)	−0.2776757600(2)
1.3	−0.5843622178747(6)	−1.4319177577(2)	1014.5891(6)	−0.2024564015(8)
1.4	−0.6016654973227(5)	−1.4081185075(9)	1215.4394(6)	−0.1462767949(6)
1.5	−0.6140732065665(4)	−1.3838768599(6)	1460.0711(5)	−0.1038202978(4)
1.6	−0.6227642582725(4)	−1.3598330956(6)	1760.9166(5)	−0.0714403619(4)
1.7	−0.6286111691169(3)	−1.3364100910(6)	2135.3438(4)	−0.04658103105(3)
1.8	−0.6322698001990(3)	−1.3138924899(4)	2608.28197(2)	−0.02741827196(2)
1.9	−0.6342403272876(3)	−1.2924821222(6)	3216.66519(5)	−0.01263235136(3)
2.0	−0.6349098149369(3)	−1.2723425412(8)	4017.2929(4)	−0.0012614557(4)
2.1	−0.6345830068397(4)	−1.2536453320(9)	5101.4406(5)	0.0073908008(4)
2.2	−0.6335059902414(3)	−1.23663808073(3)	6623.54064(2)	0.01380631807(2)
2.3	−0.6318868918692(3)	−1.2217787868(6)	8860.6709(5)	0.01825869435(3)
2.4	−0.6299193399927(4)	−1.2100571771(2)	12340.6768(10)	0.0207422929(6)
2.5	−0.6278206912406(7)	−1.203837342(4)	18102.7985(2)	0.0207216161(2)
2.6	−0.625911872660(3)	−1.208826448(7)	27932.5254(3)	0.0165374222(3)
2.7	−0.624738854739(3)	−1.233729376(9)	41831.8117(3)	0.0058327164(4)
2.8	−0.624751807635(3)	−1.261551772(7)	46630.75518(3)	−0.0043029129(3)
2.9	−0.624975673540(3)	−1.2417415006(2)	31581.0876(10)	0.0028309815(6)
3.0	−0.623922761636(2)	−1.19427276381(3)	15880.5293(6)	0.01785758648(2)
3.1	−0.6216245453716(6)	−1.15984710758(3)	8144.11562(4)	0.02690386553(2)
3.2	−0.6187230672375(4)	−1.13977971033(6)	4714.44880(2)	0.03052075754(5)
3.3	−0.6156002891964(4)	−1.12666084470(6)	2980.60180(2)	0.0316787071787(3)
3.4	−0.612422395299(3)	−1.11686308344(2)	1966.26030(6)	0.031759325633(2)
3.5	−0.6092659098249(4)	−1.10895989347(2)	1299.00384(4)	0.031306264621(3)
3.6	−0.6061710189119(4)	−1.10234996237(2)	816.49491(4)	0.03055335429(4)
3.7	−0.6031613460991(3)	−1.09674466781(2)	438.235748(2)	0.02961568227(4)
3.8	−0.6002518660529(3)	−1.09198427491(2)	119.778029(9)	0.02855775189(4)
3.9	−0.5974524429862(8)	−1.08796687633(2)	−165.6618206(2)	0.02742000247(4)
4.0	−0.5947695926241(4)	−1.08461835602(2)	−435.3590912(2)	0.02623020730(4)
4.1	−0.5922074489172(4)	−1.08187864191(2)	−700.979581(6)	0.025008842909(4)
4.2	−0.5897683425178(3)	−1.07969502425(2)	−970.533567(8)	0.023771823996(3)
4.3	−0.5874531756491(3)	−1.07801881210(2)	−1249.374589(8)	0.022531985859(3)
4.4	−0.5852616841720(3)	−1.07680369594(2)	−1540.70879(4)	0.021299925544(3)
4.5	−0.5831926345940(3)	−1.07600503748(2)	−1845.85614(4)	0.020084495935(3)
4.6	−0.5812439822480(3)	−1.07557967182(2)	−2164.40079(5)	0.018893107104(3)
4.7	−0.5794130051332(3)	−1.07548597294(2)	−2494.31355(5)	0.017731922834(2)
4.8	−0.5776964210463(3)	−1.07568401801(2)	−2832.09671(5)	0.016606005017(2)
4.9	−0.5760904915140(3)	−1.07613574171(2)	−3172.97764(6)	0.015519437003(2)
5.0	−0.5745911137275(3)	−1.07680501844(10)	−3511.15950(6)	0.014475441802(2)
5.1	−0.5731939006859(3)	−1.07765765276(9)	−3840.12323(6)	0.013476499727(2)
5.2	−0.5718942497096(3)	−1.07866129501(8)	−4152.96640(6)	0.012524462385(2)
5.3	−0.5706874000329(3)	−1.07978532482(7)	−4442.75987(6)	0.011620655706(9)
5.4	−0.5695684809826(4)	−1.08100075657(10)	−4702.90265(8)	0.010765963961(2)

5.5	−0.5685325529706(3)	−1.08228021793(9)	−4927.45687(7)	0.009960888729(9)
5.6	−0.5675746439538(3)	−1.08359803660(7)	−5111.44673(7)	0.009205580590(7)
5.7	−0.5666897840122(3)	−1.08493044676(5)	−5251.10695(6)	0.008499845835(4)
5.8	−0.5658730402471(7)	−1.08625589921(5)	−5344.0672(5)	0.007843134702(2)
5.9	−0.5651195533912(6)	−1.087555434369(2)	−5389.4600(5)	0.007234520746(3)
6.0	−0.5644245764650(6)	−1.08881305906(7)	−5387.9426(4)	0.006672682309(3)
6.5	−0.5616739737967(3)	−1.09414794218(2)	−4790.67399(2)	0.004492308525(3)
7.0	−0.55979990393723(8)	−1.09785862048(8)	−3682.070482(4)	0.003105883914(2)
7.5	−0.55849146009284(10)	−1.10059902066(2)	−2607.46464(4)	0.002184519936(3)
8.0	−0.5575714025143(3)	−1.10289688216(3)	−1772.889535(2)	0.001530740358(4)
8.5	−0.5569311006019(4)	−1.1048863731(4)	−1180.36791(5)	0.00105597977(4)
9.0	−0.5564929932563(4)	−1.10654093092(3)	−782.01696(2)	0.000716117289(3)
9.5	−0.55619780366792(3)	−1.107840676607(2)	−530.1853(2)	0.0004794663925(9)
10.0	−0.5560008468956(3)	−1.10881118102(10)	−383.35291(3)	0.000319051277(7)
11.0	−0.5557822060354(2)	−1.109993925848(3)	−267.10242(3)	0.0001427714746(2)
12.0	−0.55568225651432(4)	−1.110552136110(9)	−232.2373(2)	0.00006769807650(3)
13.0	−0.55563296951838(4)	−1.1108081704843(2)	−199.98734(2)	0.0000352129655(6)
14.0	−0.55560616167762(6)	−1.1109295754325(3)	−160.99747(5)	0.0000201962802(5)
15.0	−0.555590181110912(4)	−1.1109921111333(2)	−120.411313(2)	0.00001255007257(2)
16.0	−0.555579970036133(3)	−1.1110279581786(2)	−81.403167(2)	0.00000824886835(10)
17.0	−0.555573133690222(6)	−1.1110506535398(7)	−45.20336(4)	0.00000562434356(6)
18.0	−0.555568415321604(5)	−1.11106610287036(4)	−12.46971(4)	0.00000392932071(4)
19.0	−0.555565090350473(3)	−1.11107710345113(4)	16.309992(8)	0.00000279353946(4)
20.0	−0.555562710376694(3)	−1.11108514211306(9)	40.842073(4)	0.000002013932016(9)

Table A5: Same as for Table A1, but for $6\,^1\Sigma_g^+$ (O state).

$6\,^1\Sigma_g$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.2140023255092(10)	−1.447060963(5)	348.13537(5)	−1.455794731(5)
0.8	−0.335886648909(4)	−1.4828385094(10)	416.30256(5)	−1.0138315145(7)
0.9	−0.421710285628(3)	−1.492975713(9)	497.61987(8)	−0.721727935(6)
1.0	−0.4832638187068(7)	−1.4878903613(3)	594.60102(2)	−0.5213627240(2)
1.1	−0.527727162319(3)	−1.4705789519(2)	−1168.387049(3)	−0.3773860249(8)
1.2	−0.560088946762(6)	−1.4504219471(8)	−1180.586191(3)	−0.2752033779(5)
1.3	−0.5836627941815(6)	−1.4273362518(6)	−1194.326597(3)	−0.2000082026(4)
1.4	−0.6007221252391(5)	−1.4028264348(4)	−1210.119611(3)	−0.14384441743(3)
1.5	−0.6128869361008(4)	−1.3778627341(4)	−1228.601786(3)	−0.10139257461(3)
1.6	−0.6213348479302(9)	−1.3530735889(4)	−1250.590504(3)	−0.06900243318(2)
1.7	−0.6269366445923(5)	−1.3288649806(4)	−1277.16052(4)	−0.04411275967(2)
1.8	−0.6303458026835(4)	−1.3054963403(4)	−1309.76151(5)	−0.02489151942(2)
1.9	−0.6320590985397(5)	−1.2831300426(5)	−1350.40592(2)	−0.01000623449(3)
2.0	−0.6324585378241(6)	−1.2618646272(5)	−1401.98165(7)	0.00152622419(2)
2.1	−0.6318409488065(9)	−1.2417581726(4)	−1468.79744(8)	0.01043986905(2)
2.2	−0.6304392880171(4)	−1.2228464512(4)	−1557.58894(9)	0.01728732944(2)
2.3	−0.6284383466653(4)	−1.20516036312(3)	−1679.49918(10)	0.02248536096(9)
2.4	−0.6259867808868(4)	−1.18874955964(2)	−1854.28969(2)	0.026343334224(3)
2.5	−0.6232071194652(4)	−1.17372769826(9)	−2120.11066(2)	0.02907461627(6)
2.6	−0.6202058060270(3)	−1.1603783884(4)	−2558.11937(2)	0.03078200908(2)
2.7	−0.6170867051963(2)	−1.1493871113(4)	−3354.15059(5)	0.03140233300(2)
2.8	−0.6139682424895(9)	−1.1418029285(2)	−4869.61025(3)	0.0307619845(7)
2.9	−0.6109513005079(10)	−1.135806050(6)	−7072.1557(2)	0.0296884659(2)
3.0	−0.607984520050(3)	−1.126420436(4)	−8582.8151(2)	0.0298495347(2)
3.1	−0.604965579196(3)	−1.1153447518(3)	−8955.9046(7)	0.0305117441(7)
3.2	−0.601893387552(3)	−1.1050278308(3)	−8782.91507(3)	0.0308621701(6)
3.3	−0.598806494758(3)	−1.0959208478(2)	−8443.033329(3)	0.0308158005(6)
3.4	−0.595740596378(3)	−1.0879243374(2)	−8079.47850(6)	0.0304578986(5)
3.5	−0.592722480238(3)	−1.0808920625(2)	−7737.68105(2)	0.0298722566(5)
3.6	−0.589771654136(2)	−1.0747085622(5)	−7427.97389(3)	0.02912076279(9)
3.7	−0.5869023630600(8)	−1.0692877991(2)	−7148.69784(2)	0.0282478181(4)
3.8	−0.584125047623(2)	−1.0645636900(2)	−6894.53835(2)	0.0272858961(4)
3.9	−0.581447330977(3)	−1.0604831054(10)	−6659.51149(3)	0.02625937347(2)
4.0	−0.57887469933(8)	−1.0570017204(2)	−6437.95935(2)	0.0251869195(4)
4.1	−0.576410993974(2)	−1.0540819070(2)	−6224.76808(2)	0.0240829466(4)
4.2	−0.574058790625(3)	−1.0516920596(2)	−6015.24808(2)	0.0229584575(4)
4.3	−0.571819715484(3)	−1.0498070470(2)	−5804.82165(3)	0.0218214846(4)
4.4	−0.569694733503(2)	−1.0484097007(3)	−5588.54150(3)	0.0206772196(5)
4.5	−0.56768443716(4)	−1.0474934357(3)	−5360.39985(3)	0.0195278753(5)
4.6	−0.565789362518(3)	−1.0470662675(3)	−5112.3378(4)	0.0183722734(5)
4.7	−0.564010361903(3)	−1.0471566759(3)	−4832.8058(4)	0.0172051166(5)
4.8	−0.562349067676(3)	−1.0478218971(3)	−4504.6555(5)	0.0160158830(6)
4.9	−0.560808486465(3)	−1.0491590327(3)	−4102.0885(6)	0.0147873347(6)
5.0	−0.559393752871(3)	−1.0513179487(3)	−3586.5027(6)	0.0134939114(6)
5.1	−0.558113008001(3)	−1.0545100991(3)	−2901.7943(7)	0.0121011602(5)
5.2	−0.556978160367(3)	−1.0589951360(3)	−1972.0328(7)	0.0105694586(4)
5.3	−0.556004801071(3)	−1.0650064400(2)	−709.5929(7)	0.00886852115(3)
5.4	−0.555209840020(3)	−1.0725720624(2)	953.0760(6)	0.00700881807(2)

5.5	−0.554605475403(3)	−1.0812769350(5)	3005.9217(6)	0.00507891196(4)
5.6	−0.554190874544(3)	−1.09021079696(10)	5319.0336(5)	0.00324481287(6)
5.7	−0.553947456853(3)	−1.0983220835(4)	7679.2558(4)	0.00167944391(2)
5.8	−0.553842750631(3)	−1.104915243(8)	9888.811(4)	0.0004776308(2)
5.9	−0.553839824993(9)	−1.109820887(7)	11831.144(4)	−0.0003629215(2)
6.0	−0.553905281146(8)	−1.113223998(6)	13467.5914(3)	−0.0009022394(2)
6.5	−0.554556616403(4)	−1.1175915290(3)	17691.0988(4)	−0.0013043533(4)
7.0	−0.555073152157(3)	−1.1154348240(3)	17786.2713(2)	−0.0007555028(4)
7.5	−0.5553414869869(8)	−1.1133586067(8)	16405.1373(2)	−0.00035675103(2)
8.0	−0.55546300074328(6)	−1.11216169918(6)	14914.12107(2)	−0.000154462212(9)
8.5	−0.55551399017277(3)	−1.111553350993(3)	13723.22959(2)	−0.0000618083115(3)
9.0	−0.55553330298143(3)	−1.111256525328(6)	12854.91704(2)	−0.0000211021517(10)
9.5	−0.555538968714818(10)	−1.1111171783779(10)	12236.96221(2)	−0.00000413062615(2)
10.0	−0.555539184914083(8)	−1.1110572093276(3)	11793.72905(10)	0.00000211605005(8)
11.0	−0.555535862495673(7)	−1.1110363004284(3)	11207.58017(2)	0.00000322041481(2)
12.0	−0.555533720966736(6)	−1.1110553198214(3)	10802.20476(2)	0.00000101017599(2)
13.0	−0.555533653499766(4)	−1.1110767173675(2)	10469.48894(2)	−0.00000072387446(10)
14.0	−0.555534879773837(4)	−1.1110922534158(2)	10186.62617(3)	−0.00000160670487(7)
15.0	−0.555536678642624(3)	−1.1111021931463(2)	9948.35830(3)	−0.00000192239074(10)
16.0	−0.555538626624646(6)	−1.1111082986232(2)	9748.605212(2)	−0.00000194033587(8)
17.0	−0.555540514441146(5)	−1.1111119880602(2)	9580.608406(3)	−0.00000182112812(9)
18.0	−0.555542251438849(3)	−1.1111141712876(3)	9438.41174(2)	−0.00000164824500(2)
19.0	−0.555543806971529(3)	−1.1111154071109(2)	9317.151075(3)	−0.00000146279831(9)
20.0	−0.555545179435428(5)	−1.111116042982(4)	9212.79951(3)	−0.00000128420558(2)

Table A6: Same as for Table A1, but for $7\,^1\Sigma_g^+$.

$7\,^1\Sigma_g$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.2031026226(6)	−1.42423571(10)	−573.831(2)	−1.45432924(3)
0.8	−0.3248398062(3)	−1.45956368(8)	−579.961(9)	−1.01235509(2)
0.9	−0.41051540490(10)	−1.46925028(6)	−586.267(5)	−0.72024386(9)
1.0	−0.471920166180(4)	−1.46371156(5)	−592.9663(3)	−0.51987123(6)
1.1	−0.516552689791(9)	−1.45074580(7)	392.3021(2)	−0.37967311(5)
1.2	−0.549140355703(5)	−1.431201867(4)	468.8865(8)	−0.277434296(2)
1.3	−0.572934607636(4)	−1.408711037(6)	561.1010(3)	−0.202186016(4)
1.4	−0.590209251251(4)	−1.384781765(5)	672.8757(3)	−0.1459737589(3)
1.5	−0.602584827761(4)	−1.360389288(6)	809.508(4)	−0.103479755(4)
1.6	−0.611239689956(3)	−1.336168788(5)	978.3016(3)	−0.0710558798(3)
1.7	−0.617045605402(3)	−1.3125358749(3)	1189.5858(2)	−0.0461439201(2)
1.8	−0.620657411113(3)	−1.2897645568(2)	1458.4062(10)	−0.0269165192(9)
1.9	−0.622573847780(8)	−1.2680406209(3)	1807.45684(3)	−0.0120489081(2)
2.0	−0.6231799116910(8)	−1.2475026265(2)	2272.41926(3)	−0.0005714016(7)
2.1	−0.6227772716351(9)	−1.2282818749(3)	2912.2405(10)	0.0082250802(10)
2.2	−0.621607292156(5)	−1.210558992(2)	3830.191(8)	0.014843451(5)
2.3	−0.619870632378(3)	−1.194678933(7)	5219.785(5)	0.0195923179(3)
2.4	−0.617748981607(4)	−1.181447401(2)	7468.460(7)	0.022521068(6)
2.5	−0.615441450167(7)	−1.172978873(4)	11360.395(2)	0.023161611(2)
2.6	−0.613242851054(5)	−1.17450279(4)	17917.683(2)	0.019993425(2)
2.7	−0.611586970844(9)	−1.18772948(4)	23235.617(4)	0.013127579(2)
2.8	−0.610297993373(7)	−1.178114305(2)	15179.301(6)	0.015172029(4)
2.9	−0.608278117747(3)	−1.1438001600(2)	5680.5679(3)	0.0250883019(7)
3.0	−0.605439878414(3)	−1.1184652151(10)	2239.2655(7)	0.0308048472(5)
3.1	−0.602241084513(3)	−1.10285087526(4)	1055.5034(4)	0.03278428830(2)
3.2	−0.5989321193027(7)	−1.09149129967(2)	506.03302(2)	0.033241543409(2)
3.3	−0.595613919087(3)	−1.0821678974(5)	183.76196(2)	0.03304846691(7)
3.4	−0.5923336213943(9)	−1.0741181428(6)	−37.19408(8)	0.03251444117(2)
3.5	−0.5891179785881(9)	−1.0670405514(7)	−207.281485(3)	0.03177011595(2)
3.6	−0.5859843372776(9)	−1.0607905638(7)	−351.022338(2)	0.03088280854(2)
3.7	−0.5829448102751(9)	−1.0552844528(7)	−482.20022(5)	0.02989328858(2)
3.8	−0.5800081565592(8)	−1.0504652779(6)	−609.51946(8)	0.02882921980(2)
3.9	−0.577180773207(3)	−1.0462894731(6)	−739.02208(10)	0.02771078803(2)
4.0	−0.574467295342(5)	−1.0427211849(6)	−875.21041(2)	0.02655335143(10)
4.1	−0.5718710037173(3)	−1.0397299242(5)	−1021.57913(2)	0.02536880079(7)
4.2	−0.5693941315781(9)	−1.03728989002(4)	−1180.83964(3)	0.02416627932(5)
4.3	−0.5670381196229(7)	−1.03538036764(3)	−1354.95571(3)	0.022952528276(3)
4.4	−0.5648038502497(6)	−1.03398705128(2)	−1545.03295(3)	0.0217319657286(3)
4.5	−0.5626918857718(6)	−1.033104389670(4)	−1751.05597(3)	0.020506529303(3)
4.6	−0.5607027344729(5)	−1.03273921349(2)	−1971.41706(4)	0.01927527292(6)
4.7	−0.5588371702268(4)	−1.03291596360(4)	−2202.11318(4)	0.01803369720(8)
4.8	−0.5570966311693(5)	−1.0336835368(7)	−2435.3960(5)	0.01677285950(2)
4.9	−0.5554837063283(4)	−1.0351222071(9)	−2657.5941(4)	0.01547861337(2)
5.0	−0.5540026439204(3)	−1.0373437765(9)	−2846.05031(3)	0.01413230227(2)
5.1	−0.55265957458651(6)	−1.0404638530(5)	−2966.56157(2)	0.01271672474(9)
5.2	−0.55146155735337(6)	−1.0444992752(8)	−2977.43238(10)	0.01123535377(2)
5.3	−0.55041270870657(8)	−1.0491435623(2)	−2854.11122(2)	0.00975129341(3)
5.4	−0.5495062620854(3)	−1.0535437061(3)	−2640.22115(2)	0.0084201515(5)

5.5	−0.5487170366306(6)	−1.056548167(5)	−2470.50230(2)	0.0074338012(9)
5.6	−0.5480053893565(10)	−1.057574228(7)	−2481.95461(2)	0.0068636697(2)
5.7	−0.547334145102(3)	−1.057070595(8)	−2695.29800(2)	0.0065960868(2)
5.8	−0.546682226458(10)	−1.05595920(5)	−3027.9683(2)	0.006449181(7)
5.9	−0.54604464395(3)	−1.05494922(5)	−3386.0914(2)	0.006294926(7)
6.0	−0.54542528537(3)	−1.05436549(5)	−3713.0481(2)	0.006080848(7)
6.5	−0.54280070269(8)	−1.05777255(4)	−4552.8052(8)	0.004281362(6)
7.0	−0.54116677292(6)	−1.06616160(9)	−4348.19327(3)	0.002310277(2)
7.5	−0.54038904522(6)	−1.07382269(8)	−3616.80239(2)	0.000927387(9)
8.0	−0.54011786873(6)	−1.07816661(8)	−2998.6294(5)	0.000258641(8)
8.5	−0.54005763377(5)	−1.07987458(7)	−2738.3292(2)	0.000028315(7)
9.0	−0.54006342978(6)	−1.08048970(8)	−2736.7381(5)	−0.000040316(8)
9.5	−0.54009573505(4)	−1.081072848(3)	−2851.6811(5)	−0.0000927767(3)
10.0	−0.54016320644(4)	−1.08218587(5)	−2988.5688(4)	−0.000185945(4)
11.0	−0.54050682923(3)	−1.086909539(2)	−3114.5765(8)	−0.0005359892(2)
12.0	−0.54128587390(7)	−1.094985938(2)	−2794.1781(9)	−0.0010345159(2)
13.0	−0.54256837260(8)	−1.104773689(2)	−1852.2200(2)	−0.0015105341(2)
14.0	−0.54424234119(7)	−1.11364734(8)	−418.493(7)	−0.001797333(5)
15.0	−0.54608200238(6)	−1.11983837(6)	1148.292(5)	−0.001844958(4)
16.0	−0.5478719741(2)	−1.123143053(2)	2557.539(6)	−0.0017124441(6)
17.0	−0.54947612547(2)	−1.124227347(2)	3701.444(7)	−0.0014867704(6)
18.0	−0.55083688454(3)	−1.123889734(2)	4591.419(7)	−0.0012342203(6)
19.0	−0.55194855463(4)	−1.122763246(2)	5280.213(10)	−0.0009929546(8)
20.0	−0.55283256492(2)	−1.121277346(10)	5821.9371(3)	−0.0007806108(5)

Table A7: Same as for Table A1, but for $1\,^3\Sigma_g^+$ (a state).

$1\,^3\Sigma_g$				
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.342130928988667(7)	−1.684967556748(2)	−8221.97341966(2)	−1.429579569672(2)
0.8	−0.46143498347982(5)	−1.713637952269(8)	−8362.94950851(7)	−0.988459981637(2)
0.9	−0.544767040091894(4)	−1.717081581176(6)	−8504.450049312(2)	−0.697275001103(7)
1.0	−0.60392224803181505(5)	−1.705694057556(5)	−8646.495425121(2)	−0.497849561492(5)
1.1	−0.6462856755609065(3)	−1.685606748317(4)	−8789.318391880(3)	−0.357304906541(4)
1.2	−0.67668314180341571(7)	−1.6605580283312(2)	−8933.28743229(4)	−0.2559931206037(2)
1.3	−0.69837814548896884(4)	−1.632882613728(8)	−9078.86039579(3)	−0.181635632885(7)
1.4	−0.7136405684873686(4)	−1.6040626138235(2)	−9226.55604555(7)	−0.1262724834634(2)
1.5	−0.7240866205382896(4)	−1.575047623789(6)	−9376.93643894(3)	−0.084582921808(4)
1.6	−0.730890086928356(6)	−1.546447174066(7)	−9530.59598146(2)	−0.052916875131(5)
1.7	−0.734917974883440(2)	−1.5186497972592(2)	−9688.1546413(7)	−0.0287140279367(8)
1.8	−0.736820091741595(8)	−1.49189848327(5)	−9850.253767(2)	−0.010143499884(2)
1.9	−0.7370896537668271(2)	−1.4663394723671(3)	−10017.55353143(2)	0.0041262290350(2)
2.0	−0.7361051733454439(4)	−1.4420543471316(5)	−10190.7313291(2)	0.0150779997796(2)
2.1	−0.7341599538590402(6)	−1.41908144023(5)	−10370.48075063(7)	0.023446889282(3)
2.2	−0.7314832061423001(6)	−1.397430280530(8)	−10557.5107906(2)	0.029789150798(5)
2.3	−0.7282553924169136(8)	−1.3770914298961(2)	−10752.5451159(2)	0.0345301543207(7)
2.4	−0.724619525233251(3)	−1.35804322450(6)	−10956.3212378(8)	0.037998260818(3)
2.5	−0.720689588359196(5)	−1.34025641143(2)	−11169.5894849(6)	0.04044910612(5)
2.6	−0.71655688134612(2)	−1.32369733771(2)	−11393.1117060(4)	0.04208324038(6)
2.7	−0.712294847112937(2)	−1.30833013350(5)	−11627.6596546(3)	0.043059096565(2)
2.8	−0.707962778269134(5)	−1.29411818877(10)	−11874.0130389(3)	0.04350263134(4)
2.9	−0.703608685724174(5)	−1.28102512808(9)	−12132.9572405(3)	0.04351456668(4)
3.0	−0.699271535123230(3)	−1.269015423838(7)	−12405.280740(10)	0.0431758821360(2)
3.1	−0.694983001681094(7)	−1.25805474389(6)	−12691.772315(3)	0.042552019183(2)
3.2	−0.6907688547753517(9)	−1.248110098883(2)	−12993.218114(2)	0.04169612833342(3)
3.3	−0.6866500553689703(7)	−1.23914983267(4)	−13310.398728(2)	0.040651599416(6)
3.4	−0.68264362870430 45(10)	−1.23114348419(4)	−13644.086422(2)	0.039454050946(6)
3.5	−0.6787633595262160(6)	−1.22406153835(5)	−13995.042683(5)	0.038132908773(3)
3.6	−0.675020345825230(3)	−1.21787507632(4)	−14364.016212(3)	0.036712670927(5)
3.7	−0.6714234386847724(9)	−1.21255533240(6)	−14751.741424(3)	0.035213931072(8)
3.8	−0.6679795895349028(10)	−1.208073163407(2)	−15158.937380(3)	0.0336542146479(3)
3.9	−0.66469412144608(3)	−1.20439843936(8)	−15586.30683(5)	0.032048667573(2)
4.0	−0.661570937686215(3)	−1.20149937039(7)	−16034.53475(5)	0.030410626247(8)
4.1	−0.658612678362044(3)	−1.19934179403(5)	−16504.285341(2)	0.028752088462(3)
4.2	−0.655820834391176(4)	−1.19788845990(4)	−16996.195926(3)	0.027084097352(3)
4.3	−0.653195827155049(9)	−1.197098363415(2)	−17510.86593(4)	0.025417044394(2)
4.4	−0.65073706182336(3)	−1.19692619478(3)	−18048.83873(5)	0.02376089291(2)
4.5	−0.6484429623517(5)	−1.197321980995(3)	−18610.57430(6)	0.022125320824(10)
4.6	−0.6463109963342(5)	−1.19823100232(6)	−19196.41159(8)	0.020519780509(4)
4.7	−0.644337697996883(4)	−1.19959405664(10)	−19806.52038(10)	0.0189534764592(3)
4.8	−0.6425186973868(10)	−1.20134812213(2)	−20440.84514(2)	0.017435265134(2)
4.9	−0.6408487629943(2)	−1.20342743014(2)	−21099.04542(2)	0.015973488947(2)
5.0	−0.639321863500910(10)	−1.20576490884(4)	−21780.43994(3)	0.01457576363(5)
5.1	−0.63793125205253(2)	−1.2082939037(4)	−22483.96317(3)	0.01324874519(4)
5.2	−0.63666957360658(2)	−1.2109500327(5)	−23208.14328(3)	0.01199790663(6)
5.3	−0.635528992850(2)	−1.2136730066(6)	−23951.1086(4)	0.01082735454(7)
5.4	−0.63450133739944(2)	−1.2164082391(7)	−24710.6264(5)	0.00973971031(9)

5.5	−0.63357824894624(4)	−1.2191081030(8)	−25484.1723(6)	0.00873607178(2)
5.6	−0.6327513339942(7)	−1.2217327356(10)	−26269.0256(6)	0.00781605935(2)
5.7	−0.6320123060258(6)	−1.2242503580(2)	−27062.3803(8)	0.00697793930(2)
5.8	−0.6313531121181(2)	−1.2266371369(2)	−27861.4608(9)	0.00621880815(3)
5.9	−0.63076603896819(3)	−1.2288766615(2)	−28663.6309(10)	0.00553481634(3)
6.0	−0.63024379552804(3)	−1.23095913917(6)	−29466.48802(2)	0.004921408649(8)
6.5	−0.6283849655891246(10)	−1.2390110259897(9)	−33430.525107(7)	0.00273213925977(2)
7.0	−0.627343969517241(4)	−1.243799572991(2)	−37251.58960(8)	0.0015554808632(3)
7.5	−0.6267388331983872(6)	−1.2465060235609(8)	−40988.908399(6)	0.00092955237812(9)
8.0	−0.6263678024076574(10)	−1.248035496746(2)	−44792.39099(3)	0.0005875135087(3)
8.5	−0.626127410224462(3)	−1.248930190624(2)	−48825.17746(2)	0.0003911329205(2)
9.0	−0.6259640651384734(10)	−1.249484822983(10)	−53205.33483(6)	0.0002714785882(10)
9.5	−0.625848897568859(3)	−1.2498492915111(7)	−57938.66742(5)	0.00019457932912(7)
10.0	−0.625765155314512(3)	−1.2500909629370(2)	−62842.86269(2)	0.0001439347692(5)
11.0	−0.625651263865481(2)	−1.2502789583653(3)	−71504.08597(6)	0.00009305176051(2)
12.0	−0.625565960913511(6)	−1.2501556386917(2)	−76365.63521(6)	0.00008135692794(2)
13.0	−0.625485558864006(3)	−1.2499400391390(2)	−77981.77830(6)	0.00007931373762(6)
14.0	−0.6254088253710753(8)	−1.24979193092672(3)	−78266.14296(4)	0.000073265701102(5)
15.0	−0.6253403831152288(5)	−1.249732537596432(3)	−78227.30909(5)	0.000063215242268(6)
16.0	−0.6252826990251769(6)	−1.24973015278010(5)	−78164.21351(4)	0.000052202829391(7)
17.0	−0.62523562891080(3)	−1.24975399344689(2)	−78127.18911(4)	0.000042192022042(10)
18.0	−0.6251977430164360(3)	−1.24978573484174(5)	−78109.748539(3)	0.000033875066174(4)
19.0	−0.6251673111090794(3)	−1.24981680625318(6)	−78101.313249(2)	0.000027253471841(4)
20.0	−0.6251427558519418(2)	−1.249844080178546(3)	−78095.991640(2)	0.0000220715762669(2)

Table A8: Same as for Table A1, but for $2\,^3\Sigma_g^+$ (h state).

		$2\,^3\Sigma_g$		
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.2472644426042(5)	−1.508591821293(3)	−2223.996593(2)	−1.44866133727(2)
0.8	−0.36844181348963(9)	−1.542348734490(2)	−2286.178846(6)	−1.006831384389(2)
0.9	−0.45357315052141(3)	−1.550542429225(3)	−2349.4423343(2)	−0.714884586870(2)
1.0	−0.51445061587705(3)	−1.543586639649(3)	−2413.7914678(3)	−0.514685407895(2)
1.1	−0.558459323262524(4)	−1.52763415794(4)	−2479.33920046(3)	−0.373377737650(3)
1.2	−0.590426867896656(10)	−1.506445557816(2)	−2546.2807505(7)	−0.271326518352(2)
1.3	−0.613619506234056(5)	−1.482377683548(9)	−2614.8720080(8)	−0.196260516215(6)
1.4	−0.630310459796666(3)	−1.456935234569(6)	−2685.3854072(7)	−0.140224510697(4)
1.5	−0.642119737089215(5)	−1.431093609378(7)	−2757.9483347(10)	−0.097902756800(4)
1.6	−0.650225634282811(8)	−1.405500555971(2)	−2831.8353339(2)	−0.065655804628(7)
1.7	−0.655501642316257(5)	−1.380631447839(4)	−2901.7680511(2)	−0.040957743063(2)
1.8	−0.658611819722805(9)	−1.357061916457(2)	−2931.9295740(2)	−0.022132376117(8)
1.9	−0.660107400109173(10)	−1.336938465676(2)	−2614.4783071(5)	−0.008801929188(8)
2.0	−0.660567972914286(9)	−1.322621705762(2)	−1451.2091995(3)	−0.000742879967(5)
2.1	−0.660250897704916(7)	−1.305844067405(2)	−1069.0484489(3)	0.006979870479(6)
2.2	−0.659216201994195(8)	−1.288829863122(2)	−1092.8270950(2)	0.013455700394(6)
2.3	−0.657609692818079(7)	−1.272803111293(2)	−1242.4122766(2)	0.018441858410(6)
2.4	−0.655570311845531(7)	−1.257973017408(2)	−1466.7685624(2)	0.022153169285(6)
2.5	−0.65321394290149(6)	−1.244386304349(2)	−1758.0144672(2)	0.024816632581(5)
2.6	−0.65063552709149(3)	−1.23205227859(4)	−2120.028438(5)	0.026622605997(2)
2.7	−0.64791284889068(3)	−1.22096886799(4)	−2561.554468(5)	0.027724751775(2)
2.8	−0.645109902827123(10)	−1.21113012448(4)	−3094.178559(5)	0.028246314707(2)
2.9	−0.642279614139089(10)	−1.202528642830(4)	−3731.520483(5)	0.028286408775(10)
3.0	−0.639465977332637(8)	−1.195155945719(2)	−4488.7085212(9)	0.027925336315(5)
3.1	−0.63670571216767(3)	−1.18900169605(5)	−5381.815495(6)	0.027228944607(2)
3.2	−0.63402952500903(3)	−1.18405203596(5)	−6427.106878(6)	0.026252191893(2)
3.3	−0.631463046232689(9)	−1.180287218422(3)	−7640.0208279(2)	0.025042083044(6)
3.4	−0.629027500845529(9)	−1.177678720454(3)	−9033.8522729(2)	0.023640082717(7)
3.5	−0.626740161589626(10)	−1.176186125791(3)	−10618.1758616(8)	0.022084056397(7)
3.6	−0.624614631336522(10)	−1.175754197096(2)	−12397.12135707(3)	0.020409740438(5)
3.7	−0.62266100321433(3)	−1.176310675374(3)	−14367.7007975(5)	0.018651711096(6)
3.8	−0.62088595035570(3)	−1.17776538888(6)	−16518.456917(5)	0.016843818905(2)
3.9	−0.61929279931485(4)	−1.18001116913(6)	−18828.726532(5)	0.015019084485(2)
4.0	−0.61788163880669(3)	−1.182926830552(3)	−21268.7643419(3)	0.013209111765(7)
4.1	−0.61664950609552(3)	−1.186382097952(3)	−23800.8451636(3)	0.011443149814(7)
4.2	−0.61559067676645(3)	−1.190243953054(3)	−26381.280056(4)	0.009747000114(7)
4.3	−0.61469706202116(3)	−1.194383538354(4)	−28963.095733(6)	0.008141996672(7)
4.4	−0.61395869544520(3)	−1.198682617060(3)	−31498.996761(6)	0.006644266780(6)
4.5	−0.61336427341449(3)	−1.203038685555(3)	−33944.197032(8)	0.005264413616(6)
4.6	−0.61290170375755(3)	−1.207368133492(3)	−36258.774522(10)	0.004007668266(6)
4.7	−0.61255861730502(3)	−1.211607246315(3)	−38409.338865(2)	0.002874465595(6)
4.8	−0.61232280524364(4)	−1.215711230223(3)	−40369.954524(10)	0.001861329222(6)
4.9	−0.61218255865255(5)	−1.219651722268(3)	−42122.388209(2)	0.000961917355(5)
5.0	−0.61212690161203(3)	−1.223413389749(3)	−43655.823426(2)	0.000168082695(5)
5.1	−0.61214572276421(5)	−1.226990229422(3)	−44966.206636(2)	−0.000529173313(5)
5.2	−0.61222982021667(5)	−1.230382082446(3)	−46055.373200(3)	−0.001138931156(5)
5.3	−0.61237088044463(6)	−1.233591728667(3)	−46930.067207(3)	−0.001669805241(5)
5.4	−0.612561413542328(7)	−1.236622753762(3)	−47600.933901(3)	−0.002129616051(4)

5.5	−0.612794665583829(9)	−1.239478226302(3)	−48081.536248(3)	−0.002525253661(4)
5.6	−0.613064525058694(7)	−1.242160099716(3)	−48387.43013(4)	−0.002862687428(4)
5.7	−0.613365435474786(6)	−1.244669177108(3)	−48535.32345(4)	−0.003147071256(4)
5.8	−0.613692321260887(6)	−1.247005445530(2)	−48542.33878(5)	−0.0033828970703(4)
5.9	−0.614040529789983(6)	−1.249168593768(2)	−48425.39408(5)	−0.0035741583370(3)
6.0	−0.61440578910524(6)	−1.251158561535(2)	−48200.70944(5)	−0.0037244972208(3)
6.5	−0.616362022343828(3)	−1.258574472688(7)	−45943.385563(9)	−0.0039769889231(10)
7.0	−0.6182895759240(9)	−1.262253378187(6)	−42669.509615(2)	−0.0036677466199(7)
7.5	−0.6199870919219(8)	−1.2632147602742(8)	−38979.491515(7)	−0.0030987435241(7)
8.0	−0.6213785081438(4)	−1.262498850257(4)	−35024.92851(5)	−0.0024677292462(5)
8.5	−0.62246238897501(3)	−1.2609057936315(4)	−30773.74760(6)	−0.00188011949194(4)
9.0	−0.6232734542866(2)	−1.2589703967490(3)	−26164.81291(6)	−0.00138038757510(3)
9.5	−0.6238593009777(6)	−1.2570219144576(2)	−21217.05458(5)	−0.00097929605286(2)
10.0	−0.62426832745319(4)	−1.2552513542959(2)	−16122.89771(4)	−0.00067146993895(2)
11.0	−0.62472449687396(4)	−1.2525906023479(10)	−7163.75867(4)	−0.00028560078182(8)
12.0	−0.62490922800235(3)	−1.2511283967020(6)	−2102.035093(3)	−0.00010916172477(5)
13.0	−0.624977636045535(5)	−1.2504592957763(8)	−358.197574(3)	−0.00003877105272(6)
14.0	−0.625001000657470(5)	−1.2501737150160(5)	5.943015(3)	−0.000012265264356(3)
15.0	−0.625007604725696(3)	−1.25005396037364(4)	17.494828(2)	−0.000002583394816(2)
16.0	−0.625008244306664(3)	−1.25000564516774(3)	−12.452819(2)	0.000000677715349(2)
17.0	−0.6250070343963621(3)	−1.24998837760918(2)	−26.307626(2)	0.000001511246091(10)
18.0	−0.6250054985429428(4)	−1.24998425324141(2)	−26.483327(2)	0.000001485769137(7)
19.0	−0.6250041409427775(4)	−1.24998521093635(10)	−21.348868(2)	0.000001214260484(5)
20.0	−0.6250030754316002(3)	−1.24998771479535(9)	−15.599054(2)	0.000000921803392(4)

Table A9: Same as for Table A1, but for $3\,^3\Sigma_g^+$ (g state).

$3\,^3\Sigma_g$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.2385025849011(6)	−1.4963345319(2)	−38.81523(2)	−1.4561848030(2)
0.8	−0.3604285808126(4)	−1.5322772198(8)	−42.92934(2)	−1.0142750728(9)
0.9	−0.446299293025778(9)	−1.5426020441(4)	−48.56839(8)	−0.7222260645(4)
1.0	−0.50790540933734(4)	−1.53772722565(2)	−56.3012687(3)	−0.52191640697(2)
1.1	−0.552631673439913(7)	−1.52381155759(7)	−66.8085611(5)	−0.38049837337(6)
1.2	−0.58530594998959(3)	−1.50462175193(9)	−80.90244484(2)	−0.27834154329(6)
1.3	−0.60919508154909(3)	−1.48251953024(8)	−99.5584151(2)	−0.20317643626(5)
1.4	−0.62657290121361(3)	−1.45901079025(4)	−123.982293(4)	−0.147046419876(3)
1.5	−0.63905964591136(3)	−1.435062497884(3)	−155.805672(4)	−0.104628804041(2)
1.6	−0.64783256224535(3)	−1.411285954309(2)	−197.838076(5)	−0.072263018637(10)
1.7	−0.653760067134403(10)	−1.388019909414(2)	−257.822133(5)	−0.047352808909(8)
1.8	−0.657485408507765(5)	−1.365209208559(8)	−374.4857834(2)	−0.027910217524(4)
1.9	−0.659451216919321(5)	−1.3410321800411(2)	−859.1071992(6)	−0.0116472348434(10)
2.0	−0.659842081203761(3)	−1.313322011251(5)	−2213.945338149(9)	0.0031810755782(3)
2.1	−0.658994131399812(5)	−1.2904522658063(3)	−2816.85032338(6)	0.0131123795206(10)
2.2	−0.657312396926138(4)	−1.2702461047592(2)	−3048.60767488(2)	0.0201721314059(8)
2.3	−0.655018414880138(4)	−1.2514884868800(2)	−3195.93555649(2)	0.0254558012523(7)
2.4	−0.652265508883909(3)	−1.2339544639239(2)	−3317.55815530(2)	0.0294068974350(6)
2.5	−0.6491718595144174(6)	−1.2175663357511(2)	−3430.28202045(10)	0.0323109533111(5)
2.6	−0.6458311108734671(5)	−1.2022750590158(2)	−3540.50791238(7)	0.0343796779735(5)
2.7	−0.6423182646669432(3)	−1.1880385108346(2)	−3651.20798508(8)	0.0357770438886(4)
2.8	−0.6386937390663425(7)	−1.1748166545817(10)	−3763.968420989(3)	0.03663243698249(4)
2.9	−0.6350063807381684(7)	−1.1625704965189(9)	−3879.714487257(3)	0.03704905688190(3)
3.0	−0.6312957710664394(5)	−1.1512619898449(10)	−3999.001846166(3)	0.03710985076264(3)
3.1	−0.6275940215589652(5)	−1.1408541520911(2)	−4122.14009649(5)	0.0368819003312(4)
3.2	−0.6239271868347954(8)	−1.1313111924996(2)	−4249.24176561(4)	0.03641974411563(3)
3.3	−0.620316385777730(3)	−1.1225985975654(2)	−4380.233254157(3)	0.03576793151213(3)
3.4	−0.616778697120659(3)	−1.1146831684209(10)	−4514.843134253(3)	0.03496300759426(3)
3.5	−0.6133278789814176(5)	−1.1075330164557(9)	−4652.574539200(2)	0.03403506900203(3)
3.6	−0.6099749498852328(6)	−1.1011175256243(10)	−4792.664564186(3)	0.03300899281836(3)
3.7	−0.6067286600175318(8)	−1.0954072885505(8)	−4934.031881126(3)	0.03190541391474(2)
3.8	−0.6035958748919856(5)	−1.0903740213119(7)	−5075.21310027(4)	0.03074150749266(2)
3.9	−0.6005818886613732(4)	−1.0859904595263(5)	−5214.28837608(4)	0.02953161994781(10)
4.0	−0.5976906805119581(4)	−1.0822302363618(5)	−5348.79721584(8)	0.02828778116555(7)
4.1	−0.5949251246627084(4)	−1.07906774139731(3)	−5475.64639323(9)	0.027020123884902(3)
4.2	−0.5922871622211345(4)	−1.07647795781658(6)	−5591.01334509(10)	0.025737230148970(9)
4.3	−0.5897779413674219(3)	−1.07443627403622(7)	−5690.25052980(2)	0.024446420627585(4)
4.4	−0.5873979309254238(5)	−1.07291826426464(3)	−5767.79907517(3)	0.02315399945141(10)
4.5	−0.5851470112343226(4)	−1.07189943017758(3)	−5817.12381717(3)	0.02186546495357(9)
4.6	−0.5830245452737091(3)	−1.07135489230306(7)	−5830.68676725(3)	0.020585695270513(4)
4.7	−0.5810294321416363(3)	−1.0712590142669(5)	−5799.98245394(2)	0.01931911702476(9)
4.8	−0.5791601441748224(3)	−1.0715849356402(2)	−5715.66675176(2)	0.01806986514779(3)
4.9	−0.5774147481915913(3)	−1.0723039808626(3)	−5567.8207091(4)	0.0168419419430(5)
5.0	−0.5757909105447989(5)	−1.073384906256(4)	−5346.4014180(8)	0.0156393829667(8)
5.1	−0.5742858850147584(7)	−1.074792952528(6)	−5041.9395588(2)	0.0144664348043(2)
5.2	−0.5728964823529467(10)	−1.076488700429(9)	−4646.5397635(3)	0.0133277431302(2)
5.3	−0.571619021058419(3)	−1.078426801929(2)	−4155.2108012(4)	0.0122285358845(3)
5.4	−0.570449261522866(3)	−1.080554796238(9)	−3567.4778722(3)	0.0111747642236(2)

5.5	−0.569382330811155(3)	−1.082812416184(2)	−2889.092925(4)	0.0101731355341(2)
5.6	−0.568412653201142(4)	−1.085131989323(2)	−2133.470905(5)	0.0092309494784(3)
5.7	−0.567533910643625(4)	−1.087440603325(2)	−1322.306732(6)	0.0083556522742(3)
5.8	−0.56673906341833(3)	−1.08966444980(8)	−484.802288(3)	0.007554082249(2)
5.9	−0.56602045848605(3)	−1.09173508216(9)	344.804431(3)	0.006831497426(2)
6.0	−0.56537003696941(3)	−1.09359639806(9)	1131.153196(4)	0.006190612646(2)
6.5	−0.56286817037142(3)	−1.09914196637(6)	3576.977919(3)	0.004091442211(8)
7.0	−0.56109533347634(3)	−1.10048032670(6)	3449.223635(9)	0.003101477179(7)
7.5	−0.55971290178636(3)	−1.101019576734(3)	2121.058528(4)	0.0024541635784(3)
8.0	−0.55862502858928(4)	−1.10197294266(4)	578.264670(5)	0.001909639315(4)
8.5	−0.55779084808599(3)	−1.103338628616(3)	−797.369947(7)	0.0014403608889(3)
9.0	−0.55717053934505(3)	−1.104841654337(2)	−1908.066322(5)	0.0010554915948(2)
9.5	−0.55672088993132(3)	−1.106249989045(2)	−2771.914146(8)	0.0007570306124(9)
10.0	−0.55640056949059(3)	−1.107440981442(9)	−3447.895521(3)	0.0005360157540(7)
11.0	−0.55601501173250(3)	−1.109097075234(8)	−4480.800658(7)	0.0002666316573(5)
12.0	−0.555821527469240(6)	−1.1100088210000(2)	−5363.608736(2)	0.000136186161527(3)
13.0	−0.555720547680827(5)	−1.1104892908200(6)	−6227.97843(3)	0.00007321573397(5)
14.0	−0.555664773488572(3)	−1.1107440074176(10)	−7046.97408(3)	0.00004182425426(2)
15.0	−0.5556319984108463(6)	−1.1108828046994(5)	−7738.68238(7)	0.00002541280815(5)
16.0	−0.5556115375550769(5)	−1.1109613656691(5)	−8258.78968(6)	0.00001635684007(4)
17.0	−0.5555980481004045(3)	−1.11100794101183(2)	−8624.43110(4)	0.000011067952293(2)
18.0	−0.5555887361504259(5)	−1.11103702790855(9)	−8884.19002(5)	0.000007802466239(6)
19.0	−0.5555820661958067(4)	−1.111056196020460(10)	−9089.528091(3)	0.0000056808616397(9)
20.0	−0.5555771501550850(5)	−1.1110695298928(4)	−9286.47452(2)	0.000004238520869(2)

Table A10: Same as for Table A1, but for $4\,^3\Sigma_g^+$.

		$4\,^3\Sigma_g$		
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.2175366462959(8)	−1.452017695(4)	−895.02753(7)	−1.452777718(5)
0.8	−0.3391200341581(6)	−1.4869056185(2)	−924.491096(2)	−1.0108319377(2)
0.9	−0.4246449797467(3)	−1.4961690725(7)	−954.627473(3)	−0.7187545700(7)
1.0	−0.4859026209772(3)	−1.4902235849(7)	−985.43982(4)	−0.5184183429(6)
1.1	−0.5302776857524(3)	−1.4752245091(4)	−1016.98684(6)	−0.37697194324(3)
1.2	−0.5625977483805(4)	−1.45493506910(3)	−1049.37470(6)	−0.27478297695(2)
1.3	−0.5861292362673(3)	−1.43171438056(7)	−1082.753842(2)	−0.19958146771(4)
1.4	−0.60314561224114(10)	−1.40706854125(3)	−1117.30952(7)	−0.14341236912(2)
1.5	−0.61526708911014(8)	−1.38197264460(5)	−1153.198824(2)	−0.100958977590(3)
1.6	−0.623671993926(3)	−1.35707068066(10)	−1190.17274(4)	−0.06857918300(6)
1.7	−0.6292334545987(4)	−1.33282793812(9)	−1225.06732(4)	−0.04374178172(5)
1.8	−0.63261468663583(10)	−1.3098144612(5)	−1229.90792(2)	−0.02476949333(3)
1.9	−0.6343615806667(3)	−1.28963307176(6)	−1016.94636(2)	−0.011005216012(2)
2.0	−0.6349213450542(3)	−1.27078434399(4)	−775.69751(3)	−0.0004708269451(5)
2.1	−0.6345170451868(3)	−1.25176163547(5)	−783.180318(2)	0.008224978526(2)
2.2	−0.6333398728935(3)	−1.23362389826(3)	−874.48915(2)	0.01502538523(2)
2.3	−0.6315650288673(3)	−1.21659424974(3)	−1007.14286(2)	0.02023296000(10)
2.4	−0.6293361615865(5)	−1.20070709757(3)	−1173.40169(2)	0.02415217734(2)
2.5	−0.6267691483979(4)	−1.18595564669(2)	−1373.40924(5)	0.02703306004(5)
2.6	−0.6239574579658(3)	−1.17231900225(2)	−1609.82508(5)	0.02907535142(6)
2.7	−0.62097668432818(9)	−1.15976965891(9)	−1886.314552(3)	0.030438411016(3)
2.8	−0.61788813050889(8)	−1.14827621665(2)	−2206.89885(4)	0.03125001584(5)
2.9	−0.6147416012432(4)	−1.13780437917(3)	−2575.49350(5)	0.03161338735(7)
3.0	−0.6115775727355(3)	−1.12831711041(3)	−2995.43870(5)	0.03161267835(7)
3.1	−0.6084288772193(5)	−1.11977431085(2)	−3468.95670(4)	0.03131723987(4)
3.2	−0.6053220106340(4)	−1.11213224778(2)	−3996.528918(4)	0.03078492921(5)
3.3	−0.6022781492998(4)	−1.10534296108(3)	−4576.22845(5)	0.03006464773(8)
3.4	−0.5993139457932(3)	−1.09935388768(2)	−5203.08725(4)	0.02919823644(6)
3.5	−0.5964421635567(3)	−1.0941079622(4)	−5868.61582(5)	0.02822181856(9)
3.6	−0.5936722018878(4)	−1.08954442359(3)	−6560.615848(3)	0.02716666116(6)
3.7	−0.5910105556259(7)	−1.08560046526(2)	−7263.414516(3)	0.02605963405(5)
3.8	−0.5884612450640(5)	−1.08221370170(3)	−7958.591511(2)	0.02492336537(5)
3.9	−0.5860262403108(7)	−1.07932522506(3)	−8626.168273(2)	0.02377621937(5)
4.0	−0.5837058910232(4)	−1.07688284512(2)	−9246.108562(5)	0.02263223423(5)
4.1	−0.58149935900828(8)	−1.07484402387(3)	−9799.8806929(2)	0.02150114491(5)
4.2	−0.57940504059565(8)	−1.07317807054(3)	−10271.795253(9)	0.02038857396(5)
4.3	−0.57742096030837(8)	−1.07186734242(3)	−10649.876662(2)	0.01929641353(5)
4.4	−0.57554511796444(7)	−1.07090742771(3)	−10926.138311(3)	0.01822336550(5)
4.5	−0.57377577654270(5)	−1.07030646857(3)	−11096.270824(4)	0.01716557434(5)
4.6	−0.57211168479137(7)	−1.07008382801(3)	−11158.88059(5)	0.01611729165(5)
4.7	−0.57055223283147(7)	−1.07026816178(3)	−11114.51058(6)	0.01507155402(5)
4.8	−0.56909753736306(4)	−1.07089461086(6)	−10964.745668(2)	0.014020929971(2)
4.9	−0.56774844285343(4)	−1.07200030108(7)	−10711.778616(2)	0.012958486657(2)
5.0	−0.5665064053669(4)	−1.07361673425(9)	−10358.906894(3)	0.011879215297(2)
5.1	−0.56537320000348(4)	−1.07575734324(8)	−9912.497244(3)	0.010782167993(2)
5.2	−0.56435037553321(4)	−1.07839935217(9)	−9385.788818(4)	0.009673345942(2)
5.3	−0.56343840382454(4)	−1.08146252631(8)	−8804.11234(4)	0.008568732327(2)
5.4	−0.56263558449166(4)	−1.08479396895(9)	−8209.37676(4)	0.007495777783(2)

5.5	−0.56193698161947(5)	−1.08817416301(9)	−7659.71586(4)	0.006490872769(2)
5.6	−0.56133388196085(5)	−1.09135554861(8)	−7220.46161(4)	0.005591467020(2)
5.7	−0.56081423091580(5)	−1.09412515151(7)	−6947.395113(4)	0.004825142163(2)
5.8	−0.56036408129457(4)	−1.09636054109(5)	−6869.94060(4)	0.004201314051(7)
5.9	−0.55996952940666(4)	−1.09804892993(4)	−6983.542485(3)	0.003710191336(5)
6.0	−0.55961838626197(3)	−1.099265077785(3)	−7254.386899(3)	0.0033286157897(4)
6.5	−0.55826552204585(3)	−1.1021603882283(2)	−9274.483324(3)	0.0022108701328(8)
7.0	−0.55735669711355(3)	−1.104514274668(9)	−10175.510789(3)	0.0014570170799(2)
7.5	−0.556771892089421(10)	−1.106643535406(2)	−10010.336701(3)	0.0009200331696(2)
8.0	−0.556402866207961(6)	−1.108132144295(9)	−9446.23805(4)	0.0005841985151(2)
8.5	−0.556165439419370(6)	−1.109079353894(2)	−8800.41041(6)	0.0003825323463(2)
9.0	−0.556007320666745(3)	−1.109677185085(8)	−8177.33716(5)	0.0002597173610(9)
9.5	−0.5558982388819202(8)	−1.110064754108(9)	−7597.75384(7)	0.0001822867006(9)
10.0	−0.5558206192617401(4)	−1.110325157555(6)	−7054.29582(6)	0.0001316080969(6)
11.0	−0.5557215766072552(6)	−1.110635137376(2)	−6019.4757(4)	0.0000734559853(2)
12.0	−0.5556643565522509(8)	−1.1107997761872(3)	−4986.112089(3)	0.00004407807645(2)
13.0	−0.5556290919589019(10)	−1.1108948736324(2)	−3944.61350(5)	0.00002794694503(2)
14.0	−0.555606300007258(6)	−1.1109548162542(2)	−2965.266397(4)	0.00001841312574(10)
15.0	−0.555591101913952(3)	−1.1109959078123(2)	−2142.6881002(2)	0.00001241973438(10)
16.0	−0.5555807783014083(3)	−1.1110256407852(2)	−1524.03156(5)	0.00000849473860(9)
17.0	−0.555573681918567(3)	−1.1110475556968(2)	−1093.11060(5)	0.00000587106708(6)
18.0	−0.5555687535933527(3)	−1.1110637030405(10)	−803.78237(7)	0.00000410023035(5)
19.0	−0.5555652935109072(4)	−1.1110755557852(9)	−610.72249(8)	0.00000289638087(5)
20.0	−0.5555628353286600(7)	−1.1110842483725(5)	−480.37971(4)	0.000002071114243(2)

Table A11: Same as for Table A1, but for $5\,^3\Sigma_g^+$.

$5\,^3\Sigma_g$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.21402096724(5)	−1.44711348(4)	−63.192(2)	−1.45581650(5)
0.8	−0.335907516563(5)	−1.482898344(2)	−73.0952(10)	−1.013854138(3)
0.9	−0.4217334214735(8)	−1.493042281(6)	−84.94770(2)	−0.721750487(6)
1.0	−0.483289150953(3)	−1.4879621269(3)	−99.14804(2)	−0.5213838250(3)
1.1	−0.527959195692(5)	−1.473815093(7)	−116.1601(2)	−0.379906092(7)
1.2	−0.5605711360815(3)	−1.4543661722(2)	−136.52363(2)	−0.2776865833(9)
1.3	−0.5843915059866(3)	−1.4319753300(7)	−160.86090(2)	−0.2024556292(5)
1.4	−0.6016938216558(2)	−1.4081469615(5)	−189.90192(2)	−0.14625665585(3)
1.5	−0.6140980334512(9)	−1.38384746811(4)	−224.56312(9)	−0.10376760081(2)
1.6	−0.6227812208365(3)	−1.3596901635(5)	−266.34702(2)	−0.07132982615(3)
1.7	−0.62861193910516(7)	−1.3360211592(4)	−319.87653(9)	−0.04635134176(2)
1.8	−0.63223393915706(9)	−1.3127870800(6)	−414.819364(3)	−0.02684400091(3)
1.9	−0.63409471597720(5)	−1.28870492486(5)	−740.882382(3)	−0.010797627846(4)
2.0	−0.63451060099414(5)	−1.26546156473(8)	−1110.807863(3)	0.00177981863(4)
2.1	−0.63385119869145(10)	−1.24466178562(4)	−1250.164976(10)	0.010971719886(2)
2.2	−0.63238935100535(3)	−1.22528458013(5)	−1326.806991(2)	0.017951873582(2)
2.3	−0.63031595112395(2)	−1.207104401538(3)	−1386.542446(7)	0.023272826396(2)
2.4	−0.62777811314150(3)	−1.190057600384(3)	−1440.822359(8)	0.027291094124(2)
2.5	−0.624892241963812(8)	−1.174104183874(3)	−1493.577003(5)	0.030272120021(8)
2.6	−0.621751364642482(8)	−1.159206983155(2)	−1546.522754(5)	0.032421440819(7)
2.7	−0.618430248955305(9)	−1.145328306281(3)	−1600.556412(6)	0.033900811714(8)
2.8	−0.614989220447405(10)	−1.132429824213(3)	−1656.214165(6)	0.034838791672(8)
2.9	−0.611477083666765(9)	−1.120473042444(3)	−1713.847584(6)	0.035338318927(8)
3.0	−0.607933389760105(9)	−1.109419782969(2)	−1773.697063(5)	0.035482332184(6)
3.1	−0.604390214231849(8)	−1.099232560788(3)	−1835.921971(5)	0.035338021831(6)
3.2	−0.600873561938394(6)	−1.089874852876(2)	−1900.6094159(3)	0.034960084688(4)
3.3	−0.597404485414363(6)	−1.081311284947(2)	−1967.7701745(3)	0.0343932381459(3)
3.4	−0.593999981009364(6)	−1.073507765838(2)	−2037.3248402(3)	0.0336741753472(4)
3.5	−0.590673711814572(6)	−1.066431598837(2)	−2109.0804581(3)	0.0328330927978(4)
3.6	−0.587436595090516(5)	−1.060051599489(9)	−2182.6960514(3)	0.0318948863035(3)
3.7	−0.584297283689725(10)	−1.054338253150(2)	−2257.633552(4)	0.0308800849270(4)
3.8	−0.581262565051711(7)	−1.049263955336(2)	−2333.088086(4)	0.0298055723072(3)
3.9	−0.57833769729683(3)	−1.044803398158(8)	−2407.8874304(3)	0.0286851272913(2)
4.0	−0.575526699604009(8)	−1.040934205273(2)	−2480.343282(7)	0.0275297984838(2)
4.1	−0.572832613609267(7)	−1.037637992914(6)	−2548.023694(6)	0.0263481059279(8)
4.2	−0.570257754736699(6)	−1.0349021817035(2)	−2607.390576(5)	0.025146030421385(5)
4.3	−0.567803978955034(5)	−1.03272318229436(2)	−2653.195011(5)	0.02392669200363(3)
4.4	−0.565473005504785(4)	−1.0311122084080(2)	−2677.416028(4)	0.02268950059126(2)
4.5	−0.563266868994272(3)	−1.030106366863(2)	−2667.2935719(2)	0.0214283046945(3)
4.6	−0.561188647017841(4)	−1.02979091144(4)	−2601.4688108(2)	0.020127474479(7)
4.7	−0.559243775865617(6)	−1.03034632346(8)	−2441.978328(10)	0.018753452824(2)
4.8	−0.557442655718874(6)	−1.03215239491(6)	−2116.934414(8)	0.017236024276(2)
4.9	−0.555806110005774(10)	−1.03601774182(2)	−1483.538582(2)	0.015427444531(3)
5.0	−0.55437650136961(5)	−1.04359081871(3)	−266.96031(5)	0.01303243681(6)
5.1	−0.55323321553524(5)	−1.0572688804(5)	1895.45240(8)	0.00964657855(10)
5.2	−0.55247369297009(8)	−1.0761544522(6)	4737.72409(2)	0.00553710264(2)
5.3	−0.55209171361697(9)	−1.0914214669(5)	6700.75253(8)	0.00240791704(8)
5.4	−0.55192799100474(9)	−1.09769100840(2)	6974.185855(3)	0.001141661778(3)

5.5	−0.55182334306611(8)	−1.09769190037(7)	6120.550904(2)	0.001082688321(9)
5.6	−0.55169521827926(7)	−1.094863252390(2)	4769.36231086(2)	0.0015227114585(5)
5.7	−0.55151512962629(6)	−1.091177403354(2)	3286.502393(7)	0.002079448403(5)
5.8	−0.55128142356462(6)	−1.087617909370(3)	1866.690437(10)	0.002576713407(6)
5.9	−0.55100413797947(5)	−1.084631565354(3)	607.105205(2)	0.002945205187(6)
6.0	−0.55069717304307(4)	−1.082369351772(2)	−454.333725(2)	0.003170832386(5)
6.5	−0.54912485279601(3)	−1.0799039478366(3)	−3143.601597(7)	0.00282242427002(3)
7.0	−0.5479889115932(3)	−1.0839287038(5)	−3357.148438(3)	0.00172130277(5)
7.5	−0.5473594633688(3)	−1.0882828008(6)	−2772.83365(2)	0.00085815013(7)
8.0	−0.54707283974056(9)	−1.0914545041(4)	−2166.90194(2)	0.00033639692(4)
8.5	−0.54698758843929(4)	−1.09373542381(3)	−1849.82462(6)	0.000028206243(3)
9.0	−0.5470304163084(4)	−1.0957949608(5)	−1886.94805(7)	−0.00019268091(5)
9.5	−0.54717796783111(7)	−1.09813794635(4)	−2232.62701(5)	−0.000398106388(3)
10.0	−0.54742997532512(7)	−1.10097218313(3)	−2801.660020(2)	−0.000611223247(3)
11.0	−0.54825061974345(4)	−1.10767332840(3)	−4254.64973(2)	−0.001015644447(2)
12.0	−0.54940481998475(6)	−1.11387118193(2)	−5665.6292(6)	−0.001255128497(2)
13.0	−0.55068373198642(6)	−1.11785084007(2)	−6741.4712(7)	−0.001267952007(2)
14.0	−0.55188687356460(7)	−1.11945214486(9)	−7443.3862(10)	−0.001119885552(6)
15.0	−0.55290182872230(8)	−1.11938727559(7)	−7851.4147(10)	−0.000905574543(4)
16.0	−0.55369795957433(5)	−1.11843411646(7)	−8061.0910(8)	−0.000689887332(4)
17.0	−0.55429161424507(7)	−1.11714311194(5)	−8144.8853(2)	−0.0005035225557(2)
18.0	−0.55471788148592(3)	−1.115833887457(3)	−8147.5469(10)	−0.0003554513603(2)
19.0	−0.55501475025588(3)	−1.114664652974(3)	−8090.7001(10)	−0.0002439553927(9)
20.0	−0.55521604298990(4)	−1.113695894450(2)	−7976.9437(8)	−0.0001631904235(5)

Table A12: Same as for Table A1, but for $6\,^3\Sigma_g^+$.

$6\,^3\Sigma_g$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.204455278331(7)	−1.426823331(9)	−445.1281(2)	−1.454161107(10)
0.8	−0.3261754375344(4)	−1.462097077(6)	−461.04003(10)	−1.012182752(6)
0.9	−0.4118335943341(7)	−1.4717277927(3)	−477.362550(3)	−0.7200673379(3)
1.0	−0.4732204873279(5)	−1.4661312841(2)	−494.097543(2)	−0.5196903095(8)
1.1	−0.5177206552084(6)	−1.4514634352(2)	−511.277866(3)	−0.3782019317(9)
1.2	−0.5501616021783(4)	−1.4314880000(5)	−528.96431(6)	−0.2759706630(4)
1.3	−0.5738097434873(3)	−1.4085643943(4)	−547.24608(7)	−0.20072685176(3)
1.4	−0.5909385373399(3)	−1.3841984412(4)	−566.24019(10)	−0.14451526181(3)
1.5	−0.6031681374699(4)	−1.3593635783(5)	−586.06534(2)	−0.10201820224(3)
1.6	−0.6116766334122(3)	−1.3346983111(4)	−606.63987(2)	−0.06959065270(3)
1.7	−0.6173363713965(3)	−1.3106491789(4)	−626.13716(2)	−0.04469202126(2)
1.8	−0.6208077079588(8)	−1.2877014629(3)	−626.2004(5)	−0.0256033594(2)
1.9	−0.6226192029778(7)	−1.2667660401(8)	−515.7236(5)	−0.01133033375(3)
2.0	−0.6231732429756(5)	−1.2466370147(5)	−445.63983(3)	−0.00014526434(2)
2.1	−0.6227253282822(9)	−1.2270990104(5)	−472.34613(3)	0.00873887911(2)
2.2	−0.6214918979766(6)	−1.2085958835(5)	−532.78036(3)	0.01563086930(2)
2.3	−0.6196527540366(5)	−1.1912067874(5)	−612.88286(3)	0.02091248722(2)
2.4	−0.6173523240961(5)	−1.1749346067(5)	−710.19628(3)	0.02490418396(2)
2.5	−0.6147063610312(4)	−1.1597607090(6)	−825.08130(3)	0.02786080522(2)
2.6	−0.6118078948464(5)	−1.1456571179(7)	−958.79605(3)	0.02998410452(3)
2.7	−0.6087319356108(4)	−1.1325907772(7)	−1112.88272(3)	0.03143447926(3)
2.8	−0.6055391244653(5)	−1.1205255037(9)	−1288.85343(3)	0.03234026618(3)
2.9	−0.6022785663286(6)	−1.1094229459(10)	−1487.93597(3)	0.03280489196(3)
3.0	−0.5989900347190(4)	−1.0992430045(9)	−1710.81070(3)	0.03291235499(3)
3.1	−0.5957056948999(5)	−1.0899439428(10)	−1957.32315(3)	0.03273143450(3)
3.2	−0.5924514570116(4)	−1.0814823587(9)	−2226.18496(2)	0.03231892354(3)
3.3	−0.5892480455108(5)	−1.0738131609(10)	−2514.69657(2)	0.03172210002(3)
3.4	−0.5861118529223(5)	−1.0668896944(2)	−2818.54336(2)	0.03098059159(3)
3.5	−0.5830556323886(4)	−1.0606641316(9)	−3131.72573(2)	0.03012775234(3)
3.6	−0.5800890728351(4)	−1.0550882083(9)	−3446.67719(2)	0.02919164925(3)
3.7	−0.5772192912115(4)	−1.0501143107(8)	−3754.59689(4)	0.02819574910(2)
3.8	−0.5744512673045(4)	−1.0456968347(8)	−4045.97509(6)	0.02715939472(2)
3.9	−0.5717882379577(4)	−1.0417936773(8)	−4311.23198(4)	0.02609815350(2)
4.0	−0.5692320599538(4)	−1.0383677027(9)	−4541.338816(2)	0.02502410430(2)
4.1	−0.5667835457749(4)	−1.0353881039(9)	−4728.259924(2)	0.02394609456(2)
4.2	−0.5644427757147(4)	−1.0328317732(9)	−4865.04482(6)	0.02286994720(2)
4.3	−0.5622093955100(4)	−1.0306851632(9)	−4945.38318(10)	0.02179851808(2)
4.4	−0.5600829247289(3)	−1.0289478396(5)	−4962.34014(8)	0.02073136586(10)
4.5	−0.5580631385199(3)	−1.0276406400(5)	−4905.64312(10)	0.01966347489(10)
4.6	−0.5561506787845(3)	−1.0268262151(6)	−4755.81241(2)	0.01858155272(2)
4.7	−0.5543483201351(3)	−1.0266658082(7)	−4469.97928(2)	0.01745336853(2)
4.8	−0.5526642201774(3)	−1.0275974187(10)	−3942.11826(3)	0.01619396285(2)
4.9	−0.5511219699422(4)	−1.0309781811(2)	−2876.0751(4)	0.01454403240(3)
5.0	−0.5497948104224(4)	−1.0412009954(3)	−458.4357(6)	0.0116777251(5)
5.1	−0.5488525495243(5)	−1.0610859051(2)	3255.4647(4)	0.00718023411(3)
5.2	−0.5482216749742(5)	−1.0635112431(2)	3040.97374(2)	0.00633309748(3)
5.3	−0.5474944387792(3)	−1.0512634340(2)	442.82868(2)	0.00825008370(3)
5.4	−0.5465988719421(3)	−1.0420323073(8)	−1391.16850(6)	0.00947508085(2)

5.5	−0.54563071222658(6)	−1.0375192814(5)	−2328.172260(2)	0.00977129874(8)
5.6	−0.54466117892873(4)	−1.03576790016(3)	−2760.450680(4)	0.00956329602(5)
5.7	−0.54372574264717(3)	−1.03546665863(2)	−2922.84381310(6)	0.009120145030(3)
5.8	−0.54284050402294(3)	−1.03595012032(7)	−2927.07291117(3)	0.008574290987(2)
5.9	−0.54201209281235(3)	−1.036875984696(2)	−2827.2963238(5)	0.0079912204964(3)
6.0	−0.54124234005286(3)	−1.03805305234(4)	−2652.5476247(2)	0.007405271294(6)
6.5	−0.53820662896443(3)	−1.04468443183(2)	−1176.608032(3)	0.004881357861(2)
7.0	−0.53620754594727(5)	−1.04965545134(2)	370.28529(6)	0.003251377223(3)
7.5	−0.53485051490825(7)	−1.05281722194(3)	1353.83758(8)	0.002251174384(3)
8.0	−0.53390409027887(8)	−1.05524395817(3)	1884.06147(10)	0.001570527799(3)
8.5	−0.53325353684818(5)	−1.05756630009(4)	2247.92180(2)	0.00105185572(4)
9.0	−0.53283410628561(10)	−1.0598679583(4)	2499.38259(10)	0.00064447270(4)
9.5	−0.53258823669162(8)	−1.06174596805(3)	2442.06176(6)	0.000361105824(3)
10.0	−0.53245255793205(10)	−1.06291532953(3)	2073.07478(6)	0.000198978633(2)
11.0	−0.53232359906269(7)	−1.06362309546(2)	1076.4059(4)	0.000093100242(2)
12.0	−0.53222543808464(5)	−1.06309114580(2)	148.2966(9)	0.000113310864(2)
13.0	−0.53209100731673(4)	−1.06218789382(7)	−663.6422(9)	0.000153393909(5)
14.0	−0.53192774858381(8)	−1.06150816820(5)	−1340.3971(10)	0.0001676663545(3)
15.0	−0.53176544508749(4)	−1.06123376949(4)	−1850.6395(10)	0.0001531413793(3)
16.0	−0.53162640381361(8)	−1.061273253674(3)	−2182.2470(9)	0.0001237221221(2)
17.0	−0.53151852801338(8)	−1.061464852262(3)	−2355.8167(8)	0.0000924825743(2)
18.0	−0.53143975200547(3)	−1.061689165549(2)	−2413.8257(7)	0.0000661299145(7)
19.0	−0.53138407622952(3)	−1.061888859699(2)	−2400.9134(7)	0.0000462785663(5)
20.0	−0.53134528068609(6)	−1.062047488956(2)	−2352.0007(6)	0.00003215362079(3)

Table A13: Same as for Table A1, but for $7\,^3\Sigma_g^+$.

		$7\,^3\Sigma_g$		
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.20270205342(6)	−1.42437797(7)	−43.3069(2)	−1.45567695(9)
0.8	−0.32457366275(4)	−1.460103133(4)	−50.2212(3)	−1.01369476(4)
0.9	−0.41038260617(3)	−1.470178657(2)	−58.4140(3)	−0.721570494(2)
1.0	−0.471919268627(9)	−1.46502085(6)	−68.1173(10)	−0.52118232(6)
1.1	−0.516568046016(6)	−1.450786380(4)	−79.60019(3)	−0.379682080(3)
1.2	−0.549156416485(4)	−1.431239660(2)	−93.17167(2)	−0.277439023(2)
1.3	−0.572950811085(4)	−1.408740213(2)	−109.1833(4)	−0.202183531(8)
1.4	−0.590224658554(3)	−1.384792365(7)	−128.0360(5)	−0.145959319(5)
1.5	−0.602597876241(3)	−1.360363590(5)	−150.2151(7)	−0.1034452253(3)
1.6	−0.6112476734973(8)	−1.336071834(4)	−176.5022(7)	−0.0709853046(3)
1.7	−0.6170432529446(8)	−1.312280798(5)	−209.5322(8)	−0.0459966423(3)
1.8	−0.6206310549324(9)	−1.28902038015(3)	−268.59106(10)	−0.026532372382(2)
1.9	−0.622475693774(3)	−1.2656976813(9)	−445.84794(2)	−0.0109191020(4)
2.0	−0.6229380638207(10)	−1.2437038214(2)	−591.57925(3)	0.0010861531(5)
2.1	−0.6223550234266(8)	−1.2233497025(10)	−650.75370(3)	0.0101715925(5)
2.2	−0.6208931504403(3)	−1.20605721672(2)	49.504423(3)	0.01624049280(6)
2.3	−0.6189895119019(3)	−1.1883162370(5)	55.263664(3)	0.02159251601(3)
2.4	−0.6166176582935(3)	−1.1716678180(2)	62.16987(5)	0.0256531244(6)
2.5	−0.6138932446303(3)	−1.1560829324(3)	69.45904(2)	0.0286814227(2)
2.6	−0.6109089823284(2)	−1.141529783(6)	77.46755(3)	0.0308800699(3)
2.7	−0.6077394910151(3)	−1.127972442(9)	86.2688(4)	0.032409830(4)
2.8	−0.6044450115796(4)	−1.115373116(2)	95.9439(7)	0.033398896(6)
2.9	−0.601074284522(4)	−1.103693205(3)	106.5840(10)	0.033950126(8)
3.0	−0.597666796816(3)	−1.092894014(4)	118.2915(2)	0.034146527(2)
3.1	−0.594254548219(3)	−1.08293722(5)	131.1822(3)	0.034055446(2)
3.2	−0.590863448904(2)	−1.07378514(7)	145.3870(4)	0.033731799(2)
3.3	−0.587514432124(2)	−1.06540096(9)	161.055(5)	0.033220576(3)
3.4	−0.584224345115(4)	−1.05774879(2)	178.354(6)	0.03255880(4)
3.5	−0.5810066663217(3)	−1.05079369(2)	197.478(9)	0.03177704(5)
3.6	−0.5778720858884(4)	−1.04450175(2)	218.647(2)	0.03090067(6)
3.7	−0.5748289779428(3)	−1.03884000929(6)	242.114423(6)	0.029950796378(2)
3.8	−0.57188378692583(10)	−1.03377652347(6)	268.173489(5)	0.028945013259(2)
3.9	−0.56904134541806(8)	−1.02928030823(5)	297.162464(5)	0.027898046822(2)
4.0	−0.5663051372922(3)	−1.02532138732(5)	329.475717(5)	0.026822221816(2)
4.1	−0.56367751726792(3)	−1.02187083353(5)	365.575416(6)	0.025727853904(2)
4.2	−0.56115989592781(4)	−1.01890086217(6)	406.007947(6)	0.024623554689(2)
4.3	−0.55875289798314(6)	−1.01638500866(6)	451.428040(7)	0.023516462165(2)
4.4	−0.5564565014501(3)	−1.01429849513(7)	502.639850(8)	0.022412388130(2)
4.5	−0.5542701684158(8)	−1.01261915519(9)	560.686595(10)	0.021315818144(2)
4.6	−0.55219299456554(10)	−1.0113306585(6)	627.133464(2)	0.02022941972(2)
4.7	−0.5502240112518(5)	−1.0104408284(6)	705.577833(10)	0.01915046683(2)
4.8	−0.54836420086439(3)	−1.0102622363(4)	823.699815(4)	0.01801378447(9)
4.9	−0.547035875224(3)	−1.084753834(8)	6599.4229(6)	0.0019016156(2)
5.0	−0.547042080927(3)	−1.093591004(4)	5608.8898(9)	0.0000986316(7)
5.1	−0.5467597476297(6)	−1.062530542(5)	−554.6290(9)	0.0060762654(9)
5.2	−0.54589976160050(10)	−1.03808381141(2)	−4298.06017(2)	0.01032994458(4)
5.3	−0.5448085331157(3)	−1.0303726945(7)	−5117.88955(5)	0.01117818334(2)
5.4	−0.5436985526005(3)	−1.0283555760(8)	−5175.16126(8)	0.01093361652(2)

5.5	−0.5426319195767(4)	−1.0282230503(8)	−5046.61362(2)	0.01037105252(2)
5.6	−0.5416277076520(5)	−1.0289146739(9)	−4860.79126(2)	0.00970370383(2)
5.7	−0.5406922498595(5)	−1.0300672121(10)	−4651.25728(2)	0.00900303293(2)
5.8	−0.5398272136673(6)	−1.0315228173(10)	−4427.95087(3)	0.00829855347(2)
5.9	−0.5390321638562(6)	−1.0331938811(10)	−4194.18777(3)	0.00760516045(2)
6.0	−0.5383055043094(6)	−1.0350189548(2)	−3951.56455(3)	0.00693200897(2)
6.5	−0.5355965310240(7)	−1.0447924574(9)	−2669.0351(4)	0.00406163148(2)
7.0	−0.53406823430(9)	−1.052575359(2)	−1430.804(10)	0.0022230156(2)
7.5	−0.53322840887(6)	−1.057082984(8)	−355.215(2)	0.0012498445(2)
8.0	−0.53273460674(4)	−1.059198049(2)	320.797(6)	0.0007838956(2)
8.5	−0.532403519054(10)	−1.0599763076(3)	404.691(4)	0.0005683212(4)
9.0	−0.5321475770792(3)	−1.06010107108(9)	40.25787(2)	0.000466009231(2)
9.5	−0.5319336384744(3)	−1.06017164008(2)	−359.17358(2)	0.000389014407(2)
10.0	−0.5317600795688(3)	−1.06047408337(3)	−600.64389(2)	0.000304607577(3)
11.0	−0.53153194265189(5)	−1.0612801741(2)	−887.5716(10)	0.00016215557(2)
12.0	−0.53141404185991(3)	−1.0618352624(5)	−1221.4123(10)	0.00008273511(4)
13.0	−0.53135298748719(3)	−1.06213289325(2)	−1660.6096(6)	0.000044083210(2)
14.0	−0.53131933200584(4)	−1.06228292785(5)	−2097.59639(3)	0.000025409726(4)
15.0	−0.531299186941973(4)	−1.062360316768(2)	−2425.78981(7)	0.0000158704744(9)
16.0	−0.531286213982657(3)	−1.062403638374(5)	−2638.185937(2)	0.00001054934951(3)
17.0	−0.53127740019298(3)	−1.0624302294288(3)	−2769.326626(5)	0.00000732770337(2)
18.0	−0.53127118017378(5)	−1.0624477552168(3)	−2847.148177(2)	0.00000525584060(2)
19.0	−0.53126666349152(7)	−1.0624598800126(3)	−2888.19892(7)	0.00000386563002(2)
20.0	−0.53126330751565(9)	−1.062468556433(4)	−2902.53589(2)	0.00000290292995(2)

Table A14: Same as for Table A1, but for $2\,^1\Sigma_u^+$ (B' state).

$2\,^1\Sigma_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.238540424455(3)	−1.4976393426(2)	−20811.9674(6)	−1.4579407052(3)
0.8	−0.360658634698(9)	−1.5344097324(10)	−22157.02457(2)	−1.0163655788(2)
0.9	−0.446755626041(10)	−1.5457078770(2)	−23532.99861(8)	−0.7246629166(10)
1.0	−0.508623142870(3)	−1.5419551349(7)	−24912.00436(7)	−0.5247088491(6)
1.1	−0.5536466889439(4)	−1.52931078946(2)	−26261.008577(4)	−0.38365219234(2)
1.2	−0.5866544920225(6)	−1.51153864507(2)	−27541.36163(4)	−0.28185805086(2)
1.3	−0.6109132657944(5)	−1.49099366312(3)	−28709.09273(5)	−0.20705163964(2)
1.4	−0.6286961666708(4)	−1.4691715136(6)	−29716.08727(2)	−0.1512708430(4)
1.5	−0.6416222616294(4)	−1.44702807253(3)	−30512.20949(4)	−0.10918903285(2)
1.6	−0.6508674903008(5)	−1.4251721092(6)	−31048.30132(10)	−0.07714820541(3)
1.7	−0.65730017709273(10)	−1.40398541584(3)	−31279.803292(3)	−0.05257944804(2)
1.8	−0.6615706046248(3)	−1.38370009982(3)	−31170.550596(2)	−0.03364382810(2)
1.9	−0.6641717305398(10)	−1.36444983693(3)	−30696.168572(2)	−0.01900335571(2)
2.0	−0.6654812755503(3)	−1.34630477261(3)	−29846.486963(6)	−0.00767111075(2)
2.1	−0.6657914857209(5)	−1.32929573637(3)	−28626.5430749(3)	0.00108915956(2)
2.2	−0.6653305508915(4)	−1.31343112991(3)	−27056.019743(2)	0.00783180539(10)
2.3	−0.6642782513404(3)	−1.29870855159(3)	−25167.285514(2)	0.01297737004(10)
2.4	−0.6627775294787(4)	−1.28512250903(3)	−23002.472717(3)	0.01684689580(9)
2.5	−0.6609431300195(10)	−1.2726691850(4)	−20610.170077(9)	0.01968683003(2)
2.6	−0.6588680959628(8)	−1.2613489901(4)	−18042.29798(6)	0.02168738533(2)
2.7	−0.6566286737627(7)	−1.2511674609(4)	−15351.60570(5)	0.02299625431(2)
2.8	−0.6542880231409(8)	−1.2421348950(4)	−12590.03775(7)	0.02372898258(2)
2.9	−0.6518990169876(7)	−1.2342649537(4)	−9808.01692(2)	0.02397692422(2)
3.0	−0.6495063377012(7)	−1.22757231549(4)	−7054.52026(8)	0.02381345330(9)
3.1	−0.6471480183639(7)	−1.22206936804(4)	−4377.693365(9)	0.02329892539(8)
3.2	−0.6448565350915(10)	−1.21776190231(5)	−1825.655290(8)	0.02248473995(3)
3.3	−0.6426595283874(5)	−1.2146438678(4)	552.91234(2)	0.02141672395(2)
3.4	−0.6405802157130(4)	−1.2126914738(4)	2708.81370(2)	0.02013792871(9)
3.5	−0.6386375544977(4)	−1.21185727585(4)	4593.39096(2)	0.01869080947(8)
3.6	−0.6368462232497(3)	−1.21206528333(2)	6160.78470(4)	0.01711865643(4)
3.7	−0.6352165041710(3)	−1.21320841601(2)	7371.317308(3)	0.01546610603(4)
3.8	−0.6337541660666(3)	−1.21514959664(3)	8195.53472(2)	0.01377861460(5)
3.9	−0.6324604508304(3)	−1.21772723997(2)	8618.08422(2)	0.01210093889(4)
4.0	−0.6313322510154(3)	−1.22076490242(2)	8640.44130(2)	0.01047489990(4)
4.1	−0.63036252715892(10)	−1.22408369279(2)	8281.65970(2)	0.008936917445(3)
4.2	−0.62954095915875(10)	−1.22751519141(2)	7576.80173(2)	0.007515887360(3)
4.3	−0.62885477217240(10)	−1.23091247891(2)	6573.33520(2)	0.006231875682(2)
4.4	−0.62828964146310(8)	−1.23415750220(9)	5326.29600(2)	0.005095859254(2)
4.5	−0.62783057216830(8)	−1.23716409425(8)	3893.21865(2)	0.004110455574(2)
4.6	−0.62746266747131(8)	−1.23987704400(7)	2329.70554(2)	0.003271367597(2)
4.7	−0.62717173165794(7)	−1.24226831650(6)	686.16343(2)	0.002569180173(10)
4.8	−0.62694469018290(7)	−1.24433174051(5)	−994.14257(7)	0.001991174968(6)
4.9	−0.62676983754422(6)	−1.24607731693(4)	−2675.85517(8)	0.001522930235(6)
5.0	−0.62663694133593(6)	−1.24752595056(4)	−4331.39929(9)	0.001149586424(5)
5.1	−0.62653723779872(6)	−1.248705037944(4)	−5940.28441(9)	0.000856752481(5)
5.2	−0.62646335342252(5)	−1.249645051937(3)	−7488.11205(10)	0.000631087482(4)
5.3	−0.62640918204889(5)	−1.250377075503(3)	−8965.49346(2)	0.000460620490(4)
5.4	−0.626369740200(5)	−1.25093114294(2)	−10367.0086(2)	0.000334877304(3)

5.5	−0.6263410167617(3)	−1.251335215829(10)	−11690.27931(6)	0.0002448759444(2)
5.6	−0.626319827566(4)	−1.25161462841(9)	−12935.1828(2)	0.000183040484(2)
5.7	−0.626303681077(4)	−1.25179186243(8)	−14103.2146(2)	0.000143070125(2)
5.8	−0.626290658314(4)	−1.25188654078(7)	−15196.9817(2)	0.000119788936(2)
5.9	−0.626279308035(3)	−1.25191555800(7)	−16219.8141(2)	0.000108992890(2)
6.0	−0.626268556926(3)	−1.25189328886(7)	−17175.4707(2)	0.000107304165(9)
6.5	−0.62620412050869(7)	−1.251370900147(4)	−21084.995300(9)	0.0001595909031(4)
7.0	−0.62610884069292(5)	−1.250699005517(5)	−23877.95010(5)	0.0002169536955(4)
7.5	−0.62599282551812(4)	−1.250174059432(7)	−25904.080167(2)	0.0002415455472(7)
8.0	−0.62587195912505(8)	−1.249837502984(2)	−27392.46920(2)	0.0002383019083(2)
8.5	−0.62575713629618(5)	−1.249650492490(2)	−28484.32073(9)	0.0002192682473(2)
9.0	−0.62565372378234(3)	−1.249562308219(8)	−29261.513603(3)	0.0001939043717(8)
9.5	−0.62556332677957(3)	−1.249531822226(10)	−29764.87099(9)	0.0001678769824(9)
10.0	−0.62548547617907(3)	−1.249530775730(7)	−30004.223361(9)	0.0001440176628(6)
11.0	−0.62536144681516(3)	−1.249552842365(8)	−29598.82831(9)	0.0001063682969(7)
12.0	−0.62526838382390(3)	−1.249556456196(8)	−27605.52547(2)	0.0000816926210(6)
13.0	−0.62519481217122(3)	−1.249522239372(2)	−23251.21605(3)	0.0000667219208(8)
14.0	−0.62513333817165(4)	−1.249476328095(3)	−16174.6605(8)	0.0000564534463(2)
15.0	−0.62508265371459(7)	−1.249503287821(7)	−8368.7652(4)	0.00004413464055(3)
16.0	−0.62504627268548(7)	−1.2496358173761(3)	−3242.67231(3)	0.00002854549967(3)
17.0	−0.62502458881057(3)	−1.249782768618(7)	−1087.16581(2)	0.0000156711178(5)
18.0	−0.62501315847231(3)	−1.249882675451(7)	−361.96352(6)	0.0000079800829(5)
19.0	−0.625007381376735(10)	−1.249938088589(8)	−129.417624(3)	0.0000040354823(5)
20.0	−0.625004422300836(9)	−1.249966591645(8)	−51.679889(2)	0.0000021126479(5)

Table A15: Same as for Table A1, but for $3\,^1\Sigma_u^+$ (B"$\bar{B}$ state).

$3\,^1\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.214021007253(5)	−1.447629134(7)	−8771.4525(10)	−1.456553028(8)
0.8	−0.335988249501(5)	−1.483762357(9)	−9287.41775(3)	−1.014732322(9)
0.9	−0.42190925239(4)	−1.494315950(5)	−9802.8659(2)	−0.722774940(5)
1.0	−0.483574887235(5)	−1.489707692(4)	−10303.9256(8)	−0.5225579175(4)
1.1	−0.528369903241(4)	−1.476094517(4)	−10774.5503(10)	−0.3812315550(3)
1.2	−0.561121954872(4)	−1.457239640(4)	−11196.4931(10)	−0.2791631083(3)
1.3	−0.585097432476(3)	−1.4354996960(6)	−11549.659405(2)	−0.2040806392(4)
1.4	−0.602569486863(5)	−1.4123747078(2)	−11812.88530(3)	−0.1480255243(10)
1.5	−0.615157555458(3)	−1.3888278080(2)	−11965.14833(3)	−0.1056751314(9)
1.6	−0.6240383632746(8)	−1.3654778639(2)	−11987.13664(2)	−0.0733757108(9)
1.7	−0.6300814447073(6)	−1.3427191824(2)	−11863.01396(2)	−0.0485625253(8)
1.8	−0.6339386894494(9)	−1.3207979890(2)	−11582.12896(7)	−0.0294003390(8)
1.9	−0.6361049906624(8)	−1.2998625196(2)	−11140.378631(6)	−0.0145539675(6)
2.0	−0.6369602249812(8)	−1.2799965292(2)	−10540.96805(5)	−0.0030380396(5)
2.1	−0.6367988751494(7)	−1.2612420587(10)	−9794.42054(2)	0.0058836626(4)
2.2	−0.6358512902166(7)	−1.2436150084(10)	−8917.85446(2)	0.0127670782(4)
2.3	−0.6342991712284(7)	−1.2271157536(10)	−7933.70553(2)	0.0180359082(4)
2.4	−0.6322869950164(7)	−1.2117362627(10)	−6868.18512(2)	0.0220157197(4)
2.5	−0.629930532534(3)	−1.1974647138(10)	−5749.79553(2)	0.0249585405(4)
2.6	−0.6273232575293(7)	−1.1842883080(9)	−4608.17507(2)	0.02706084885(3)
2.7	−0.624541202247(3)	−1.1721947498(9)	−3473.44436(2)	0.02847690914(3)
2.8	−0.6216466544103(10)	−1.1611726758(8)	−2376.10297(2)	0.02932879751(3)
2.9	−0.618690976162(5)	−1.1512111468(8)	−1347.40455(2)	0.02971407089(3)
3.0	−0.6157167442534(4)	−1.1422981750(7)	−420.02509(2)	0.02971177118(2)
3.1	−0.6127593513728(4)	−1.1344181687(6)	371.27340(9)	0.02938726905(2)
3.2	−0.609848165915(2)	−1.1275481784(5)	989.39748(6)	0.02879629795(2)
3.3	−0.6070073197618(8)	−1.1216529912(4)	1395.61168(4)	0.02798837829(9)
3.4	−0.6042561821753(10)	−1.1166795083(6)	1551.7087(2)	0.027009663550(2)
3.5	−0.6016095834313(9)	−1.11255146552(2)	1424.049625(3)	0.025905057523(3)
3.6	−0.5990778754349(4)	−1.10916627034(4)	989.39114(4)	0.024719300145(4)
3.7	−0.5966669494619(5)	−1.10639613624(5)	241.60922(5)	0.023496692614(3)
3.8	−0.5943783562400(3)	−1.10409523613(2)	−802.50235(5)	0.02227933588(4)
3.9	−0.5922096652745(6)	−1.10211292106(2)	−2100.67046(5)	0.02110420756(6)
4.0	−0.5901551408194(3)	−1.10031056014(3)	−3587.60740(5)	0.01999993037(7)
4.1	−0.58820670919815(6)	−1.09857752845(3)	−5182.64432(4)	0.01898436340(6)
4.2	−0.58635508584783(4)	−1.09684170675(2)	−6800.639409(3)	0.01806392023(5)
4.3	−0.584590871106421(9)	−1.09507189240(2)	−8363.012133(2)	0.017234848795(3)
4.4	−0.582905438381356(4)	−1.09327259865(5)	−9805.981240(5)	0.016485972297(2)
4.5	−0.581291512643715(3)	−1.091474111252(3)	−11084.4891919(3)	0.015801980897(6)
4.6	−0.579743429521856(9)	−1.08972139044(8)	−12171.927832(9)	0.015166406218(2)
4.7	−0.57825713674501(3)	−1.08806467671(2)	−13056.826287(2)	0.014563743997(3)
4.8	−0.57683003403914(9)	−1.08655338212(2)	−13737.873658(3)	0.01398055958(4)
4.9	−0.57546075129177(7)	−1.08523389600(3)	−14218.21830(5)	0.01340563400(5)
5.0	−0.57414895715282(9)	−1.08415189895(3)	−14499.16827(7)	0.01282920307(6)
5.1	−0.5728952980558(2)	−1.0833614565(4)	−14572.17972(10)	0.01224100777(7)
5.2	−0.5717016409956(3)	−1.0829493701(5)	−14405.57316(2)	0.01162575228(9)
5.3	−0.5705720931180(3)	−1.0831067819(7)	−13915.73184(3)	0.01095045365(2)
5.4	−0.5695165289452(3)	−1.0843906482(5)	−12890.28496(2)	0.01011896475(9)

5.5	−0.5685650013364(4)	−1.0890153029(2)	−10759.43793(3)	0.00874812723(2)
5.6	−0.5678478151802(6)	−1.109318402(4)	−6482.47790(3)	0.0047102194(6)
5.7	−0.5678863321072(10)	−1.169065086(4)	−7676.5116(5)	−0.0058407758(6)
5.8	−0.5687705428840(6)	−1.1994425023(7)	−16186.47024(5)	−0.01067265801(2)
5.9	−0.5699078864930(6)	−1.2096687541(7)	−22163.580062(2)	−0.01183948832(2)
6.0	−0.5711137815459(6)	−1.2155053732(7)	−26643.22611(6)	−0.01221296835(2)
6.5	−0.5772318632564(5)	−1.2324517146(7)	−41505.78498(2)	−0.01199815201(9)
7.0	−0.5830024167892(3)	−1.2431886824(6)	−50383.1223(9)	−0.01102626412(7)
7.5	−0.5882157819770(4)	−1.2498979412(6)	−55318.9623(7)	−0.00979551697(7)
8.0	−0.5927749983486(4)	−1.2529631039(5)	−57481.0197(5)	−0.00842663841(5)
8.5	−0.5966347589327(7)	−1.2528604651(5)	−57844.79261(3)	−0.00701069968(6)
9.0	−0.5997880958179(4)	−1.2500473055(6)	−57120.39043(2)	−0.00560790155(6)
9.5	−0.6022490876828(6)	−1.2448041820(7)	−55755.52598(2)	−0.00424273754(7)
10.0	−0.6040367511206(5)	−1.2372008025(8)	−53992.63663(2)	−0.00291273002(7)
11.0	−0.6056467620919(5)	−1.2148719831(2)	−49626.813613(2)	−0.00032531444(2)
12.0	−0.604785946817(3)	−1.1862188697(3)	−44563.66258(5)	0.00194608532(2)
13.0	−0.6020541085776(9)	−1.1606184765(3)	−40026.85038(6)	0.00334536467(2)
14.0	−0.598400117003(3)	−1.1429771097(4)	−36867.63541(2)	0.00384450888(2)
15.0	−0.594530173646(9)	−1.131425265(4)	−34879.65707(2)	0.00384233886(3)
16.0	−0.590782328490(4)	−1.123418738(4)	−33637.21597(2)	0.00363411987(3)
17.0	−0.587283406929(10)	−1.117464572(5)	−32851.58202(3)	0.00335895539(3)
18.0	−0.584067028544(7)	−1.112786064(7)	−32355.2495(5)	0.00307488852(4)
19.0	−0.581128783061(6)	−1.108964275(8)	−32049.5729(6)	0.0028049100(4)
20.0	−0.578449723123(9)	−1.105755551(10)	−31873.1507(7)	0.0025571948(5)

Table A16: Same as for Table A1, but for $4\,^1\Sigma_u^+$.

$4\,^1\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.2139061642326(5)	−1.4467298553(10)	31.19671(5)	−1.4555964670(2)
0.8	−0.3357691488807(5)	−1.4824204172(8)	37.56859(7)	−1.0136026493(9)
0.9	−0.4215682708968(9)	−1.4924559895(3)	44.9115839(3)	−0.7214660531(2)
1.0	−0.48309384018666(5)	−1.4872524425(5)	53.315363(7)	−0.5210647621(4)
1.1	−0.5277301720749(3)	−1.472965996(4)	62.873(4)	−0.379550592(4)
1.2	−0.5603046645387(5)	−1.4533607313(9)	73.688507(4)	−0.2772928352(7)
1.3	−0.58408368098118(7)	−1.4307960929(2)	85.876363(3)	−0.2020221007(2)
1.4	−0.6013406226560(3)	−1.4067770881(5)	99.565433(5)	−0.14578274480(3)
1.5	−0.61369549024474(3)	−1.38227404623(2)	114.899488(2)	−0.10325537717(9)
1.6	−0.6223258991366(3)	−1.35791499699(4)	132.039488(2)	−0.07078949920(2)
1.7	−0.628102586324313(7)	−1.33410479744(8)	151.165867(4)	−0.04582330870(5)
1.8	−0.63167890689482(3)	−1.31110070905(9)	172.481297(3)	−0.02652383070(5)
1.9	−0.633551397356628(7)	−1.28906133560(5)	196.2138343(2)	−0.011557126780(2)
2.0	−0.63410164005824(2)	−1.26807886400(4)	222.620676(5)	0.000062208058(2)
2.1	−0.63362574950514(2)	−1.24820061605(5)	251.992537(5)	0.009071849030(2)
2.2	−0.63235548912619(3)	−1.229443630222(3)	284.658835(5)	0.016030612741(2)
2.3	−0.63047362101576(3)	−1.211804626250(3)	320.993831(8)	0.021366354688(8)
2.4	−0.62812521411291(4)	−1.195266868836(2)	361.423946(5)	0.025409816412(8)
2.5	−0.62542607654748(3)	−1.179804925347(2)	406.436512(8)	0.028418891099(7)
2.6	−0.62246911326793(3)	−1.165387980344(2)	456.590319(7)	0.030596248535(6)
2.7	−0.61932916810914(4)	−1.151982155676(2)	512.528377(8)	0.032102289089(7)
2.8	−0.61606674617973(3)	−1.139552144721(2)	574.993472(6)	0.033064767014(7)
2.9	−0.61273090057467(3)	−1.128062376920(3)	644.847242(7)	0.033586008355(9)
3.0	−0.60936148970866(3)	−1.117477867863(4)	723.093721(6)	0.033748370518(10)
3.1	−0.60599095692708(3)	−1.10776487058(4)	810.908569(6)	0.033618401058(2)
3.2	−0.60264574523960(3)	−1.09889141942(5)	909.675556(4)	0.033250022207(2)
3.3	−0.59934743224656(3)	−1.09082784580(4)	1021.0322566(2)	0.032686975364(10)
3.4	−0.59611365039664(4)	−1.08354734311(9)	1146.9273477(9)	0.031964693437(3)
3.5	−0.59295884350638(3)	−1.07702666856(6)	1289.6921902(3)	0.031111719559(2)
3.6	−0.58989490061293(3)	−1.07124709335(6)	1452.129314(5)	0.030150752188(2)
3.7	−0.58693170191095(3)	−1.06619575871(8)	1637.619216(8)	0.029099363542(3)
3.8	−0.58407760840918(4)	−1.06186767220(9)	1850.243069(10)	0.027970406480(3)
3.9	−0.58133992718306(4)	−1.05826870827(2)	2094.909158(2)	0.026772088742(4)
4.0	−0.57872538841923(8)	−1.05542018948(3)	2377.447741(3)	0.02550764684(6)
4.1	−0.57624068030024(10)	−1.0533659664(4)	2704.58650(5)	0.02417448639(10)
4.2	−0.5738931054608(3)	−1.0521834439(7)	3083.60145(8)	0.02276256359(2)
4.3	−0.5716914509406(4)	−1.0520007316(2)	3521.18018(2)	0.02125166749(3)
4.4	−0.5696472023979(3)	−1.0530227927(9)	4020.47953(7)	0.01960718457(2)
4.5	−0.5677762688719(4)	−1.0555688758(2)	4574.2352(6)	0.0177741471(5)
4.6	−0.5661013514517(5)	−1.0601172711(3)	5149.81941(10)	0.0156707461(6)
4.7	−0.5646547754763(8)	−1.067329497(5)	5660.12108(5)	0.0131872454(2)
4.8	−0.5634805058732(3)	−1.0779645032(4)	5917.8525362(2)	0.01020760594(8)
4.9	−0.5626316181453(3)	−1.0925127994(6)	5597.591787(3)	0.00668376261(2)
5.0	−0.5621572857977(4)	−1.1104961714(8)	4287.94947(6)	0.00276368003(2)
5.1	−0.5620787050442(5)	−1.1300100982(10)	1704.68741(2)	−0.00114758591(2)
5.2	−0.5623698415715(6)	−1.1484365107(2)	−2100.18345(2)	−0.00455708222(2)
5.3	−0.5629625538277(7)	−1.1638081361(2)	−6831.27091(3)	−0.00714774122(2)
5.4	−0.5637684739687(4)	−1.1751059049(4)	−12291.86597(2)	−0.00880906610(6)

5.5	−0.5646864674261(4)	−1.18049946717(2)	−18776.84168(2)	−0.009295733148(3)
5.6	−0.5655311277245(3)	−1.1682843979(5)	−27191.51498(2)	−0.00664681116(9)
5.7	−0.56574153393586(7)	−1.1152714025(6)	−29870.79017(2)	0.00284415180(10)
5.8	−0.56520018163113(3)	−1.0907087990(5)	−24964.18138(2)	0.00684337315(9)
5.9	−0.56448059956602(3)	−1.08568220706(3)	−22331.44511(2)	0.00733542239(4)
6.0	−0.56375404891211(5)	−1.08463290886(3)	−20952.37192(2)	0.00714586483(5)
6.5	−0.56069048165735(10)	−1.08857388408(2)	−18356.44376(2)	0.005047242959(2)
7.0	−0.55866064529663(10)	−1.095230238608(2)	−17035.84113(2)	0.0031558645693(10)
7.5	−0.55743991868702(9)	−1.101201062320(2)	−15840.83945(2)	0.001823836674(5)
8.0	−0.55674825572483(7)	−1.105347014907(3)	−14751.65129(2)	0.001018687068(5)
8.5	−0.55636051351678(7)	−1.107804097994(3)	−13864.97814(3)	0.000578462240(5)
9.0	−0.55613552641502(6)	−1.109157221333(2)	−13199.61165(3)	0.0003459812774(3)
9.5	−0.55599687972581(4)	−1.1098941747154(4)	−12699.30114(2)	0.0002210089196(8)
10.0	−0.55590555705350(3)	−1.1103044937372(3)	−12276.02286(2)	0.00015066203696(4)
11.0	−0.555793967498227(9)	−1.110673544055(4)	−11372.11886(6)	0.00008312644915(3)
12.0	−0.555726877530804(7)	−1.1108002648423(2)	−10381.075432(3)	0.00005445751827(8)
13.0	−0.555681048545983(5)	−1.1108633289362(6)	−9624.639739(2)	0.000038366781212(4)
14.0	−0.555648509857390(7)	−1.11091438043860(3)	−9198.711820(8)	0.000027331376868(5)
15.0	−0.555625337538939(3)	−1.1109587261143(4)	−9009.5398356(2)	0.000019463264238(10)
16.0	−0.555608805601579(6)	−1.1109946922112(6)	−8950.102964(6)	0.000013932437001(3)
17.0	−0.555596911087659(7)	−1.1110222776525(9)	−8948.968539(2)	0.00001009085429(5)
18.0	−0.555588233968701(4)	−1.1110428389381(2)	−8967.711036(2)	0.00000742383329(7)
19.0	−0.555581798259419(3)	−1.1110580281541(2)	−8989.19966515(3)	0.00000555622972(9)
20.0	−0.55557694197560(3)	−1.1110692828982(3)	−9007.731703(3)	0.00000423005265(2)

Table A17: Same as for Table A1, but for $5\,^1\Sigma_u^+$.

$5\,^1\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.202698747624(8)	−1.424635071(5)	−4484.9581(6)	−1.456053679(5)
0.8	−0.324611637060(10)	−1.460538520(8)	−4735.5801(2)	−1.014144057(8)
0.9	−0.410469233105(10)	−1.470823574(7)	−4982.4899(3)	−0.722094564(7)
1.0	−0.472062106988(8)	−1.465906871(8)	−5218.1260(3)	−0.521782657(7)
1.1	−0.51677476061(5)	−1.451944726(3)	−5433.851(7)	−0.380359277(2)
1.2	−0.54943467753(3)	−1.432700440(2)	−5619.995(6)	−0.278192570(2)
1.3	−0.57330817874(3)	−1.410531616(2)	−5766.1030(3)	−0.203011737(9)
1.4	−0.59066847095(3)	−1.386940260(2)	−5861.4123(3)	−0.146859513(9)
1.5	−0.603135191497(10)	−1.362892537(2)	−5895.5510(3)	−0.104414770(9)
1.6	−0.611885418804(4)	−1.339011322(2)	−5859.4071(3)	−0.072025303(9)
1.7	−0.617789190774(4)	−1.3156956526(2)	−5746.06846(4)	−0.0471278065(10)
1.8	−0.621499031411(3)	−1.2931968217(3)	−5551.6874388(2)	−0.0278881994(10)
1.9	−0.623510562954(3)	−1.2716679486(3)	−5276.11637(4)	−0.0129720119(10)
2.0	−0.624204434706(7)	−1.2511968930(3)	−4923.18326(2)	−0.0013940118(2)
2.1	−0.623875883460(3)	−1.2318284367(3)	−4500.55415(2)	0.0075825382(9)
2.2	−0.622755926597(3)	−1.2135793604(3)	−4019.21949(3)	0.0145147694(10)
2.3	−0.62102678250(4)	−1.1964487138(3)	−3492.72869(4)	0.0198281962(10)
2.4	−0.618833237390(3)	−1.1804247734(3)	−2936.3486(4)	0.0238507089(9)
2.5	−0.616291119942(3)	−1.1654896950(3)	−2366.3243(4)	0.0268370179(8)
2.6	−0.613493682603(3)	−1.1516225454(3)	−1799.3811(4)	0.0289864691(8)
2.7	−0.610516447970(3)	−1.1388011694(2)	−1252.5440(4)	0.0304561950(7)
2.8	−0.607420915206(3)	−1.1270031726(2)	−743.27622(4)	0.0313709492(6)
2.9	−0.604257408058(3)	−1.1162061552(2)	−289.87022(3)	0.0318305727(5)
3.0	−0.601067265331(3)	−1.1063872060(2)	88.04917(2)	0.0319157749(5)
3.1	−0.597884516311(7)	−1.097521590(6)	369.13007(9)	0.0316927231(2)
3.2	−0.594737141533(3)	−1.0895805430(2)	530.324517(3)	0.03121679375(3)
3.3	−0.591647990785(2)	−1.0825281685(7)	547.75357(2)	0.03053570093(2)
3.4	−0.58863541577(7)	−1.07631778007(2)	398.84124(2)	0.029692073958(3)
3.5	−0.585713675572(4)	−1.0708884697(9)	65.9894(7)	0.0287253947(5)
3.6	−0.582893189761(4)	−1.0661633621(3)	−458.4192(7)	0.0276730604(7)
3.7	−0.580180740449(3)	−1.062051350(4)	−1166.7294(6)	0.0265703055(10)
3.8	−0.577579744019(3)	−1.058453661(4)	−2032.3449(4)	0.0254489019(10)
3.9	−0.5750907017186(8)	−1.055274975(5)	−3009.83107(2)	0.0243349816(2)
4.0	−0.5727118795011(5)	−1.052436589(4)	−4039.92985(5)	0.0232467925(10)
4.1	−0.57044017454969(4)	−1.0498875968(4)	−5058.52048(8)	0.02219335421(10)
4.2	−0.5682720441149(5)	−1.047610786(6)	−6006.59101(4)	0.0211745958(2)
4.3	−0.566204349790(3)	−1.045622570(2)	−6837.8256(7)	0.0201828209(3)
4.4	−0.5642350196979(6)	−1.0439692415(3)	−7521.72894(7)	0.0192047268(6)
4.5	−0.5623635200353(7)	−1.042723267(4)	−8042.23511(5)	0.0182230606(8)
4.6	−0.560591206703(2)	−1.041982817(5)	−8393.20913(4)	0.0172173037(10)
4.7	−0.558921660050(3)	−1.041875404(6)	−8572.69833(2)	0.0161633865(2)
4.8	−0.5573610644606(10)	−1.042562165(4)	−8577.72521(3)	0.0150333258(7)
4.9	−0.555918540232(3)	−1.044231551(4)	−8401.6685(4)	0.0137970468(8)
5.0	−0.554606051944(3)	−1.047065065(5)	−8037.0402(6)	0.0124294077(9)
5.1	−0.553437400176(3)	−1.051182772(5)	−7485.3943(7)	0.0109200055(9)
5.2	−0.552426762276(4)	−1.056656743(5)	−6769.3265(9)	0.0092686119(8)
5.3	−0.551588911394(4)	−1.063641755(4)	−5936.4492(10)	0.0074596354(6)
5.4	−0.550940811352(3)	−1.0723189756(2)	−5056.8514(8)	0.00547456429(3)

5.5	−0.550497606148(3)	−1.0823660837(7)	−4220.2221(8)	0.00338711427(7)
5.6	−0.550259504182(3)	−1.09258344798(10)	−3517.5016(7)	0.00141706435(6)
5.7	−0.550202087571(3)	−1.1015180007(5)	−3002.5642(6)	−0.00019540799(2)
5.8	−0.5502831882371(8)	−1.1084029094(4)	−2673.60053(4)	−0.00135112637(9)
5.9	−0.5504585414690(7)	−1.1132799127(4)	−2493.23931(3)	−0.00209539487(8)
6.0	−0.5506919579335(6)	−1.11656409513(3)	−2416.92949(3)	−0.00253002988(7)
6.5	−0.5520719643808(3)	−1.12143357808(8)	−2605.08026(6)	−0.002659946050(2)
7.0	−0.55324148375147(9)	−1.12051750958(5)	−2744.681263(3)	−0.002004934582(9)
7.5	−0.55408977133408(8)	−1.11876255423(4)	−2546.242879(2)	−0.001411068209(7)
8.0	−0.55467602594838(7)	−1.117001501288(2)	−2100.9937239(8)	−0.0009561811740(4)
8.5	−0.55506617184247(5)	−1.1154244137705(3)	−1558.022321(5)	−0.0006225964807(10)
9.0	−0.55531488489987(4)	−1.114109632537(5)	−1029.2418101(3)	−0.00038665141526(2)
9.5	−0.55546544660127(4)	−1.113082832888(4)	−584.673845(7)	−0.000226519966925(3)
10.0	−0.55555076835428(3)	−1.1123283105005(3)	−274.590288(3)	−0.0001226773792152(3)
11.0	−0.55561398263426(3)	−1.1114673168019(7)	−163.25934(5)	−0.00002175923032(2)
12.0	−0.555617638054840(5)	−1.1111439754057(2)	−514.054090(2)	0.00000760839199(2)
13.0	−0.555606591245903(3)	−1.1110503912403(10)	−842.6730314(10)	0.00001252240396(7)
14.0	−0.555594581646624(8)	−1.1110339552445(2)	−967.864545(2)	0.00001108628919(7)
15.0	−0.5555847236645352(6)	−1.1110400982439(2)	−937.00733(5)	0.00000862327234(9)
16.0	−0.5555772344878559(3)	−1.1110515447048(9)	−830.46230(5)	0.00000643276693(5)
17.0	−0.55557169325546418(4)	−1.1110629778741(9)	−703.52041(6)	0.00000472991982(5)
18.0	−0.55556762820741856(4)	−1.1110728804206(6)	−584.43178(7)	0.000003465333012(3)
19.0	−0.5555646487193081(3)	−1.1110809849967(5)	−483.73008(6)	0.000002542760103(2)
20.0	−0.55556245831105189(4)	−1.1110874370890(5)	−402.78092(7)	0.000001873976656(3)

Table A18: Same as for Table A1, but for $6\,^1\Sigma_u^+$.

$6\,^1\Sigma_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.202641543808(5)	−1.424176569(7)	17.23258(2)	−1.455562116(8)
0.8	−0.324500857535(3)	−1.459852575(5)	20.6958(4)	−1.013563575(5)
0.9	−0.410295833993(3)	−1.469871654(4)	24.6801(5)	−0.721422207(4)
1.0	−0.4718167774298(3)	−1.4646496340(10)	29.2380280(2)	−0.5210160792(7)
1.1	−0.51644799587222(4)	−1.45034268205(3)	34.421681(6)	−0.37949699119(2)
1.2	−0.54901687824994(2)	−1.43071481602(2)	40.288392(7)	−0.27723421627(2)
1.3	−0.5727897769928(3)	−1.4081254010(4)	46.902090(8)	−0.20195834382(4)
1.4	−0.5900400802291(3)	−1.3840793503(2)	54.334260(3)	−0.1457137070(2)
1.5	−0.60238777308499(9)	−1.3595468809(2)	62.664955(2)	−0.1031808898(6)
1.6	−0.6110104526310(3)	−1.3351558875(7)	71.983953(10)	−0.0707093639(4)
1.7	−0.61677883438837(5)	−1.311311067(6)	82.39211(3)	−0.0457372936(3)
1.8	−0.62034624836547(5)	−1.288269494(4)	94.00295(2)	−0.0264316653(2)
1.9	−0.62220920185797(3)	−1.2661895467(3)	106.94450(2)	−0.0114584963(2)
2.0	−0.62274924325695(4)	−1.2451631482(4)	121.361487(2)	0.00016766918(2)
2.1	−0.6222624476602(3)	−1.22523730934(2)	137.417930(3)	0.00918456475(7)
2.2	−0.6209805328213(2)	−1.20642870245(3)	155.300186(3)	0.01615107418(2)
2.3	−0.6190862079500(3)	−1.18873361634(2)	175.220613(3)	0.02149513024(6)
2.4	−0.6167244807978(2)	−1.17213480914(3)	197.421937(6)	0.02554756353(10)
2.5	−0.6140110887424(2)	−1.15660625298(2)	222.182531(4)	0.02856636980(5)
2.6	−0.6110388549557(2)	−1.14211643337(2)	249.82278(4)	0.03075433713(4)
2.7	−0.6078825287852(3)	−1.12863065146(2)	280.712889(2)	0.03227200226(4)
2.8	−0.6046025061957(3)	−1.11611263771(2)	315.282399(3)	0.03324727667(4)
2.9	−0.6012477142481(3)	−1.10452569267(8)	354.031987(2)	0.033782667526(3)
3.0	−0.5978578658818(4)	−1.09383351032(10)	397.548069(9)	0.033960740479(3)
3.1	−0.5944652366487(3)	−1.08400079999(2)	446.521007(9)	0.03384828171(4)
3.2	−0.5910960762671(3)	−1.07499380000(3)	501.767827(2)	0.03349948517(9)
3.3	−0.5877717401608(3)	−1.0667807662(4)	564.260477(9)	0.03295839822(2)
3.4	−0.5845096063642(3)	−1.0593325210(5)	635.160631(2)	0.03226079171(2)
3.5	−0.5813238292462(3)	−1.0526231671(7)	715.86144(5)	0.03143556895(2)
3.6	−0.5782259722003(4)	−1.0466311142(10)	808.03488(9)	0.03050578617(3)
3.7	−0.5752255562020(6)	−1.0413406411(2)	913.67855(2)	0.0294893166(5)
3.8	−0.5723305601326(6)	−1.0367443729(3)	1035.14388(4)	0.0283991440(7)
3.9	−0.5695479131869(9)	−1.032847317(5)	1175.0991(6)	0.0272432075(2)
4.0	−0.566884032335(5)	−1.029673612(7)	1336.3110(8)	0.0260236131(2)
4.1	−0.564345484236(5)	−1.027278076(2)	1520.9610(2)	0.0247348517(3)
4.2	−0.561939901191(7)	−1.025766301(3)	1728.7917(2)	0.023360357(5)
4.3	−0.559677367918(10)	−1.02532959(4)	1952.3452(3)	0.021866314(9)
4.4	−0.557572619296(2)	−1.026302710(5)	2165.05483(2)	0.0201914838(10)
4.5	−0.555648421851(3)	−1.029241072(9)	2292.77000(4)	0.0182346159(2)
4.6	−0.553939738997(4)	−1.034936003(2)	2154.1123(6)	0.015857277(4)
4.7	−0.552494223188(6)	−1.044015779(3)	1381.2751(3)	0.012972908(6)
4.8	−0.551354534192(3)	−1.055523411(5)	−516.4681(6)	0.0098303452(9)
4.9	−0.550509617707(3)	−1.065513115(4)	−3659.0237(9)	0.0072461471(8)
5.0	−0.549858443017(3)	−1.0695556705(3)	−7325.1532(10)	0.0060322431(4)
5.1	−0.549258749173(3)	−1.06727594402(4)	−10490.1113(10)	0.006125794961(2)
5.2	−0.548614881226(3)	−1.0619958838(6)	−12650.8192(8)	0.00677574589(2)
5.3	−0.547908676997(3)	−1.0571868319(5)	−13865.8296(6)	0.00728877775(2)
5.4	−0.547171579357(2)	−1.05449178440(2)	−14347.8781(5)	0.007379884131(6)

5.5	−0.546445037727(2)	−1.0538077682(8)	−14226.3188(4)	0.00710587404(2)
5.6	−0.545755698385(2)	−1.0541551696(2)	−13614.6076(4)	0.00667075485(3)
5.7	−0.545111046755(2)	−1.0547361000(2)	−12731.30057(3)	0.00622561290(3)
5.8	−0.544510214674(6)	−1.055441000(10)	−11820.4877(10)	0.0057895568(2)
5.9	−0.543954125096(6)	−1.056493042(2)	−11023.5822(7)	0.0053246115(2)
6.0	−0.543447051824(7)	−1.058047370(2)	−10377.5313(4)	0.0048077890(2)
6.5	−0.541776292713(7)	−1.071273367(2)	−8587.2512(5)	0.0018891105(2)
7.0	−0.541331654425(7)	−1.081104033(9)	−7161.3645(6)	0.0002227537(2)
7.5	−0.541289909323(5)	−1.081885087(4)	−5672.14737(3)	0.0000926308(5)
8.0	−0.541181860253(5)	−1.079650697(5)	−4597.14632(3)	0.0003391279(5)
8.5	−0.540972160924(3)	−1.0779420786(2)	−3932.21314(2)	0.00047085214(2)
9.0	−0.540737779255(3)	−1.0774795113(2)	−3530.09725(7)	0.00044400525(2)
9.5	−0.540546319996(3)	−1.0781699992(2)	−3309.86328(7)	0.00030764639(2)
10.0	−0.540441347155(3)	−1.0798488587(2)	−3261.61182(6)	0.00010338357(2)
11.0	−0.540590594603(3)	−1.0858128650(2)	−3803.15758(5)	−0.00042106144(2)
12.0	−0.541303924753(3)	−1.0946731750(2)	−5356.08241(6)	−0.00100544379(2)
13.0	−0.542575402077(3)	−1.1047973888(2)	−7663.35938(3)	−0.00151127574(2)
14.0	−0.544253876152(4)	−1.1137549124(2)	−9982.0715(5)	−0.00180336858(2)
15.0	−0.546098788249(4)	−1.1199324115(2)	−11681.6164(6)	−0.00184898900(2)
16.0	−0.547891392065(3)	−1.1232032591(2)	−12603.2024(8)	−0.00171377969(2)
17.0	−0.549495899070(6)	−1.1242591586(3)	−12897.1536(10)	−0.00148631532(2)
18.0	−0.550855689336(4)	−1.1239028468(3)	−12782.6318(10)	−0.00123285935(2)
19.0	−0.551965794737(6)	−1.1227654529(3)	−12439.7143(2)	−0.00099125597(10)
20.0	−0.552848073525(3)	−1.1212737750(2)	−11990.8930(2)	−0.00077888140(9)

Table A19: Same as for Table A1, but for $7\,^1\Sigma_u^+$.

$7\,^1\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.1965562674(5)	−1.4121946(5)	−2592.734(3)	−1.4558315(6)
0.8	−0.31844497168(5)	−1.44799578(6)	−2733.102(9)	−1.01388229(6)
0.9	−0.40427435518(5)	−1.45816139(6)	−2870.156(9)	−0.72179186(5)
1.0	−0.4658348636(2)	−1.45310759(3)	−2999.38(6)	−0.52143787(3)
1.1	−0.51051090051(5)	−1.43899057(5)	−3115.668(2)	−0.37997161(4)
1.2	−0.54312988844(4)	−1.41957374(5)	−3213.344(2)	−0.27776163(4)
1.3	−0.56695813656(5)	−1.39721527(5)	−3286.354(2)	−0.20253769(4)
1.4	−0.58426889886(6)	−1.37341821(6)	−3328.555(2)	−0.14634315(4)
1.5	−0.59668192667(3)	−1.349150228(4)	−3334.151(6)	−0.103857583(2)
1.6	−0.60537448219(7)	−1.32503611(4)	−3298.206(5)	−0.071429470(2)
1.7	−0.61121685295(6)	−1.30147711(4)	−3217.199(4)	−0.046496124(2)
1.8	−0.61486186757(7)	−1.278726811(2)	−3089.5080(9)	−0.027223931(10)
1.9	−0.61680548867(6)	−1.256940429(3)	−2915.7465(5)	−0.012278659(10)
2.0	−0.61742871595(7)	−1.236207489(3)	−2698.87518(2)	−0.000675028(10)
2.1	−0.61702711596(4)	−1.216573699(3)	−2444.0686(8)	0.008324063(9)
2.2	−0.61583198344(7)	−1.19805581(4)	−2158.3682(3)	0.015276431(2)
2.3	−0.61402573097(7)	−1.180651776(4)	−1850.2049(3)	0.020608559(2)
2.4	−0.61175322987(5)	−1.164347568(3)	−1528.9026(3)	0.024649538(9)
2.5	−0.60913026530(4)	−1.149121933(2)	−1204.2656(3)	0.027655439(7)
2.6	−0.60624990564(4)	−1.134949499(2)	−886.3307(2)	0.029827043(5)
2.7	−0.60318734535(4)	−1.121802818(2)	−585.3199(2)	0.031322916(4)
2.8	−0.60000361643(7)	−1.10965363(2)	−311.790(5)	0.03226914(4)
2.9	−0.59674845137(7)	−1.09847348(10)	−76.9231(7)	0.032766697(3)
3.0	−0.59346249975(6)	−1.0882337450(3)	107.12175(2)	0.0328970848(6)
3.1	−0.59017904458(6)	−1.07890503(5)	226.967(7)	0.032726791(2)
3.2	−0.58692532206(5)	−1.070456078(3)	268.088(10)	0.032310801(5)
3.3	−0.5837235207(2)	−1.062851839(6)	215.502(2)	0.0316955157(2)
3.4	−0.58059151863(9)	−1.056051324(2)	55.378(10)	0.030921092(6)
3.5	−0.57754341332(5)	−1.050005534(2)	−222.227(5)	0.030023226(6)
3.6	−0.57458990810(6)	−1.04465666(6)	−619.703(8)	0.029034211(2)
3.7	−0.57173863658(3)	−1.039939829(3)	−1128.1385(2)	0.027983093(7)
3.8	−0.568994520991(7)	−1.035788656(2)	−1725.00476(3)	0.026894839(5)
3.9	−0.56636025444(2)	−1.032144325(2)	−2374.9103(4)	0.025788765(4)
4.0	−0.563836955134(6)	−1.02896679(4)	−3034.053(4)	0.024676780(10)
4.1	−0.561424980109(8)	−1.026245643(3)	−3657.1654(4)	0.023562029(8)
4.2	−0.55912484278(3)	−1.02400947(6)	−4204.208(6)	0.022438145(2)
4.3	−0.55693819400(4)	−1.02233540(8)	−4643.969(8)	0.021288600(2)
4.4	−0.55486890009(6)	−1.02136259(2)	−4952.973(9)	0.020085276(3)
4.5	−0.55292431640(8)	−1.02131104(2)	−5109.518(8)	0.01878613(4)
4.6	−0.55111672431(10)	−1.02249083(2)	−5083.474(4)	0.01733535(4)
4.7	−0.54946423512(10)	−1.02525181(2)	−4824.707(6)	0.01567589(4)
4.8	−0.5479896236(3)	−1.02986034(2)	−4264.218(2)	0.01377477(4)
4.9	−0.5467181810(3)	−1.03657654(2)	−3362.105(3)	0.011604044(2)
5.0	−0.5456800818(2)	−1.0458544145(5)	−2199.0782(2)	0.009101149826(9)
5.1	−0.54490499451(10)	−1.05713340(5)	−1009.814(2)	0.006407174(2)
5.2	−0.54438443098(8)	−1.06723096(10)	−92.839(8)	0.004141903(2)
5.3	−0.54403937782(5)	−1.07232365(10)	353.7003(2)	0.002972661(2)
5.4	−0.54374804748(5)	−1.07107240(2)	276.3446(2)	0.003041425(3)

5.5	−0.54340186291(3)	−1.06492121(7)	−306.91685(4)	0.003978639(2)
5.6	−0.542943778177(5)	−1.056900679(3)	−1284.0602(7)	0.005176228(5)
5.7	−0.5423749700448(7)	−1.0497762462(3)	−2415.09973(2)	0.0061357358(4)
5.8	−0.541730622372(5)	−1.044697916(2)	−3461.5699(2)	0.0066833325(3)
5.9	−0.541050202482(8)	−1.041535834(2)	−4310.820(4)	0.0068753509(4)
6.0	−0.54036358648(2)	−1.039774811(2)	−4956.762(6)	0.0068253935(4)
6.5	−0.5372957390352(7)	−1.0403341026(5)	−6364.8799(4)	0.00527036546(7)
7.0	−0.5351121055207(3)	−1.045619996389(2)	−6536.66657(4)	0.0035148878074(2)
7.5	−0.5337080158909(5)	−1.05104268813(6)	−6232.16911(2)	0.002183112486(2)
8.0	−0.532851179857(4)	−1.0551963414(2)	−5767.340(4)	0.00131325230(3)
8.5	−0.532337574887(3)	−1.0579885050(2)	−5374.6277(4)	0.00078666408(5)
9.0	−0.5320290194529(9)	−1.05978713198(7)	−5132.6386(2)	0.000474545213(2)
9.5	−0.5318423866878(4)	−1.06095281892(5)	−5016.711985(6)	0.000287574155(3)
10.0	−0.5317292665811(4)	−1.0617130057(6)	−4974.21909(2)	0.00017455274(5)
11.0	−0.5316140103275(3)	−1.06237460306(2)	−5056.07680(5)	0.000077583418(9)
12.0	−0.5315491139527(3)	−1.06240695652(2)	−5331.35268(2)	0.000057605949(2)
13.0	−0.5314948265179(3)	−1.06232347995(9)	−5490.21635(2)	0.000051244083(7)
14.0	−0.5314469154046(10)	−1.0622728796(5)	−5355.34502(3)	0.000044353660(3)
15.0	−0.531406369096(4)	−1.0622618172(2)	−4984.8838(3)	0.00003672806(10)
16.0	−0.531373303038(4)	−1.0622738665(2)	−4518.0693(4)	0.00002954622(6)
17.0	−0.531346928831(5)	−1.0622961940(3)	−4060.9393(3)	0.00002339198(9)
18.0	−0.531326139881(6)	−1.0623216396(2)	−3663.4204(3)	0.00001836890(5)
19.0	−0.531309849441(6)	−1.0623466891(6)	−3337.9999(3)	0.000014368932(2)
20.0	−0.53129711748324(5)	−1.0623697789719(3)	−3080.0970(4)	0.000011222799719(3)

Table A20: Same as for Table A1, but for $8\,^1\Sigma_u^+$.

$8\,^1\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.465693148443(5)	−1.45238010024(2)	17.5358657(2)	−0.520993803353(9)
1.1	−0.510322026051(2)	−1.438063738210(7)	20.6275253(2)	−0.379472441916(3)
1.2	−0.542888337542(4)	−1.41842548023(2)	24.1267667(5)	−0.277207337623(8)
1.3	−0.566658429219(5)	−1.39582464821(2)	28.07210192(8)	−0.201929069052(7)
1.4	−0.583905681935(4)	−1.37176610392(2)	32.50661638(2)	−0.145681957176(5)
1.5	−0.596250072236(2)	−1.347220002257(6)	37.47858887(5)	−0.103146571857(2)
1.6	−0.6048691871190(8)	−1.322814164698(3)	43.04220498(8)	−0.0706723690376(9)
1.7	−0.6106337303137(4)	−1.298953201107(2)	49.25838382(10)	−0.0456974944001(4)
1.8	−0.614197018055(2)	−1.275894079710(6)	56.19574785(6)	−0.026388913111(2)
1.9	−0.6160555415697(7)	−1.253795057001(4)	63.931762840(6)	−0.0114126178217(10)
2.0	−0.616590830522(2)	−1.2327479091662(8)	72.55408162(5)	0.000216875936(2)
2.1	−0.616098938183(6)	−1.2127994724504(2)	82.16213556(2)	0.009237335188(6)
2.2	−0.61481155687(2)	−1.19396621163(3)	92.869021(4)	0.0162076827735(10)
2.3	−0.612911366089(8)	−1.17624416846(2)	104.803775(3)	0.0215558972694(9)
2.4	−0.6105433389656(6)	−1.159615806431(2)	118.11405984(9)	0.0256128631252(2)
2.5	−0.6078231723758(4)	−1.1440547454198(9)	132.96944376(10)	0.02863663973270(9)
2.6	−0.6048436420466(3)	−1.1295290485910(7)	149.5653820(2)	0.03083009057776(8)
2.7	−0.601679441649(2)	−1.1160035092425(2)	168.1280521(2)	0.032353842241(2)
2.8	−0.5983909016304(10)	−1.1034412447891(5)	188.9203101(2)	0.0333359137386(9)
2.9	−0.5950268717287(7)	−1.0918048126334(6)	212.2490375(2)	0.0338789416626(7)
3.0	−0.5916269733028(3)	−1.081057001468(2)	238.4742490(2)	0.0340656483793(3)
3.1	−0.5882233730089(3)	−1.071161411942(4)	268.0203989(2)	0.0339630109922(9)
3.2	−0.5848421905002(3)	−1.062082916757(5)	301.39038230(2)	0.033625457576(2)
3.3	−0.5815046250901(4)	−1.053788079349(6)	339.1826922(3)	0.033097324494(2)
3.4	−0.5782278664546(4)	−1.046245612301(7)	382.1119129(5)	0.032414741355(2)
3.5	−0.5750258404714(5)	−1.03942697507(2)	431.0318070(10)	0.031607058822(3)
3.6	−0.5719098319556(7)	−1.03330725451(2)	486.957793(2)	0.030697891501(5)
3.7	−0.568889020916(2)	−1.02786656063(3)	551.079365(4)	0.029705805731(7)
3.8	−0.565970968462(2)	−1.02309234511(5)	624.737534(6)	0.02864462943(2)
3.9	−0.56316209451(2)	−1.0189833990(4)	709.30362(5)	0.02752327949(8)
4.0	−0.56046820648(2)	−1.0155569960(6)	805.79720(7)	0.0263448542(2)
4.1	−0.55789517626(4)	−1.012862112(2)	913.8187(2)	0.0251044488(3)
4.2	−0.55544994231(7)	−1.011004625(3)	1028.6622(2)	0.0237845857(5)
4.3	−0.5531421684(2)	−1.010195556(5)	1133.5010(2)	0.0223462281(10)
4.4	−0.55098712164(3)	−1.0108359086(10)	1178.371027(6)	0.0207132579(3)
4.5	−0.54901019239(6)	−1.013603266(3)	1028.05311(7)	0.0187593598(5)
4.6	−0.5472499526(10)	−1.01917252(4)	375.008(3)	0.016375517(8)
4.7	−0.54574143551(2)	−1.0264679964(6)	−1192.575445(6)	0.0138329520(2)
4.8	−0.54445616768(2)	−1.03087701312(5)	−3554.04324(3)	0.01209069212(2)
4.9	−0.543277933792(9)	−1.02944938756(4)	−5761.61933(3)	0.01165438367(2)
5.0	−0.542106228321(7)	−1.02522876298(5)	−7156.35631(3)	0.01179673873(2)

Table A21: Same as for Table A1, but for $9\,^1\Sigma_u^+$.

	$9\,^1\Sigma_u$			
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46567859703(3)	−1.4523257273(2)	2.371662(2)	−0.5209685332(2)
1.1	−0.51030481589(2)	−1.43799860715(10)	2.8389724(8)	−0.37944452307(7)
1.2	−0.542868199239(8)	−1.41834841084(6)	3.3658702(5)	−0.27717667697(3)
1.3	−0.566635083266(5)	−1.39573439068(3)	3.9565579(4)	−0.20189555703(2)
1.4	−0.583878836951(3)	−1.37166132564(2)	4.6155973(3)	−0.145645465527(8)
1.5	−0.596219422965(2)	−1.34709927219(2)	5.3479434(2)	−0.103106950843(5)
1.6	−0.604834412121(2)	−1.322675934880(7)	6.15898323(9)	−0.070629444149(3)
1.7	−0.6105944892952(8)	−1.298795784634(5)	7.05458014(7)	−0.045651062379(2)
1.8	−0.6141529487651(6)	−1.275715624444(3)	8.04112294(6)	−0.0263387371746(10)
1.9	−0.6160062561699(4)	−1.253593514009(2)	9.12558203(4)	−0.0113584219310(6)
2.0	−0.6165359113217(3)	−1.232520994626(2)	10.31557214(3)	0.0002754140086(4)
2.1	−0.6160379326163(2)	−1.2125446215028(7)	11.61942304(2)	0.0093005922523(2)
2.2	−0.61474397153723(10)	−1.1936805220906(5)	13.04625911(2)	0.01627610044719(2)
2.3	−0.61283665970117(6)	−1.1759243318644(3)	14.606089015(7)	0.02162999458173(6)
2.4	−0.61046091380702(4)	−1.1592580226922(2)	16.309906786(5)	0.02569325205078(3)
2.5	−0.60773236409172(3)	−1.14365461667205(9)	18.169806122(4)	0.02872404460456(2)
2.6	−0.60474370724376(2)	−1.12908144591727(6)	20.199109654(3)	0.030925372527022(9)
2.7	−0.601569542717653(10)	−1.11550240366023(4)	22.412515444(2)	0.032458030287064(5)
2.8	−0.598270088045028(6)	−1.10287949069371(2)	24.826263279(2)	0.033450244784408(3)
2.9	−0.594894056768207(4)	−1.09117386700873(2)	27.458323742(2)	0.034004912595753(3)
3.0	−0.591480904777409(3)	−1.080346554979362(10)	30.3286135754(9)	0.034205084858485(2)
3.1	−0.588062596003195(2)	−1.070358897122490(7)	33.4592414361(8)	0.034118159639968(2)
3.2	−0.584664999329707(2)	−1.061172841600273(6)	36.8747888821(6)	0.0337991115809814(9)
3.3	−0.5813090004188324(10)	−1.052751107852087(4)	40.6026323042(7)	0.0332929978744175(6)
3.4	−0.5780113916133233(7)	−1.045057270146031(4)	44.6733125811(7)	0.0326369156119456(7)
3.5	−0.5747855879936831(6)	−1.038055786493163(5)	49.1209605422(10)	0.031861539855487(2)
3.6	−0.5716422064619846(8)	−1.031711992962891(10)	53.983787932(2)	0.030992338878077(3)
3.7	−0.568589536340687(2)	−1.02599207808316(2)	59.304655572(3)	0.030050539080597(3)
3.8	−0.565633923646694(3)	−1.02086304809087(2)	65.13173293(3)	0.029053894526975(6)
3.9	−0.562780086388447(5)	−1.01629269089313(5)	71.51926656(2)	0.028017303047120(10)
4.0	−0.560031374546647(8)	−1.01224954441574(10)	78.52847890(3)	0.02695330116939(3)
4.1	−0.55738998555406(2)	−1.0087028733638(5)	86.2286245(3)	0.0258724628645(2)
4.2	−0.55485714388014(3)	−1.0056226571974(5)	94.69823639(7)	0.02478372156259(10)
4.3	−0.55243325160154(2)	−1.0029795914413(2)	104.02659524(5)	0.02369463064227(4)
4.4	−0.55011801550314(2)	−1.0007451056965(6)	114.3153515(2)	0.0226115739340(2)
4.5	−0.54791055536378(6)	−0.998891422151(4)	125.6784165(3)	0.0215399307947(9)
4.6	−0.5458095022605(7)	−0.9973928911(2)	138.07530(3)	0.02048393769(4)
4.7	−0.544052874(7)	−1.01530618(6)	−2146.643(8)	0.015489270(8)
4.8	−0.542603982(7)	−1.020640210(6)	−1187.640(4)	0.013451610(4)
4.9	−0.541369125(5)	−1.02765209(6)	−260.940(2)	0.01124207(2)
5.0	−0.540341440322(4)	−1.0333277369(2)	236.242023(4)	0.00947102875(3)

Table A22: Same as for Table A1, but for $10\,^1\Sigma_u^+$.

$10\,^1\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46209096234(8)	−1.4454439155(8)	−1880.2926(4)	−0.5212619908(7)
1.1	−0.50674832441(9)	−1.4312480140(9)	−1950.0337(4)	−0.3797739683(7)
1.2	−0.53934645377(6)	−1.4117434394(6)	−2007.4726(2)	−0.2775421099(4)
1.3	−0.56315166089(7)	−1.3892887064(7)	−2048.8067(2)	−0.2022964497(5)
1.4	−0.58043723261(8)	−1.3653874368(9)	−2070.2210(2)	−0.1460806940(5)
1.5	−0.59282298801(4)	−1.3410081261(4)	−2068.16656(5)	−0.1035747667(3)
1.6	−0.60148629275(3)	−1.3167765912(3)	−2039.69361(2)	−0.0711275036(2)
1.7	−0.60729757134(7)	−1.2930952340(6)	−1982.79645(3)	−0.0461765243(3)
1.8	−0.6109098159(3)	−1.270218814(3)	−1896.7121(3)	−0.026888434(2)
1.9	−0.6128191681(7)	−1.24830360(7)	−1782.113(3)	−0.01192909(4)
2.0	−0.6134068111(2)	−1.227439968(2)	−1641.16812(5)	−0.0003131731(6)
2.1	−0.6129684765(2)	−1.2076739425(10)	−1477.41247(8)	0.0086966717(4)
2.2	−0.6117355950(5)	−1.189022163(5)	−1295.53176(10)	0.015658649(2)
2.3	−0.6098906679(5)	−1.171481828(5)	−1101.0379(2)	0.020999786(2)
2.4	−0.6075785938(5)	−1.155037572(4)	−899.9566(2)	0.025049840(2)
2.5	−0.6049151149(5)	−1.139666170(4)	−698.5761(2)	0.028065624(2)
2.6	−0.6019931793(5)	−1.125339719(4)	−503.3085(2)	0.030248708(2)
2.7	−0.5988877826(5)	−1.112027775(4)	−320.6835(2)	0.0317584408(10)
2.8	−0.5956596807(7)	−1.099698733(5)	−157.4698(2)	0.0327216529(10)
2.9	−0.5923582605(6)	−1.088320626(4)	−20.8858(3)	0.0332399637(7)
3.0	−0.5890237681(5)	−1.077861431(3)	81.1619(3)	0.0333953684(5)
3.1	−0.5856890471(4)	−1.068288915(2)	139.9172(4)	0.0332545738(2)
3.2	−0.5823808885(3)	−1.0595700126(7)	145.8427(4)	0.03287242636(2)
3.3	−0.5791210747(3)	−1.051669758432(4)	89.1246(4)	0.0322946637(2)
3.4	−0.5759271760(2)	−1.0445499475(5)	−39.1598(3)	0.0315601188(3)
3.5	−0.5728131524(2)	−1.0381679302(8)	−245.0724(2)	0.0307023926(3)
3.6	−0.56978981830(6)	−1.0324763433(9)	−529.18244(6)	0.0297509147(3)
3.7	−0.56686523726(5)	−1.027424824(2)	−883.90709(4)	0.0287312569(4)
3.8	−0.564045126181(2)	−1.0229646434(2)	−1291.956392(2)	0.02766463392(3)
3.9	−0.5613333460108(4)	−1.01905653506(5)	−1727.051858(5)	0.02656670691(2)
4.0	−0.558732533834(4)	−1.0156810067(3)	−2157.24712(3)	0.02544601523(7)
4.1	−0.556244899681(9)	−1.0128505189(5)	−2549.67261(4)	0.02430226353(10)
4.2	−0.55387320709(2)	−1.0106244628(7)	−2874.26888(6)	0.0231242741(2)
4.3	−0.55162200330(4)	−1.009130215(2)	−3103.82712(7)	0.0218869282(3)
4.4	−0.54949920580(8)	−1.008589623(3)	−3208.03557(7)	0.0205474519(5)
4.5	−0.54751783895(6)	−1.009316878(2)	−3139.56942(2)	0.0190486223(3)
4.6	−0.5456961464(3)	−1.011568558(5)	−2816.2125(3)	0.0173529858(10)
4.7	−0.543813030658159(8)	−0.9962192557154(10)	152.0310702(3)	0.0194482565108(3)
4.8	−0.541919053733511(2)	−0.99534871929512(7)	167.60881311(2)	0.01843528920248(2)
4.9	−0.5401251261214282(8)	−0.99475659431216(3)	184.842990753(6)	0.017447685291980(6)
5.0	−0.538428600477727(2)	−0.99441944609552(7)	204.05034258(2)	0.01648755097199(2)

Table A23: Same as for Table A1, but for $11\,^1\Sigma_u^+$.

$11\,^1\Sigma_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46200181622(4)	−1.4449858909(2)	11.277637(2)	−0.5209822584(2)
1.1	−0.50662948034(2)	−1.43066464431(8)	13.2594652(8)	−0.37945971240(5)
1.2	−0.539194458336(6)	−1.41102098669(4)	15.5025792(6)	−0.27719339168(3)
1.3	−0.56296309305(2)	−1.38841421557(7)	18.031790(2)	−0.20191386882(4)
1.4	−0.580208761190(6)	−1.36434916343(4)	20.8748588(3)	−0.14566545789(2)
1.5	−0.592551434454(6)	−1.33979595030(3)	24.0628992(2)	−0.10312872093(2)
1.6	−0.601168694135(5)	−1.3153823559(4)	27.63084(8)	−0.0706531048(3)
1.7	−0.606931237290(3)	−1.29151294083(2)	31.6179846(3)	−0.045676744854(5)
1.8	−0.610492372355(2)	−1.26844461393(2)	36.068587(4)	−0.026366594013(7)
1.9	−0.612348581451(5)	−1.24633556148(4)	41.0326592(5)	−0.01138863083(2)
2.0	−0.61288138360(2)	−1.2252774758(2)	46.566786(3)	0.00024264569(5)
2.1	−0.612386819635(8)	−1.20531709301(8)	52.735204(2)	0.00926502203(3)
2.2	−0.611096567328(6)	−1.18647075819(6)	59.6110031(9)	0.01623744385(3)
2.3	−0.60919328919(2)	−1.16873436973(9)	67.277608(5)	0.02158791680(3)
2.4	−0.606821938319(4)	−1.15209021855(4)	75.830560(2)	0.02564735754(2)
2.5	−0.604098188105(3)	−1.13651171656(3)	85.379612(2)	0.028673863858(9)
2.6	−0.601114786550(4)	−1.12196667488(3)	96.0513572(8)	0.030870345468(7)
2.7	−0.597946394514(3)	−1.10841958001(3)	107.992356(2)	0.032397484822(7)
2.8	−0.594653303466(3)	−1.09583317372(3)	121.373048(2)	0.033383369006(7)
2.9	−0.591284316610(2)	−1.08416955050(3)	136.392512(2)	0.033930718179(7)
3.0	−0.587878999461(3)	−1.07339092427(4)	153.284383(2)	0.034122358217(10)
3.1	−0.584469451242(3)	−1.06346017587(5)	172.324155(4)	0.03402539568(2)
3.2	−0.581081709598(4)	−1.05434126785(6)	193.838143(6)	0.03369442230(2)
3.3	−0.577736873300(7)	−1.04599960017(4)	218.2140(2)	0.03317398376(2)
3.4	−0.574452007619(7)	−1.0384023814(2)	245.91455(2)	0.03250048054(3)
3.5	−0.571240882941(9)	−1.0315190997(2)	277.48808(3)	0.03170361892(5)
3.6	−0.56811458750(2)	−1.0253222254(3)	313.58106(5)	0.03080748599(8)
3.7	−0.56508204977(3)	−1.0197883501(6)	354.93400(9)	0.0298312836(2)
3.8	−0.56215050506(3)	−1.0149001423(7)	402.3408(2)	0.0287897021(2)
3.9	−0.55932594654(6)	−1.010649860(2)	456.5035(3)	0.0276928291(5)
4.0	−0.5566136189(2)	−1.007045942(4)	517.6105(8)	0.0265453239(9)
4.1	−0.55401865480(5)	−1.004125966(2)	584.1621(2)	0.0253442301(4)
4.2	−0.55154705223(8)	−1.001983206(3)	649.6624(2)	0.0240740235(7)
4.3	−0.5492073951(2)	−1.000821619(7)	693.1435(2)	0.022696086(2)
4.4	−0.5470140331(4)	−1.00105511(3)	652.0757(5)	0.021130218(5)
4.5	−0.544991781(2)	−1.00333940(5)	357.604(3)	0.019254259(10)
4.6	−0.543173148(3)	−1.00765734(6)	−505.698(8)	0.01710630(2)
4.7	−0.5415565087(10)	−1.01080993(2)	−2013.376(4)	0.015383635(2)
4.8	−0.540059788(2)	−1.009558892(8)	−3511.580(3)	0.014700142(2)
4.9	−0.5386019047(3)	−1.0063333176(5)	−4450.1499(7)	0.014463365654(5)
5.0	−0.5371723036(2)	−1.003881689(2)	−4800.1643(5)	0.0140925837(2)

Table A24: Same as for Table A1, but for $12\,{}^1\Sigma_u^+$.

$12\,{}^1\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46199256413(3)	−1.4449513536(2)	1.554529(2)	−0.5209662253(2)
1.1	−0.506618541223(8)	−1.43062327771(3)	1.8576056(4)	−0.37944199569(2)
1.2	−0.53918166090(2)	−1.41097203887(8)	2.1993266(10)	−0.27717393089(5)
1.3	−0.562948259402(7)	−1.38835688923(5)	2.5824677(6)	−0.20189259264(3)
1.4	−0.580191705736(5)	−1.36428260755(3)	3.0100436(5)	−0.14564228291(2)
1.5	−0.592531962567(3)	−1.33971924972(2)	3.4853386(3)	−0.103103549726(9)
1.6	−0.601146600657(2)	−1.31529451940(2)	4.0119303(3)	−0.070625823802(6)
1.7	−0.6069063047846(3)	−1.291412886212(2)	4.59372135(4)	−0.0456472215548(8)
1.8	−0.6104643690743(4)	−1.268331151398(2)	5.23497284(6)	−0.0263346740273(5)
1.9	−0.61231725894517(5)	−1.2462073723162(4)	5.940344670(6)	−0.0113541339084(2)
2.0	−0.61284647391452(3)	−1.2251330872826(2)	6.714938296(4)	0.00027993027323(7)
2.1	−0.61234803199535(2)	−1.20515484774751(9)	7.564346932(2)	0.00930534106819(3)
2.2	−0.611053584187250(6)	−1.18628877651144(5)	8.494711196(2)	0.01628108721048(2)
2.3	−0.609145761506255(3)	−1.16853050335276(3)	9.5127822902(7)	0.021635225939020(7)
2.4	−0.606769479916485(2)	−1.15186199323331(2)	10.6259934092(5)	0.025698736083190(4)
2.5	−0.6040403687665298(10)	−1.136256259946467(6)	11.8425406432(2)	0.028729791034637(2)
2.6	−0.6010511236809920(10)	−1.1216806256904033(9)	13.1714747990(4)	0.0309313929506066(10)
2.7	−0.597876342850460(2)	−1.108098971932870(8)	14.622805815(2)	0.032464338432610(4)
2.8	−0.594576242315171(2)	−1.09547328558416(2)	16.207621734(3)	0.033456856802204(8)
2.9	−0.591199533868059(3)	−1.08376471033490(4)	17.938224560(5)	0.03401184737973(2)
3.0	−0.587785671358042(5)	−1.07293424950595(7)	19.828285749(9)	0.03421236440337(3)
3.1	−0.584366616344855(5)	−1.06294322343577(2)	21.893024628(2)	0.034125809436755(3)
3.2	−0.580968234970722(3)	−1.05375355457062(2)	24.149413606(2)	0.033807161053383(3)
3.3	−0.577611409738688(2)	−1.045327932640607(8)	26.616415018(3)	0.033301480859627(2)
3.4	−0.57431292936535(3)	−1.0376298977110(2)	29.315255163(4)	0.03264587088815(3)
3.5	−0.57108620478248(4)	−1.0306238685490(7)	32.26974254(6)	0.0318710117188(2)
3.6	−0.56794184816067(7)	−1.024275136345(3)	35.50663895(10)	0.0310023777712(7)
3.7	−0.56488814344257(4)	−1.0185498384700(8)	39.0560940(2)	0.0300612022744(2)
3.8	−0.561931430546394(3)	−1.01341492305608(6)	42.952155651(10)	0.02906524685176(2)
3.9	−0.559076420587214(4)	−1.00883811224597(5)	47.233374172(5)	0.02802941767396(2)
4.0	−0.556326455777606(4)	−1.00478786984658(3)	51.943522013(3)	0.026966260427157(6)
4.1	−0.55368372482509(2)	−1.00123337748547(7)	57.132454854(4)	0.025886359064564(10)
4.2	−0.551149442437021(9)	−0.99814452236469(5)	62.857147170(4)	0.024798657740321(7)
4.3	−0.548723999835585(10)	−0.9954919003214(2)	69.182873102(6)	0.02371072077902(3)
4.4	−0.54640709197592(2)	−0.9932468536137(3)	76.183253510(5)	0.02262893871322(6)
4.5	−0.544197829993(2)	−0.99138246328(2)	83.824663(5)	0.021558488156(4)
4.6	−0.5422583545(6)	−1.002794866(5)	−1385.1518(10)	0.0177656179(9)
4.7	−0.5405639972(4)	−1.005430299(2)	−659.9034(8)	0.0161058924(6)
4.8	−0.5390417875(3)	−1.009295884(5)	−45.5608(2)	0.0143307688(10)
4.9	−0.53768684976(8)	−1.012154244(4)	142.2628(2)	0.0129019297(8)
5.0	−0.5364254827(4)	−1.01036069(3)	−111.245(2)	0.012498054(5)

Table A25: Same as for Table A1, but for $13\,^1\Sigma_u^+$.

$13\,^1\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.4596661920(3)	−1.440495467(3)	−1255.6059(3)	−0.521163084(3)
1.1	−0.5043130569(4)	−1.42625530(3)	−1300.7047(3)	−0.37966289(3)
1.2	−0.5368994683(4)	−1.406701532(4)	−1337.302(2)	−0.277418830(3)
1.3	−0.5606917414(4)	−1.384192895(4)	−1362.856(2)	−0.202161086(3)
1.4	−0.5779631852(4)	−1.360233364(4)	−1374.844(2)	−0.145933567(3)
1.5	−0.5903336607(5)	−1.335791919(5)	−1370.942(2)	−0.103416399(3)
1.6	−0.5989805960(5)	−1.311494977(5)	−1349.252(2)	−0.070958616(3)
1.7	−0.6047744964(4)	−1.287745603(4)	−1308.5359(8)	−0.045998006(2)
1.8	−0.6083684493(5)	−1.264799224(5)	−1248.4042(5)	−0.026701292(3)
1.9	−0.6102587005(5)	−1.242812721(5)	−1169.4435(3)	−0.011734379(2)
2.0	−0.6108265343(5)	−1.221876824(5)	−1073.23676(10)	−0.000111878(2)
2.1	−0.6103677778(5)	−1.202037809(5)	−962.28106(8)	0.008903689(2)
2.2	−0.6091139355(5)	−1.183312170(4)	−839.8186(3)	0.015870773(2)
2.3	−0.6072475541(5)	−1.165696632(5)	−709.6220(3)	0.021216729(2)
2.4	−0.6049135425(4)	−1.149175002(3)	−575.7831(3)	0.0252717012(10)
2.5	−0.6022276110(3)	−1.133722869(3)	−442.5494(2)	0.0282929411(6)
2.6	−0.5992826313(3)	−1.119310817(2)	−314.23960(5)	0.0304824790(4)
2.7	−0.5961534758(3)	−1.105906610(2)	−195.24925(7)	0.0320001267(5)
2.8	−0.5929007321(3)	−1.093476622(2)	−90.144352(7)	0.0329731579(4)
2.9	−0.5895735759(3)	−1.081986748(2)	−3.81358(4)	0.0335035874(3)
3.0	−0.5862120075(2)	−1.0714028515(10)	58.36405(9)	0.0336737211(2)
3.1	−0.5828485988(2)	−1.0616908290(5)	90.4087(2)	0.03355044150(5)
3.2	−0.5795098620(2)	−1.0528163149(3)	85.7963(2)	0.033188565361(3)
3.3	−0.57621731699(10)	−1.04474404431(5)	37.8284(2)	0.03263351190(8)
3.4	−0.57298832144(8)	−1.0374370241(3)	−59.5172(2)	0.0319234172(2)
3.5	−0.56983671435(6)	−1.0308558163(6)	−210.15580(7)	0.0310907463(2)
3.6	−0.5667733246(2)	−1.024958542(3)	−413.9842(2)	0.0301633631(7)
3.7	−0.56380640358(4)	−1.019702407(2)	−664.95795(8)	0.0291649730(4)
3.8	−0.56094204810(3)	−1.0150476238(6)	−949.9859(2)	0.0281148611(2)
3.9	−0.55818468222(7)	−1.010964063(4)	−1249.4768(2)	0.0270270005(10)
4.0	−0.5555376549(2)	−1.007440707(8)	−1539.6786(7)	0.025908651(2)
4.1	−0.5530040012(4)	−1.00449834(2)	−1795.714(2)	0.024758453(4)
4.2	−0.5505874340(7)	−1.00220753(3)	−1993.107(3)	0.023563651(5)
4.3	−0.5482936711(4)	−1.00071348(2)	−2104.9849(9)	0.022296248(3)
4.4	−0.5461320525(6)	−1.00024724(2)	−2091.6716(6)	0.020912923(3)
4.5	−0.5441160611(8)	−1.00100481(2)	−1881.9720(3)	0.019383846(3)
4.6	−0.54209479555673(4)	−0.989868540520(4)	92.4390825(8)	0.0205045762160(7)
4.7	−0.54009622195321(2)	−0.98868126279935(2)	102.12989445(4)	0.019470464065328(3)
4.8	−0.53819993505445(2)	−0.9877950121655(2)	112.864817404(6)	0.01845934540487(4)
4.9	−0.53640349841137(2)	−0.9871851685157(10)	124.87188973(10)	0.0174738425116(2)
5.0	−0.53470424410258(5)	−0.986828504749(2)	138.3527495(2)	0.0165159966913(4)

Table A26: Same as for Table A1, but for $14\,^1\Sigma_u^+$.

$14\,^1\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.45960651665(3)	−1.4401887360(2)	7.6572755(2)	−0.5209757027(2)
1.1	−0.504233491594(8)	−1.42586471328(5)	9.00007666(4)	−0.37945248190(3)
1.2	−0.536797712033(5)	−1.40621798496(3)	10.5198992(4)	−0.27718546741(2)
1.3	−0.560565518698(3)	−1.38360783395(2)	12.2336034(2)	−0.201905228119(7)
1.4	−0.577810285857(2)	−1.359539075407(7)	14.16003821(3)	−0.145656074067(4)
1.5	−0.590151982299(4)	−1.33498180851(2)	16.3203555(4)	−0.103118562606(10)
1.6	−0.598768185915(3)	−1.31056378821(2)	18.73829287(4)	−0.070642135236(3)
1.7	−0.6045295897824(9)	−1.2866895451919(9)	21.44055102(4)	−0.045664920963(2)
1.8	−0.6080894976823(8)	−1.263615953327(5)	24.45722806(2)	−0.026353865534(2)
1.9	−0.6099443862887(4)	−1.241501156597(3)	27.82231747(2)	−0.011374938957(2)
2.0	−0.6104757682582(2)	−1.220436796983(2)	31.57430715(2)	0.00025736977819(9)
2.1	−0.609979676977(2)	−1.20046955038(3)	35.756881(6)	0.009280858847(2)
2.2	−0.6086877814796(6)	−1.181615689505(4)	40.4197781(8)	0.016254487934(2)
2.3	−0.6067827340127(4)	−1.163871025725(6)	45.6197570(5)	0.021606279261(3)
2.4	−0.6044094756242(3)	−1.147217744948(3)	51.4218410(7)	0.0256671692919(7)
2.5	−0.6016836654313(2)	−1.131629131540(2)	57.9007539(6)	0.0286952797291(5)
2.6	−0.5986980345651(4)	−1.117072841282(2)	65.1426892(8)	0.03089354917222(10)
2.7	−0.5955272238102(3)	−1.103513170171(3)	73.2474665(8)	0.0324226953515(6)
2.8	−0.5922315006422(4)	−1.09091262481(2)	82.331173(2)	0.033410848739(4)
2.9	−0.5888596394328(2)	−1.079233007070(10)	92.529416(3)	0.033960783378(4)
3.0	−0.5854511708230(3)	−1.068436163453(4)	104.0013317(9)	0.0341553927310(10)
3.1	−0.5820381515357(4)	−1.058484508762(6)	116.9345025(10)	0.034061869132(2)
3.2	−0.5786465669773(5)	−1.049341407341(9)	131.5509518(7)	0.033734914567(3)
3.3	−0.5752974510670(10)	−1.04097148122(3)	148.1142410(5)	0.033219218459(6)
3.4	−0.572007787651(2)	−1.03334091094(4)	166.9373982(6)	0.032551371871(10)
3.5	−0.5687912435177(9)	−1.02641780517(10)	188.390546(6)	0.03176133767(3)
3.6	−0.565658773161(2)	−1.02017274701(5)	212.904886(5)	0.03087355536(2)
3.7	−0.562619129477(3)	−1.01457969342(9)	240.964170(3)	0.02990772041(3)
3.8	−0.559679312987(5)	−1.0096175596(2)	273.06067(2)	0.02887922798(4)
3.9	−0.55684499669(9)	−1.005273149(3)	309.5543(6)	0.0277991908(6)
4.0	−0.55412098017(2)	−1.0015468671(4)	350.27752(5)	0.02667377331(10)
4.1	−0.55151176786(3)	−0.9984644630(10)	393.39448(8)	0.0255022129(3)
4.2	−0.54902246905(6)	−0.996102550(3)	432.12134(10)	0.0242719972(5)
4.3	−0.5466604490(2)	−0.994644675(5)	444.78123(3)	0.0229479589(10)
4.4	−0.5444384978(3)	−0.99448077(2)	365.3846(4)	0.021453689(3)
4.5	−0.5423787327(5)	−0.99612138(2)	22.258(2)	0.019696908(4)
4.6	−0.5405014950(7)	−0.99867039(2)	−803.168(3)	0.017898390(3)
4.7	−0.5387753560(7)	−0.998730065(3)	−1895.677(2)	0.0167703499(8)
4.8	−0.5371271383(4)	−0.996333500(6)	−2726.1621(8)	0.016233495(2)
4.9	−0.5355293738(3)	−0.994143458(3)	−3126.5788(4)	0.0156969976(7)
5.0	−0.5339921205(2)	−0.992799150(2)	−3085.07009(7)	0.0150370182(3)

Table A27: Same as for Table A1, but for $2\,^3\Sigma_u^+$ (e state).

$2\,^3\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.2451495173345(3)	−1.5178592583(5)	25493.236221(3)	−1.4679431767(6)
0.8	−0.36833209609689(5)	−1.55875842295(3)	25761.805922(3)	−1.02761778844(3)
0.9	−0.4556059526533(3)	−1.57441151800(2)	25254.146888(6)	−0.73688845855(2)
1.0	−0.51872729888455(3)	−1.57493143496(4)	23869.239373(4)	−0.537476837196(4)
1.1	−0.56503249449268(5)	−1.566129161162(2)	21651.626345(8)	−0.396421974706(10)
1.2	−0.5992935895477(2)	−1.551461994285(2)	18795.2027280(2)	−0.294062345991(2)
1.3	−0.6247230795477(9)	−1.53308944686(7)	15589.43598(3)	−0.21818714443(6)
1.4	−0.64354985483349(9)	−1.51244790940(4)	12336.7746429(2)	−0.160962999814(2)
1.5	−0.657363112434248(6)	−1.490549543068(3)	9283.8424020(8)	−0.117215545466(2)
1.6	−0.66732378820258(3)	−1.468131090654(2)	6590.2055196(4)	−0.083427196405(10)
1.7	−0.67429778540326(2)	−1.445731002563(2)	4331.506815(5)	−0.057138489269(8)
1.8	−0.678942138555728(10)	−1.423736760526(2)	2520.5432410(3)	−0.036584713008(6)
1.9	−0.6817623790110(3)	−1.402420026233(9)	1131.4669114(9)	−0.020471193795(4)
2.0	−0.683151888034877(6)	−1.381965139986(9)	119.3851194(2)	−0.007830681958(4)
2.1	−0.683419654413064(10)	−1.362492230756(8)	−566.55695774(2)	0.0020700371761(3)
2.2	−0.682810323097895(6)	−1.344075386779(6)	−975.6655027(2)	0.0097932997349(3)
2.3	−0.681518956969674(8)	−1.326756482077(7)	−1152.04903857(2)	0.0157745355925(3)
2.4	−0.679702073874316(5)	−1.310555427766(6)	−1133.3127171(2)	0.0203536333257(2)
2.5	−0.677486001519539(7)	−1.295477632825(6)	−950.5240523(3)	0.0237977480859(2)
2.6	−0.674973267207350(3)	−1.281519362565(5)	−628.7842126(3)	0.0263181430189(2)
2.7	−0.67224752754603(4)	−1.268671544268(5)	−188.0285392(3)	0.0280827817867(2)
2.8	−0.669377400742445(4)	−1.256922431437(5)	356.1371312(3)	0.0292258464454(2)
2.9	−0.666419465423273(4)	−1.246259419509(5)	991.6508352(3)	0.0298550039095(2)
3.0	−0.663420620078305(5)	−1.236670209897(4)	1709.2872003(3)	0.0300570100865(2)
3.1	−0.660419946811376(5)	−1.228143443892(5)	2502.025673(5)	0.0299020805583(2)
3.2	−0.657450186116804(4)	−1.220668868944(4)	3364.4769579(4)	0.0294473447782(2)
3.3	−0.654538901907307(4)	−1.214237054544(5)	4292.3449408(2)	0.0287396209911(2)
3.4	−0.651709395361588(4)	−1.208838642447(5)	5281.9015223(7)	0.0278176906696(2)
3.5	−0.648981410606303(4)	−1.204463098524(5)	6329.4562462(8)	0.0267142064824(2)
3.6	−0.646371663739601(5)	−1.201096936575(5)	7430.811511(4)	0.0254573308069(10)
3.7	−0.643894218703247(3)	−1.198721415812(4)	8580.708151(8)	0.0240721679986(10)
3.8	−0.641560728869722(4)	−1.197309782334(5)	9772.285663(10)	0.0225820198435(2)
3.9	−0.639380562008245(3)	−1.196824235199(5)	10996.605230(2)	0.0210094586710(10)
4.0	−0.637360828579427(3)	−1.197212943422(5)	12242.308092(2)	0.0193771784340(10)
4.1	−0.635506338738168(4)	−1.198407594922(5)	13495.49914(4)	0.0177085567204(9)
4.2	−0.633819520844898(4)	−1.200322071372(4)	14739.94519(4)	0.0160278500757(9)
4.3	−0.632300341455545(3)	−1.202852845111(4)	15957.64855(5)	0.0143599622791(8)
4.4	−0.630946270507275(3)	−1.205881523498(5)	17129.79551(5)	0.0127297767081(9)
4.5	−0.629752332465679(4)	−1.209279606069(4)	18237.99396(7)	0.0111611241917(8)
4.6	−0.628711272602945(3)	−1.212915035298(4)	19265.62978(8)	0.0096755456322(7)
4.7	−0.627813848138214(3)	−1.216659657913(4)	20199.11920(9)	0.0082910719923(7)
4.8	−0.627049230707203(3)	−1.220396443460(4)	21028.84059(9)	0.0070212537404(6)
4.9	−0.626405485630473(3)	−1.2240253450318(4)	21749.59700(10)	0.0058746175978(6)
5.0	−0.625870080464611(3)	−1.2274670244728(3)	22360.56852(2)	0.0048546272913(5)
5.1	−0.625430373331476(3)	−1.2306641709147(3)	22864.82174(2)	0.0039601128918(5)
5.2	−0.625074039719545(3)	−1.2335806358555(3)	23268.51815(2)	0.0031860468430(5)
5.3	−0.624789411056880(3)	−1.2361989466696(3)	23579.98891(2)	0.0025245048008(4)
5.4	−0.624565714566977(3)	−1.2385168885852(3)	23808.82415(2)	0.0019656556572(4)

5.5	−0.624393217796996(3)	−1.2405437929091(3)	23965.08075(2)	0.0014986623063(4)
5.6	−0.624263290644980(3)	−1.2422970111106(3)	24058.66190(2)	0.00111242324631(3)
5.7	−0.624168402402467(3)	−1.2437988664044(2)	24098.87948(2)	0.00079612954395(3)
5.8	−0.624102072144993(2)	−1.24507420905887(4)	24094.182300(3)	0.00053964400536(4)
5.9	−0.62405878907694(3)	−1.24614858246903(3)	24052.019085(3)	0.000333728082177(3)
6.0	−0.624033916433984(3)	−1.24704693606655(3)	23978.80123(4)	0.000170149466901(3)
6.5	−0.624071951793777(3)	−1.24965075888221(3)	23305.381560(2)	−0.000231823891485(3)
7.0	−0.624211780405681(3)	−1.2505133982066(5)	22341.66219(4)	−0.00029854819931(6)
7.5	−0.624355079362741(10)	−1.2507199130779(9)	21179.674595(3)	−0.00026796724699(2)
8.0	−0.624477359273812(5)	−1.2507253196615(2)	19788.72720(2)	−0.00022132513924(2)
8.5	−0.624577609803405(5)	−1.2506967628496(3)	18102.0223(4)	−0.00018135802857(3)
9.0	−0.62466041682866(7)	−1.250683792432(4)	16060.6665(7)	−0.0001514398638(4)
9.5	−0.6247303865304555(4)	−1.250691215206(5)	13650.8486(7)	−0.0001295202259(5)
10.0	−0.6247907605363017(9)	−1.250707041423(6)	10945.9725(10)	−0.0001125520351(6)
11.0	−0.624888518903934(4)	−1.250690749552(5)	5517.64445(2)	−0.0000830647040(4)
12.0	−0.6249561630483466(10)	−1.2505373403604(3)	1833.15679(4)	−0.00005208452198(2)
13.0	−0.624994023194899(3)	−1.2503139356552(3)	374.5620(8)	−0.00002506840503(2)
14.0	−0.625009826714532(3)	−1.2501360929307(10)	54.04789(2)	−0.00000831710726(6)
15.0	−0.62501366827014881(8)	−1.2500353205178(10)	41.44572(8)	−0.00000053226517(6)
16.0	−0.6250125745234676(7)	−1.2499906637361(6)	58.42833(3)	0.000002155331930(3)
17.0	−0.6250100921666303(5)	−1.2499761354575(4)	58.28547(3)	0.000002591110336(2)
18.0	−0.6250076441545968(3)	−1.24997489940513(2)	47.46800(2)	0.000002243828004(8)
19.0	−0.6250056545181464(4)	−1.2499783650740(4)	34.80546(3)	0.000001733892748(2)
20.0	−0.62500415715332536(3)	−1.24998278221234(4)	24.21534(3)	0.0000012766047159(4)

Table A28: Same as for Table A1, but for $3\,^3\Sigma_u^+$ (f state).

$3\,^3\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.216737782218(8)	−1.455736815(8)	9585.51214(3)	−1.460373216(8)
0.8	−0.339106607001(9)	−1.4933536766(3)	9431.52780(3)	−1.0189255783(3)
0.9	−0.425460109053(9)	−1.5054041924(2)	8971.3636(4)	−0.7272044158(2)
1.0	−0.4875729698923(3)	−1.50218526943(2)	8202.308586(2)	−0.52703932965(2)
1.1	−0.5328100652784(5)	−1.4897325337(6)	7176.64627(4)	−0.3855567301(4)
1.2	−0.5659783856276(4)	−1.47171571244(4)	5990.596688(3)	−0.28313245099(3)
1.3	−0.5903260471867(6)	−1.45044398343(3)	4757.11040(4)	−0.20753222235(2)
1.4	−0.6081126328929(3)	−1.42741714398(2)	3576.93993(5)	−0.15085134157(2)
1.5	−0.62094959568497(6)	−1.40363329040(10)	2520.838892(3)	−0.10782273269(6)
1.6	−0.63001086155816(6)	−1.37976510140(5)	1626.062360(2)	−0.074839611429(3)
1.7	−0.63616723493092(4)	−1.35626583817(4)	902.509285(2)	−0.049371393123(2)
1.8	−0.64007464588366(5)	−1.33343714911(8)	342.1466026(3)	−0.02960436519(4)
1.9	−0.64223363942751(5)	−1.31147482328(8)	−72.487071(9)	−0.01421449706(4)
2.0	−0.6430304536764(3)	−1.2905006820(6)	−362.25841(4)	−0.00221988732(3)
2.1	−0.64276599526070(8)	−1.27058511752(6)	−547.8464924(4)	0.007117558570(3)
2.2	−0.64167665933086(10)	−1.25176307430(5)	−647.939554(5)	0.014359201980(2)
2.3	−0.6399495303538(5)	−1.23404537078(4)	−678.553826(4)	0.019936386925(2)
2.4	−0.63773363516721(3)	−1.217426712592(2)	−652.9710503(3)	0.024183565726(4)
2.5	−0.635148375657781(9)	−1.201891364816(2)	−581.9737587(9)	0.027362154600(4)
2.6	−0.63228991710785(9)	−1.187417177801(10)	−474.19391767(3)	0.0296779447749(4)
2.7	−0.62923607600263(3)	−1.173978461834(8)	−336.47977039(4)	0.0312939593229(3)
2.8	−0.626050094269150(5)	−1.161548063422(7)	−174.23841277(3)	0.0323400446843(2)
2.9	−0.6227835791239(3)	−1.150098895134(8)	8.2589593(3)	0.0329200907288(3)
3.0	−0.61947881242838(3)	−1.139605100182(6)	207.6061474(4)	0.0331175082249(2)
3.1	−0.616170580166219(3)	−1.130042983651(6)	421.0131066(5)	0.0329994118325(2)
3.2	−0.612887634475419(3)	−1.121391807846(5)	646.0599768(7)	0.0326198315952(2)
3.3	−0.609653873013346(5)	−1.113634525083(5)	880.4272304(9)	0.0320221881646(2)
3.4	−0.60648930019790(4)	−1.106758504373(4)	1121.5642837(4)	0.0312412047125(2)
3.5	−0.6034108199369055(9)	−1.100756297616(4)	1366.2416687(2)	0.0303043835022(9)
3.6	−0.6004328984262034(8)	−1.095626488733(4)	1609.9042369(2)	0.0292331411441(9)
3.7	−0.5975681276628707(10)	−1.091374686058(4)	1845.6989711(2)	0.0280436673698(8)
3.8	−0.5948277154304132(5)	−1.088014785031(4)	2062.9822599(2)	0.0267475383761(8)
3.9	−0.59222192694515(3)	−1.08557082504(6)	2245.005853(2)	0.025352058682(2)
4.0	−0.58976051127683(3)	−1.08408029378(6)	2365.322927(2)	0.023860182193(2)
4.1	−0.58745317306753(3)	−1.08360110444(6)	2382.233706(3)	0.022269571146(2)
4.2	−0.58531022466225(3)	−1.08422797965(6)	2230.334160(3)	0.020569635636(2)
4.3	−0.58334374566032(3)	−1.08613302527(6)	1808.224609(3)	0.018733596755(2)
4.4	−0.58157006861058(3)	−1.08966910882(6)	963.348597(3)	0.016697961000(2)
4.5	−0.58001568253228(3)	−1.09563768432(4)	−512.085447(3)	0.014309706831(8)
4.6	−0.57873180704421(3)	−1.105964869566(2)	−2788.570799(2)	0.0111953792438(2)
4.7	−0.57782791905779(2)	−1.124994527705(2)	−5406.1975314(2)	0.0065236830661(3)
4.8	−0.577514960007280(9)	−1.15838230809(10)	−5385.74047(6)	−0.000698414182(2)
4.9	−0.57800569887875(4)	−1.19982640948(2)	1939.87789(2)	−0.00894183913(4)
5.0	−0.5792134011485(3)	−1.2317408251(8)	14150.2642(4)	−0.01466280458(2)
5.1	−0.58084420547256(9)	−1.2514213320(6)	25947.9653(4)	−0.01759469039(2)
5.2	−0.5826800667043(3)	−1.2638319558(7)	35772.5026(4)	−0.01893688892(2)
5.3	−0.5846042157393(3)	−1.2722688950(7)	43735.1832(5)	−0.01944537049(2)
5.4	−0.58655366424522(4)	−1.27832108902(9)	50175.6487(8)	−0.019484029728(2)

5.5	−0.58849155614466(4)	−1.28278242792(9)	55387.1321(9)	−0.019236239207(2)
5.6	−0.59039482635739(5)	−1.28609565324(9)	59599.1936(10)	−0.018804642951(2)
5.7	−0.59224848771210(5)	−1.28853596525(9)	62992.1331(2)	−0.018252454356(2)
5.8	−0.59404270393580(3)	−1.29028984482(4)	65709.77732(8)	−0.017621454646(7)
5.9	−0.59577112642299(3)	−1.29149191624(4)	67868.41107(9)	−0.016940620916(6)
6.0	−0.59742986449210(2)	−1.29224390329(4)	69563.03568(10)	−0.016230695717(6)
6.5	−0.60464358337705(3)	−1.291558471514(3)	73399.01587(2)	−0.012657123809(4)
7.0	−0.610164283471734(3)	−1.287009364116(2)	73222.92683(3)	−0.0095258281675(3)
7.5	−0.614274655129412(6)	−1.281197184414(2)	71750.01220(2)	−0.0070197165540(2)
8.0	−0.617281722559672(8)	−1.275349858133(10)	70223.69172(3)	−0.0050983016267(10)
8.5	−0.619453749372869(8)	−1.270031235888(9)	69216.74658(3)	−0.0036616161344(8)
9.0	−0.621006626945171(6)	−1.265459723947(6)	68968.85627(3)	−0.0026051633396(5)
9.5	−0.622107040260207(6)	−1.261675932869(5)	69525.28607(3)	−0.0018380897210(4)
10.0	−0.622880687353616(4)	−1.2586354242806(3)	70778.86914(2)	−0.00128740495734(2)
11.0	−0.623797094063254(3)	−1.2544573630076(10)	74273.30868(2)	−0.00062392498919(5)
12.0	−0.624243509019488(2)	−1.2521995910830(4)	76920.09974(9)	−0.0003093810870029(2)
13.0	−0.6244723143861125(7)	−1.25111417658852(5)	77865.57213(6)	−0.000166888293562(2)
14.0	−0.6246021841113039(5)	−1.25061585729774(6)	77955.99703(6)	−0.000100820648225(4)
15.0	−0.6246845979773363(3)	−1.25038135585660(10)	77880.301890(3)	−0.000067477326795(2)
16.0	−0.6247419164849900(2)	−1.25026437626316(5)	77840.62798(4)	−0.000048783955824(6)
17.0	−0.62478449223931143(7)	−1.25020132104251(6)	77845.417060(3)	−0.000037196268464(5)
18.0	−0.62481754638225007(5)	−1.250163829745373(3)	77870.311510(3)	−0.0000293742767152(3)
19.0	−0.62484396080291682(3)	−1.250138912083569(2)	77898.773037(2)	−0.0000237363409334(10)
20.0	−0.62486547583059293(7)	−1.250120551515117(9)	77923.958298(3)	−0.00001947999269654(4)

Table A29: Same as for Table A1, but for $4\,^3\Sigma_u^+$.

$4\,^3\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.2139062298985(5)	−1.4467300627(5)	30.20853(5)	−1.4555965756(6)
0.8	−0.3357692262666(4)	−1.4824206725(5)	36.37159(5)	−1.0136027749(6)
0.9	−0.42156836168352(7)	−1.4924562994(4)	43.488180(2)	−0.7214661956(4)
1.0	−0.48309394608072(10)	−1.48725281401(3)	51.639049(2)	−0.52106492185(3)
1.1	−0.52773029481435(10)	−1.47296643600(3)	60.916029(3)	−0.37955076943(2)
1.2	−0.56030480586979(7)	−1.45336124748(2)	71.423124(2)	−0.27729302979(2)
1.3	−0.584083842621311(6)	−1.43079669108(4)	83.278025(4)	−0.202022312184(3)
1.4	−0.601340806245561(7)	−1.406777773440(3)	96.614048(4)	−0.145782972106(2)
1.5	−0.613695697286332(4)	−1.38227482241(3)	111.582474(2)	−0.10325561856(2)
1.6	−0.62232613092061(5)	−1.35791586529(3)	128.355415(2)	−0.07078975215(2)
1.7	−0.62810284384050(6)	−1.33410575620(4)	147.129271(10)	−0.04582356972(2)
1.8	−0.631679190729689(9)	−1.31110175281(8)	168.1289102(7)	−0.02652409520(4)
1.9	−0.633551707577880(5)	−1.28906245415(5)	191.6127490(2)	−0.011557388945(3)
2.0	−0.634101976090493(5)	−1.26808004161(5)	217.8789550(3)	0.000061955285(3)
2.1	−0.63362611000514(2)	−1.24820183078(5)	247.273076(5)	0.009071613919(2)
2.2	−0.632355871872489(6)	−1.229444853805(3)	280.1974893(3)	0.016030404518(9)
2.3	−0.630474022839470(8)	−1.211805824916(2)	317.1231993(3)	0.021366182940(7)
2.4	−0.628125630913351(6)	−1.195268005986(2)	358.6047144(10)	0.025409689934(6)
2.5	−0.625426503465334(7)	−1.179805967378(3)	405.2989885(10)	0.028418815821(8)
2.6	−0.622469545133671(5)	−1.165388907939(2)	457.9898138(2)	0.030596223973(6)
2.7	−0.619329600357573(7)	−1.151982984289(2)	517.6196168(2)	0.032102302380(4)
2.8	−0.616067176539832(3)	−1.139552960523(8)	585.3314699(3)	0.0330647830561(3)
2.9	−0.612731332038507(3)	−1.128063398739(2)	662.525426(4)	0.033585953565(4)
3.0	−0.609361935607286(5)	−1.117479553085(9)	750.9353133(2)	0.0337481060431(3)
3.1	−0.605991449491318(5)	−1.107768096160(2)	852.7353695(3)	0.033617678330(5)
3.2	−0.602646349976706(4)	−1.098897793223(9)	970.6913618(7)	0.0332484083534(3)
3.3	−0.599348272155293(4)	−1.090840248223(2)	1108.3798292(2)	0.032683726087(5)
3.4	−0.596114947132426(3)	−1.083570885955(7)	1270.5146933(2)	0.0319585318556(2)
3.5	−0.592960988433888(7)	−1.077070431400(9)	1463.4489703(3)	0.0311004415622(3)
3.6	−0.589898580089736(6)	−1.071327360920(3)	1695.973421(9)	0.030130499794(8)
3.7	−0.586938124473674(3)	−1.066342278406(2)	1980.642295(6)	0.029063235281(4)
3.8	−0.58408893175049(3)	−1.062136301151(2)	2336.086013(9)	0.027905674302(5)
3.9	−0.581360097730429(4)	−1.058768425949(3)	2791.291064(10)	0.026654299875(6)
4.0	−0.578761889481352(5)	−1.056374911771(3)	3394.095587(2)	0.025287216798(7)
4.1	−0.576308447892993(6)	−1.05526880791(5)	4229.480938(3)	0.023743436067(2)
4.2	−0.574024159276663(9)	−1.05622536558(9)	5462.48202(5)	0.021862607853(3)
4.3	−0.57196145313725(3)	−1.06141071495(3)	7444.21049(10)	0.01918888170(5)
4.4	−0.570256295832041(6)	−1.07738391599(7)	10923.51276(4)	0.014347426290(2)
4.5	−0.56925521998132(3)	−1.11683847384(2)	16791.18885(8)	0.00481599247(5)
4.6	−0.56931892019938(4)	−1.1627071086(4)	24518.02923(2)	−0.00523244960(7)
4.7	−0.57005222059822(6)	−1.1787386052(5)	33739.05439(3)	−0.00822003489(9)
4.8	−0.57075934261579(8)	−1.1660989328(5)	41469.93228(3)	−0.00512088491(9)
4.9	−0.57098780944278(9)	−1.13925409720(3)	42239.59079(3)	0.00055541259(6)
5.0	−0.57071026269754(9)	−1.11862355549(3)	37788.72877(2)	0.00455939398(4)
5.1	−0.57015055440259(10)	−1.10786136540(3)	33004.50628(10)	0.00636073400(4)
5.2	−0.56947541445587(10)	−1.10243299900(3)	29261.27381(7)	0.00702265960(4)
5.3	−0.56876166746158(10)	−1.09934731965(3)	26416.36622(6)	0.00720302175(4)
5.4	−0.56804129874973(3)	−1.09729115700(4)	24189.339867(6)	0.007183600092(7)

5.5	−0.56732775261242(3)	−1.09572679330(4)	22388.787193(5)	0.007077947622(6)
5.6	−0.56662705643123(3)	−1.09444029495(4)	20899.289750(4)	0.006931038913(6)
5.7	−0.56594233389912(3)	−1.09335193984(4)	19650.559508(4)	0.006760127711(6)
5.8	−0.56527561680270(3)	−1.092436412726(4)	18597.2725690(3)	0.006571520841(5)
5.9	−0.56462854119154(3)	−1.091688608421(4)	17707.9269865(3)	0.006367537960(5)
6.0	−0.56400258290111(4)	−1.091109101137(4)	16958.9551419(3)	0.006149344111(5)
6.5	−0.5612327606064(3)	−1.09067196694(4)	14757.127653(4)	0.004891316043(5)
7.0	−0.55913015922880(3)	−1.09361620171(4)	14114.6550523(3)	0.003520588106(5)
7.5	−0.55769133047783(3)	−1.09833440122(4)	14004.0950519(3)	0.002273101299(4)
8.0	−0.55680641218793(3)	−1.10301839383(4)	13636.951280(4)	0.001324303819(4)
8.5	−0.55631038364416(4)	−1.10657605571(4)	12462.680877(2)	0.000711142538(4)
9.0	−0.55605203326245(3)	−1.108884225313(2)	10078.85403(6)	0.0003577601346(2)
9.5	−0.55592312161897(3)	−1.110118039447(2)	6871.951156(3)	0.0001819161885(2)
10.0	−0.55585213473268(2)	−1.110565716563(7)	4237.11644(6)	0.0001138552903(5)
11.0	−0.555761041228978(7)	−1.1106825428259(4)	1651.52890(3)	0.00007632178473(2)
12.0	−0.555695256979466(5)	−1.1107224510777(2)	668.6441(7)	0.00005567190677(2)
13.0	−0.555648716718361(4)	−1.1108023412648(2)	227.7096(2)	0.00003808401323(9)
14.0	−0.555617551323114(10)	−1.1108847221827(2)	23.9664(2)	0.00002502717597(8)
15.0	−0.555597235558680(4)	−1.1109510740138(2)	−57.3499(2)	0.00001622647357(8)
16.0	−0.5555840553908489(6)	−1.1109991593077(2)	−73.3890(8)	0.00001055946712(6)
17.0	−0.555575429534386(3)	−1.1110324620354(9)	−57.0872(7)	0.00000696453137(4)
18.0	−0.5555696933710385(9)	−1.1110551902412(7)	−27.66360(3)	0.000004677583377(4)
19.0	−0.5555658052586013(3)	−1.11107073147400(4)	4.3930(4)	0.000003204160168(2)
20.0	−0.5555631172449833(4)	−1.1110814739(8)	34.012(3)	0.00000223803(4)

Table A30: Same as for Table A1, but for $5\,^3\Sigma_u^+$.

		$5\,^3\Sigma_u$		
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.204068665129(5)	−1.428673309(7)	4633.161286(4)	−1.457908541(7)
0.8	−0.326175387839(3)	−1.465275473(5)	4503.9110(8)	−1.016155871(5)
0.9	−0.412239095498(5)	−1.476250061(2)	4227.17319(3)	−0.724190967(9)
1.0	−0.474042043214(8)	−1.471955313(7)	3809.1177(2)	−0.523871227(5)
1.1	−0.518958982599(6)	−1.458491883(5)	3281.3242(3)	−0.382339925(4)
1.2	−0.551807651512(6)	−1.439582888(4)	2693.2641(3)	−0.2799729872(3)
1.3	−0.575846083804(2)	−1.4175683318(4)	2098.5593(2)	−0.2045201263(3)
1.4	−0.593341620396(2)	−1.3939543341(2)	1542.1098(6)	−0.1480507809(7)
1.5	−0.605910726312(4)	−1.3697265024(2)	1053.2985(8)	−0.1052700332(2)
1.6	−0.614729712369(4)	−1.3455347723(2)	645.7499(5)	−0.0725470922(9)
1.7	−0.6206696779206(6)	−1.3218067450(2)	320.98418(2)	−0.0473337583(6)
1.8	−0.6243854138104(5)	−1.2988200244(6)	73.04327(2)	−0.02780510930(3)
1.9	−0.6263754750308(7)	−1.2767499500(8)	−107.631267(3)	−0.0126310526(4)
2.0	−0.6270236958692(4)	−1.2557018366(6)	−231.58845(2)	−0.00082722240(3)
2.1	−0.6266284549644(4)	−1.2357330585(5)	−308.88908(9)	0.00834469117(2)
2.2	−0.6254236673803(3)	−1.21686830732(3)	−348.41880(4)	0.01544501247(2)
2.3	−0.62359407492495(6)	−1.19911018912(4)	−357.67701(2)	0.02090346119(2)
2.4	−0.6212865355921(2)	−1.18244661660(2)	−342.81668(9)	0.02505268941(7)
2.5	−0.61861846085074(7)	−1.16685598827(2)	−308.796097(5)	0.02815237337(6)
2.6	−0.6156841910794(3)	−1.15231083823(9)	−259.56636(4)	0.030406747665(3)
2.7	−0.61255986194178(5)	−1.13878043363(8)	−198.256795(4)	0.031977514909(3)
2.8	−0.60930715425560(4)	−1.12623265798(8)	−127.343531(2)	0.032993446619(3)
2.9	−0.60597621006599(7)	−1.11463542804(6)	−48.798825(3)	0.033557583481(2)
3.0	−0.60260792142856(6)	−1.10395783687(7)	35.773549(4)	0.033752668664(2)
3.1	−0.59923574508731(3)	−1.09417119044(6)	125.005767(2)	0.033645257980(2)
3.2	−0.59588715899875(3)	−1.08525011092(5)	217.617808(2)	0.033288814712(2)
3.3	−0.59258485128439(3)	−1.07717392795(5)	312.222449(2)	0.032725992307(2)
3.4	−0.58934771653027(3)	−1.06992870159(6)	407.027040(3)	0.031990215138(2)
3.5	−0.58619172840682(3)	−1.06351049358(6)	499.323675(3)	0.031106560926(2)
3.6	−0.58313076477269(3)	−1.05793111776(6)	584.547117(3)	0.030091781052(2)
3.7	−0.58017749255980(8)	−1.05322905198(4)	654.42642(9)	0.02895295490(8)
3.8	−0.57734450480454(3)	−1.04949188477(7)	693.153136(4)	0.027683453903(2)
3.9	−0.57464612716543(3)	−1.04690689736(9)	668.97006(4)	0.026252655634(2)
4.0	−0.57210194150471(3)	−1.04588747408(10)	514.58308(4)	0.024579102232(3)
4.1	−0.56974498676975(4)	−1.04742480400(2)	79.51461(4)	0.022454919399(3)
4.2	−0.56764355975593(4)	−1.05412265258(2)	−977.66828(4)	0.019324873079(4)
4.3	−0.56595716303017(4)	−1.07227529717(2)	−3246.646175(3)	0.01386954160(4)
4.4	−0.56495931100542(7)	−1.10274354033(2)	−6201.38660(2)	0.006176154929(3)
4.5	−0.56448663890060(6)	−1.10577577636(9)	−6784.48315(7)	0.005155000321(3)
4.6	−0.56369607815871(4)	−1.07844992886(5)	−4650.36444(4)	0.010639614665(2)
4.7	−0.56247094953253(4)	−1.06257608355(10)	−1926.88363(4)	0.013269322450(2)
4.8	−0.56112314955822(6)	−1.05774145565(3)	375.42076(6)	0.01343850906(5)
4.9	−0.55981501750065(7)	−1.0577742482(4)	2416.45173(10)	0.01262362995(7)
5.0	−0.55861225549086(10)	−1.0603035834(6)	4383.87267(2)	0.01138418552(10)
5.1	−0.5575449034520(3)	−1.0643939652(7)	6321.09743(3)	0.00994036112(2)
5.2	−0.5566268868706(3)	−1.0694974871(9)	8144.48294(3)	0.00841467050(2)
5.3	−0.5558615569826(3)	−1.0751490683(10)	9695.89944(3)	0.00690076334(2)
5.4	−0.5552438275193(4)	−1.0809322893(10)	10825.22830(3)	0.00547321588(2)

5.5	−0.5547623306292(4)	−1.0865219927(10)	11461.93906(3)	0.00418230336(2)
5.6	−0.5544019453523(4)	−1.09170482460(2)	11632.34687(4)	0.003053404661(3)
5.7	−0.5541460201101(5)	−1.09636187893(2)	11427.991891(3)	0.002093010753(3)
5.8	−0.5539778962742(5)	−1.10044012911(2)	10961.701760(7)	0.001295804041(2)
5.9	−0.5538818213437(5)	−1.10393093398(2)	10336.867828(5)	0.000649611645(2)
6.0	−0.5538434717999(5)	−1.10685638761(10)	9634.207386(2)	0.000138425999(2)
6.5	−0.55413754947794(5)	−1.11478516523(6)	6326.28333(6)	−0.001001548657(8)
7.0	−0.55466149848350(4)	−1.11633791674(4)	4161.63392(9)	−0.001002131397(5)
7.5	−0.55509589755677(3)	−1.115605447053(3)	2905.43503(2)	−0.0007218202586(2)
8.0	−0.55538346752639(3)	−1.114257579695(5)	2339.32374(2)	−0.0004363305803041(3)
8.5	−0.555542697349489(6)	−1.112887305665(7)	2587.31146(5)	−0.0002119895255(10)
9.0	−0.5556069910575(4)	−1.1117282620(2)	4035.566(8)	−0.00005714221(2)
9.5	−0.55561257480207(3)	−1.11101579830(5)	6382.0148(2)	0.000022036979(4)
10.0	−0.55559539624365(5)	−1.1107942920(5)	8279.0400(3)	0.00003965004(5)
11.0	−0.5555627344581741(4)	−1.110869302054(2)	9760.8670(2)	0.0000232878966(9)
12.0	−0.5555469461346367(2)	−1.110975858636(9)	10019.8455(5)	0.0000098361361(7)
13.0	−0.555540690864199(4)	−1.111035970655(8)	9977.10893(2)	0.0000034931595(5)
14.0	−0.555538837382522(3)	−1.1110694538241(3)	9842.00688(2)	0.00000058721006(2)
15.0	−0.5555389985481027(8)	−1.1110889963511(2)	9670.66741(2)	−0.00000073328366(9)
16.0	−0.5555400544556883(7)	−1.1111007807111(2)	9483.95776(2)	−0.00000129198748(6)
17.0	−0.555541459141185(3)	−1.1111079869457(2)	9290.49393(2)	−0.00000147462726(6)
18.0	−0.5555429437012050(3)	−1.1111124261525(7)	9090.37732(3)	−0.00000147437500(4)
19.0	−0.5555443812475581(3)	−1.1111152242601(5)	8875.20366(2)	−0.000001392724472(2)
20.0	−0.5555457206482823(10)	−1.1111171379432(6)	8626.32591(2)	−0.000001284832331(3)

Table A31: Same as for Table A1, but for $6\,^3\Sigma_u^+$.

$6\,^3\Sigma_u$				
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.20264159869(3)	−1.424176741(3)	16.411(6)	−1.45556220(10)
0.8	−0.324500922089(6)	−1.459852787(8)	19.7004(4)	−1.013563678(9)
0.9	−0.4102959095911(4)	−1.4698719108(2)	23.498130(2)	−0.7214223241(2)
1.0	−0.47181686544168(3)	−1.4646499410(2)	27.848596(2)	−0.5210162102(2)
1.1	−0.51644809768165(5)	−1.4503430450(2)	32.802755(3)	−0.3794971360(2)
1.2	−0.5490169952310(4)	−1.4307152401(3)	38.418806(2)	−0.2772343747(2)
1.3	−0.5727899104778(3)	−1.4081258908(2)	44.763142(2)	−0.2019585153(9)
1.4	−0.5900402314657(5)	−1.3840799095(2)	51.911625(9)	−0.1457138904(7)
1.5	−0.60238794318267(5)	−1.3595475114(6)	59.95114391(10)	−0.10318108333(4)
1.6	−0.61101064249595(4)	−1.3351565895(4)	68.9815032(4)	−0.07070956529(2)
1.7	−0.61677904464738(3)	−1.31131183856(2)	79.1177725(2)	−0.04573749957(9)
1.8	−0.62034647927793(4)	−1.2882703276(5)	90.493146(7)	−0.02643187168(3)
1.9	−0.62220945321848(9)	−1.2661904325(4)	103.2624760(6)	−0.01145869795(2)
2.0	−0.62274951429236(4)	−1.24516407170(3)	117.606660(6)	0.00016747844(9)
2.1	−0.62226273693076(4)	−1.22523825059(2)	133.738132(7)	0.00918439204(6)
2.2	−0.62098083814168(5)	−1.20642963641(3)	151.907786(6)	0.01615092721(2)
2.3	−0.6190865263551(3)	−1.18873451422(2)	172.4138060(2)	0.02149501674(6)
2.4	−0.61672480860268(3)	−1.17213564145(2)	195.61302875(3)	0.02554748990(4)
2.5	−0.6140114217709(6)	−1.15660699608(9)	221.935758(7)	0.028566338985(3)
2.6	−0.61103918906181(6)	−1.14211708169(10)	251.905303(7)	0.03075434478(4)
2.7	−0.6078828608738(5)	−1.12863123983(2)	286.164138(4)	0.03227203034(4)
2.8	−0.60460283608384(3)	−1.11611328063(10)	325.509448(5)	0.03324728269(4)
2.9	−0.60124804793325(4)	−1.10452665297(6)	370.94228477(10)	0.033782566515(2)
3.0	−0.59785822118043(4)	−1.09383531882(5)	423.73686839(7)	0.033960374514(2)
3.1	−0.594465652863831(6)	−1.08400446565(8)	485.540413(8)	0.033847367767(3)
3.2	−0.59109663081579(3)	−1.07500118412(8)	558.5205494(4)	0.033497524224(2)
3.3	−0.58777257749395(6)	−1.06679526253(5)	645.589353(4)	0.032954512865(2)
3.4	−0.58451098923173(4)	−1.05936032893(9)	750.755402(5)	0.032253426333(3)
3.5	−0.58132623212150(3)	−1.05267576815(6)	879.699665(8)	0.031421913170(2)
3.6	−0.57823025808934(3)	−1.04673033283(2)	1040.764588(3)	0.030480606486(3)
3.7	−0.575233333286372(3)	−1.04152968924(8)	1246.758687(3)	0.029442425050(2)
3.8	−0.57234491321941(3)	−1.03711405685(2)	1518.50956(4)	0.028309413049(3)
3.9	−0.56957518557946(4)	−1.03360600987(2)	1892.569270(9)	0.02706265674(5)
4.0	−0.56693848452347(3)	−1.03136647612(3)	2440.04031(6)	0.02562762323(7)
4.1	−0.56446441971930(4)	−1.0316524291(8)	3318.29995(6)	0.02372595373(2)
4.2	−0.56224794803340(8)	−1.0403068006(4)	4889.15679(2)	0.0200450227(8)
4.3	−0.5606740177601(4)	−1.077091512(7)	7150.0079(2)	0.0102922149(2)
4.4	−0.55994545373723(3)	−1.08876504563(3)	9839.53132(2)	0.00707405951(5)
4.5	−0.55900120287592(4)	−1.0656276156(4)	12490.46946(2)	0.01163884226(8)
4.6	−0.55772547583469(6)	−1.0539403062(5)	14311.15471(3)	0.01337187944(2)
4.7	−0.55639585136161(9)	−1.0516766937(7)	16355.9628(4)	0.01300319341(2)
4.8	−0.55515258951886(4)	−1.05375680349(3)	18725.53390(2)	0.01178091157(5)
4.9	−0.55404786648140(5)	−1.05759428540(3)	20917.75516(2)	0.01030641787(6)
5.0	−0.55308743703514(5)	−1.06146142451(3)	22196.72466(2)	0.00894268991(6)
5.1	−0.55224889167781(6)	−1.06428309206(3)	22066.28215(7)	0.00788523359(5)
5.2	−0.55149983290654(6)	−1.06587120858(3)	20600.027229(4)	0.00714008793(4)
5.3	−0.55081447245266(6)	−1.06672001996(2)	18309.2379221(7)	0.006586589612(3)
5.4	−0.55018084097031(6)	−1.06750200476(2)	15784.535810(2)	0.006085125403(2)

5.5	−0.54959886360296(5)	−1.06871012273(8)	13452.755038(2)	0.005543200814(10)
5.6	−0.54907475467068(5)	−1.07056381445(3)	11522.6794(2)	0.00492601694(4)
5.7	−0.54861599449434(4)	−1.07306702332(3)	10037.3676(2)	0.00423946766(4)
5.8	−0.5482282896171(4)	−1.07609690285(3)	8947.5291(2)	0.003510289032(4)
5.9	−0.5479142166369(4)	−1.07946947934(3)	8166.4732(10)	0.002772704057(3)
6.0	−0.5476728801721(3)	−1.08297956137(2)	7601.9218(2)	0.002061033161(3)
6.5	−0.54733590850223(3)	−1.09680332814(2)	5763.706(2)	−0.000327924791(2)
7.0	−0.5476505500369(3)	−1.10012777503(3)	3578.694(9)	−0.000689524994(4)
7.5	−0.54789732096216(5)	−1.09771469209(2)	1353.839(4)	−0.000256006689(3)
8.0	−0.54791390795675(3)	−1.09460655679(9)	−250.8861(2)	0.000152657391(9)
8.5	−0.54779080633619(3)	−1.09308939765(2)	−1047.7228(5)	0.000293201767(2)
9.0	−0.54766059484044(3)	−1.09355651168(9)	−1169.29858(8)	0.000196075333(8)
9.5	−0.54761795573200(3)	−1.09562723219(8)	−792.297534(2)	−0.000041191656(8)
10.0	−0.54771131233150(3)	−1.09878739642(5)	−38.82181(2)	−0.000336477176(5)
11.0	−0.54833738428699(2)	−1.10646856169(6)	2216.1308(7)	−0.000890344829(5)
12.0	−0.54941102480008(3)	−1.11332695028(6)	4747.8412(10)	−0.001208741724(4)
13.0	−0.55066230440924(3)	−1.11762575548(4)	6804.9398(9)	−0.0012539343585(3)
14.0	−0.55185835746226(5)	−1.11936438607(4)	8120.1908(7)	−0.0011176907962(3)
15.0	−0.55287346787947(3)	−1.11935687579(4)	8812.2859(7)	−0.0009073293355(3)
16.0	−0.55367202817534(6)	−1.11842761629(4)	9108.5124(10)	−0.0006927224956(2)
17.0	−0.55426859745281(3)	−1.117146411744(3)	9200.1512(5)	−0.0005064245199(2)
18.0	−0.55469764773037(5)	−1.115840888626(2)	9214.7057(6)	−0.0003580885092(9)
19.0	−0.55499698239659(3)	−1.114672654608(2)	9230.9125(5)	−0.0002462468323(6)
20.0	−0.55520039556637(4)	−1.113703683919(2)	9300.8685(6)	−0.0001651446393(4)

Table A32: Same as for Table A1, but for $7\,^3\Sigma_u^+$.

$7\,^3\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.7	−0.19734116211(7)	−1.41449150(8)	2591.694(2)	−1.45687026(10)
0.8	−0.31933803910(6)	−1.45067691(6)	2502.424(2)	−1.01500104(7)
0.9	−0.40528158588(4)	−1.461216656(3)	2331.332(5)	−0.722948316(3)
1.0	−0.46695746289(5)	−1.456494460(2)	2084.126(6)	−0.522579535(2)
1.1	−0.51174459948(4)	−1.442636387(2)	1780.212(7)	−0.381042899(2)
1.2	−0.54446506629(4)	−1.423385048(2)	1447.904(8)	−0.278712430(9)
1.3	−0.56838072475(5)	−1.401090443(2)	1116.674(2)	−0.203329995(10)
1.4	−0.58576177452(3)	−1.377259207(8)	810.357(4)	−0.146954041(5)
1.5	−0.59822641281(3)	−1.352870662(7)	543.901(4)	−0.104278558(4)
1.6	−0.60695165876(3)	−1.328565068(9)	323.637(9)	−0.071663594(5)
1.7	−0.612808536545(8)	−1.3047596789(3)	149.4905(2)	−0.0465544741(2)
1.8	−0.616451243723(7)	−1.2817226538(2)	17.5644(2)	−0.0271223147(5)
1.9	−0.618377448729(5)	−1.2596214182(2)	−77.7715(2)	−0.0120350109(5)
2.0	−0.618969968931(4)	−1.2385549460(10)	−142.5155(9)	−0.0003075041(4)
2.1	−0.618526140451(8)	−1.2185756217(9)	−182.2828(8)	0.0087984092(4)
2.2	−0.617278870265(4)	−1.1997041922(3)	−201.9751(9)	0.0158425220(9)
2.3	−0.615411955804(3)	−1.1819400729(2)	−205.6960(7)	0.0212538429(8)
2.4	−0.61307138423(10)	−1.1652684889(7)	−196.79248(2)	0.02536428314(3)
2.5	−0.6103737679588(10)	−1.1496654525(6)	−177.95044(10)	0.02843283339(2)
2.6	−0.607412712187(5)	−1.1351012514(8)	−151.30386(4)	0.03066314346(3)
2.7	−0.6042636697986(9)	−1.1215429146(10)	−118.54057(2)	0.03221645369(4)
2.8	−0.6009876785649(8)	−1.1089559855(10)	−80.99706(2)	0.03322120415(3)
2.9	−0.5976342640258(9)	−1.09730584402(2)	−39.74244(2)	0.03378023587(2)
3.0	−0.5942437152586(10)	−1.086558770720(2)	4.34332(2)	0.03397621993(5)
3.1	−0.5908488872944(7)	−1.0766829303(8)	50.48937(2)	0.03387575623(3)
3.2	−0.5874766471411(4)	−1.0676494787(4)	97.934890(2)	0.03353244234(10)
3.3	−0.584149056339(3)	−1.0594340994(3)	145.7824(9)	0.0329890949(7)
3.4	−0.5808843706931(3)	−1.05201952138(3)	192.742201(3)	0.03227918235(8)
3.5	−0.5776979403236(7)	−1.0454001857(8)	236.6322(5)	0.03142734141(3)
3.6	−0.5746031230138(3)	−1.03959182024(3)	273.31368(5)	0.03044845161(7)
3.7	−0.5716124201410(3)	−1.03465321806(3)	294.22761(6)	0.02934368168(5)
3.8	−0.5687393378746(3)	−1.03074215741(3)	280.13790(8)	0.02808855746(6)
3.9	−0.5660024575704(3)	−1.0282822256(4)	183.31805(9)	0.02659556142(10)
4.0	−0.5634370247983(7)	−1.0285599249(2)	−130.48644(6)	0.02457853118(3)
4.1	−0.5611364044543(3)	−1.0361998544(2)	−1084.70558(10)	0.0209934035(4)
4.2	−0.5593851269583(4)	−1.0631072764(2)	−3530.37743(2)	0.0132530899(4)
4.3	−0.558292990692(3)	−1.066069866(2)	−4195.850(9)	0.011747934(5)
4.4	−0.5567687626320(10)	−1.035806344(5)	−759.1967(7)	0.0176661776(10)
4.5	−0.554952260223(3)	−1.0281617696(3)	1865.3267(2)	0.0181650557(5)
4.6	−0.553189345327(2)	−1.028451373(6)	4221.7402(3)	0.0169407211(2)
4.7	−0.551586044062(5)	−1.032463679(10)	6838.183(4)	0.0150443424(2)
4.8	−0.550190627456(6)	−1.038687393(2)	9378.050(5)	0.0128528879(3)
4.9	−0.549007351538(7)	−1.044587847(2)	10650.4009(3)	0.0109034400(2)
5.0	−0.54798612477(5)	−1.047741129(2)	9854.151(4)	0.0096462241(2)
5.1	−0.547057231855(6)	−1.0481788165(2)	7660.0502(3)	0.009006989642(2)
5.2	−0.546175316319(5)	−1.0473415616(3)	5234.558(8)	0.0086555906(7)
5.3	−0.545323938182(5)	−1.0462619047(3)	3241.522(2)	0.0083747116(7)
5.4	−0.54450038958813(8)	−1.0452858087(4)	1841.41867(2)	0.00809536490(8)

5.5	$-0.5437049279452(2)$	$-1.04443086441(3)$	968.58136(2)	0.00781436209(5)
5.6	$-0.54293728995319(3)$	$-1.04365106346(2)$	499.32584(2)	0.007539913651(3)
5.7	$-0.542196645715466(6)$	$-1.042930141342(9)$	315.10243(10)	0.0072742368576(3)
5.8	$-0.541482275985524(5)$	$-1.042286243923(3)$	319.91553(10)	0.007013501388(5)
5.9	$-0.54079397323849(3)$	$-1.04175125920(4)$	442.28337(8)	0.006751980894(6)
6.0	$-0.54013205931739(4)$	$-1.04135317031(5)$	632.20329(6)	0.006485158054(7)
6.5	$-0.53724191005752(8)$	$-1.04162801343(8)$	1793.8959468(7)	0.005054739491(2)
7.0	$-0.5350770965360(7)$	$-1.0447944342(7)$	2768.95600(9)	0.00362282269(9)
7.5	$-0.5335891607150(3)$	$-1.049420967303(2)$	3500.61749(6)	0.0023676472168(8)
8.0	$-0.5326670154818(4)$	$-1.0544637587(8)$	3880.521576(5)	0.00135878403(10)
8.5	$-0.5322240493022(6)$	$-1.061007802(4)$	3045.2083(8)	0.0004047408(5)
9.0	$-0.5321575636059(9)$	$-1.0644963284(2)$	2711.20216(2)	$-0.00002013346(2)$
9.5	$-0.5321898303680(6)$	$-1.0652013577(6)$	3220.86128(2)	$-0.00008649441(6)$
10.0	$-0.5322317602668(5)$	$-1.0652092494(5)$	3777.26056(3)	$-0.00007457288(4)$
11.0	$-0.5322679381490(3)$	$-1.06444800414(2)$	4703.6156(5)	0.000007988378(2)
12.0	$-0.5322142236734(3)$	$-1.06326963838(2)$	5166.2122(7)	0.000096567414(10)
13.0	$-0.53208544998747(9)$	$-1.06216783638(7)$	5139.5541(2)	0.000154081815(5)
14.0	$-0.53192029435751(8)$	$-1.06146548150(5)$	4796.3624(2)	0.0001696505152(4)
15.0	$-0.53175677405773(8)$	$-1.06121025820(5)$	4314.1146(2)	0.0001535526608(3)
16.0	$-0.53161794461763(8)$	$-1.061267530655(3)$	3805.2965(2)	0.0001230224113(2)
17.0	$-0.53151101539029(7)$	$-1.061468528807(2)$	3329.5797(2)	0.0000913824690(9)
18.0	$-0.53143336373603(6)$	$-1.061696340906(2)$	2912.6162(2)	0.0000650214759(6)
19.0	$-0.53137873381095(5)$	$-1.061896645738(10)$	2558.9594(9)	0.00004530641493(4)
20.0	$-0.53134082845386(5)$	$-1.062054757448(7)$	2262.2137(7)	0.00003134497299(2)

Table A33: Same as for Table A1, but for $8\,^3\Sigma_u^+$.

$8\,^3\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46569321127(2)	−1.4523803188(2)	17(2)	−0.52099389626(8)
1.1	−0.51032209866(3)	−1.4380639962(2)	19.4749173(7)	−0.37947254445(2)
1.2	−0.54288842086(2)	−1.4184257811(2)	22.79738378(7)	−0.27720744950(7)
1.3	−0.56665852417(2)	−1.39582499502(9)	26.553339(2)	−0.20192918976(5)
1.4	−0.583905789357(10)	−1.37176649892(7)	30.7891874(5)	−0.14568208586(4)
1.5	−0.596250192871(8)	−1.34722044655(4)	35.55831394(3)	−0.10314670721(2)
1.6	−0.604869321549(7)	−1.32281465790(4)	40.9223581(5)	−0.07067250925(2)
1.7	−0.610633878907(4)	−1.29895374081(2)	46.9527604(3)	−0.045697637055(7)
1.8	−0.614197180909(2)	−1.275894661033(10)	53.73267150(8)	−0.026389055120(4)
1.9	−0.616055718437(3)	−1.25379567210(2)	61.3593343(5)	−0.011412755384(8)
2.0	−0.616591020735(2)	−1.23274854676(2)	69.9470587(2)	0.000216747356(5)
2.1	−0.6160991405894(10)	−1.212800117614(6)	79.6309743(3)	0.009237220745(2)
2.2	−0.614811769775(2)	−1.19396684600866(4)	90.57181255(7)	0.016207587970(2)
2.3	−0.6129115872740(9)	−1.176244771414(2)	102.9620540(2)	0.0215558274493(2)
2.4	−0.6105435657082(5)	−1.1596163575946(10)	117.0339300(2)	0.02561282242569(3)
2.5	−0.60782340166511(10)	−1.1440552300885(9)	133.0699626(4)	0.0286366292967(3)
2.6	−0.60484387103559(7)	−1.1295294678863(3)	151.4170410(2)	0.03083010545571(6)
2.7	−0.60167966849585(9)	−1.1160038984462(3)	172.5055029(3)	0.03235386612796(2)
2.8	−0.5983911270442(2)	−1.1034417058885(5)	196.8754411(2)	0.0333359100712(3)
2.9	−0.5950271016794(5)	−1.0918055716694(10)	225.2136447(2)	0.0338788385136(2)
3.0	−0.59162722373893(9)	−1.081058509848(2)	258.4065748(2)	0.0340653125432(7)
3.1	−0.588223678032(2)	−1.07116452741(2)	297.618159(2)	0.033962202791(5)
3.2	−0.5848426166478(2)	−1.062089232814(5)	344.4072100(3)	0.033623750150(2)
3.3	−0.58150529672639(7)	−1.0538005420275(7)	400.91041511(5)	0.0330939549774(2)
3.4	−0.578229012066(2)	−1.046269719293(7)	470.1386824(3)	0.032408324953(2)
3.5	−0.575027880320(3)	−1.03947322867(10)	556.4796(3)	0.03159500913(3)
3.6	−0.571913552811(2)	−1.033396531122(5)	666.604758(2)	0.0306751595835(6)
3.7	−0.568895950121(7)	−1.02804299081(5)	811.221946(2)	0.029661867415(8)
3.8	−0.565984259369(5)	−1.02345841753(3)	1008.845009(2)	0.028555289791(6)
3.9	−0.5631889563913(3)	−1.019815168749(10)	1294.977847(9)	0.027323780521(3)
4.0	−0.5605283085442(3)	−1.017807856002(8)	1747.934400(6)	0.025812190272(2)
4.1	−0.5580633368016(7)	−1.02160122631(4)	2544.03605(2)	0.023054987144(9)
4.2	−0.5561310011644(8)	−1.05067496362(3)	3214.236524(3)	0.014663580645(5)
4.3	−0.5546868497918(6)	−1.039737149263(2)	4283.754210(2)	0.0161945465856(5)
4.4	−0.5529235450321(6)	−1.024820484680(4)	5500.174494(3)	0.0184151375873(7)
4.5	−0.5510900863801(10)	−1.02118676747(4)	7061.99459(2)	0.017998534508(7)
4.6	−0.549358297703(3)	−1.02273950744(3)	9395.514893(3)	0.016516758253(4)
4.7	−0.547802308316(2)	−1.02707715198(4)	12053.54942(2)	0.014580311628(8)
4.8	−0.546430873775(2)	−1.03053212850(4)	13148.441955(10)	0.012985337302(6)
4.9	−0.545171036023(2)	−1.02974011440(2)	11388.055400(2)	0.012367746459(2)
5.0	−0.543938554485(2)	−1.026325611995(2)	8325.085977(2)	0.0123102993944(4)

Table A34: Same as for Table A1, but for $9\,^3\Sigma_u^+$.

$9\,^3\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46567859703(4)	−1.4523257273(3)	2.371658(2)	−0.5209685333(2)
1.1	−0.51030481589(2)	−1.4379986072(2)	2.838967(2)	−0.37944452308(8)
1.2	−0.542868199241(10)	−1.41834841084(6)	3.3658637(7)	−0.27717667697(4)
1.3	−0.566635083267(5)	−1.39573439068(4)	3.9565501(4)	−0.20189555704(2)
1.4	−0.583878836952(3)	−1.37166132564(2)	4.6155876(3)	−0.145645465528(8)
1.5	−0.596219422966(2)	−1.347099272198(10)	5.3479315(2)	−0.103106950845(5)
1.6	−0.6048344121213(10)	−1.322675934884(6)	6.15896878(7)	−0.070629444151(3)
1.7	−0.6105944892961(6)	−1.298795784639(4)	7.05456275(5)	−0.045651062381(2)
1.8	−0.6141529487662(4)	−1.275715624451(3)	8.04110228(4)	−0.0263387371768(8)
1.9	−0.6160062561714(3)	−1.253593514017(2)	9.12555783(3)	−0.0113584219336(5)
2.0	−0.6165359113236(2)	−1.2325209946360(9)	10.31554426(2)	0.0002754140056(3)
2.1	−0.6160379326185(2)	−1.2125446215141(7)	11.61939161(2)	0.0093005922490(2)
2.2	−0.61474397153974(9)	−1.1936805221035(5)	13.046224674(10)	0.0162761004436(2)
2.3	−0.61283665970405(7)	−1.1759243318787(4)	14.606052759(6)	0.02162999457798(8)
2.4	−0.61046091381028(5)	−1.15925802270758(2)	16.30987091(4)	0.02569325204701(4)
2.5	−0.60773236409537(4)	−1.1436546166889(2)	18.169774356(4)	0.02872404460072(2)
2.6	−0.60474370724779(2)	−1.12908144593522(6)	20.199087989(3)	0.030925372523212(9)
2.7	−0.60156954272206(2)	−1.11550240367950(4)	22.412513215(3)	0.032458030283193(6)
2.8	−0.598270088049840(8)	−1.10287949071547(3)	24.826294693(2)	0.033450244780076(4)
2.9	−0.594894056773514(5)	−1.09117386703622(2)	27.458410085(2)	0.034004912589933(3)
3.0	−0.591480904783457(4)	−1.08034655502010(2)	30.3287863525(10)	0.034205084848939(2)
3.1	−0.588062596010558(3)	−1.070358897192268(8)	33.4595468781(8)	0.034118159622209(2)
3.2	−0.584664999339589(2)	−1.061172841730627(6)	36.8752944019(6)	0.0337991115464223(9)
3.3	−0.5813090004336343(10)	−1.052751108104073(4)	40.6034357790(5)	0.0332929978070289(6)
3.4	−0.5780113916376585(7)	−1.045057270636149(3)	44.6745557478(6)	0.0326369154821080(4)
3.5	−0.5747855880362596(6)	−1.038055787443618(2)	49.1228484090(6)	0.0318615396082574(2)
3.6	−0.5716422065391783(6)	−1.0317119948041999(10)	53.9866169802(7)	0.03099233840948792(3)
3.7	−0.5685895364836935(7)	−1.0259920816812618(5)	59.308854515(2)	0.0300505381854388(3)
3.8	−0.5656339239171400(9)	−1.0208630553174123(3)	65.137919361(3)	0.0290538927675959(6)
3.9	−0.562780086917758(2)	−1.016292706372706(3)	71.528309505(4)	0.0280172993494385(2)
4.0	−0.5600313756636609(5)	−1.012249582987697(4)	78.541425745(2)	0.0269532920849061(7)
4.1	−0.5573899884676057(5)	−1.00870302163381(2)	86.2442618770(5)	0.025872428122293(3)
4.2	−0.554857182991407(9)	−1.005638526922(7)	93.6929195(5)	0.024779961681(2)
4.3	−0.55280844979(2)	−1.0148609073(5)	500.9298(2)	0.0211060447(2)
4.4	−0.55071047444(2)	−1.01091716187(6)	2220.49878(9)	0.020569042503(8)
4.5	−0.548725638750(10)	−1.0118340720(2)	4031.6572(2)	0.01902604567(3)
4.6	−0.546921463709(9)	−1.0156285768(3)	6157.1413(2)	0.01700311969(4)
4.7	−0.545323957921(5)	−1.01998170996(8)	7456.92657(5)	0.01503536295(2)
4.8	−0.543882595922(3)	−1.020700686435(4)	6330.52298(2)	0.0139717719598(3)
4.9	−0.5425048677276(9)	−1.018209887613(10)	3902.185578(5)	0.013632622008(3)
5.0	−0.5411565573047(3)	−1.015798206589(6)	1968.037207(2)	0.013302981604(2)

Table A35: Same as for Table A1, but for $10\,^3\Sigma_u^+$.

$10\,^3\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46278819416(2)	−1.44753035959(8)	1265.973793(2)	−0.521953971222(8)
1.1	−0.50751266843(2)	−1.43348594106(4)	1075.711486(10)	−0.380418731098(3)
1.2	−0.540171626191(8)	−1.41407457222(2)	870.012187(4)	−0.278109433202(4)
1.3	−0.564028717202(5)	−1.391650395964(5)	666.779477(2)	−0.202763816589(3)
1.4	−0.581355439424(3)	−1.367719757872(3)	480.1768926(5)	−0.146434913592(2)
1.5	−0.593770743459(2)	−1.343258634830(2)	318.83674975(4)	−0.1038114319425(8)
1.6	−0.6024519200959(7)	−1.3189025033303(3)	186.1714225(7)	−0.0712491644629(8)
1.7	−0.6082699048055(5)	−1.2950636405751(7)	81.7930722(3)	−0.0461904888026(2)
1.8	−0.6118785734837(3)	−1.2720057308256(7)	3.0989269(5)	−0.02680476881014(6)
1.9	−0.6137751452288(3)	−1.2498924795306(8)	−53.4760332(7)	−0.0117590468806(2)
2.0	−0.6143419351550(3)	−1.2288198940162(10)	−91.6539514(10)	−0.0000680118531(3)
2.1	−0.6138757714003(2)	−1.208838026027(2)	−114.881151(2)	0.0090064365589(4)
2.2	−0.6126090735637(2)	−1.189965774822(2)	−126.144534(2)	0.0160238055933(4)
2.3	−0.6107251845222(2)	−1.172201049334(2)	−127.932034(2)	0.0214127477002(4)
2.4	−0.6083696730523(2)	−1.155527789709(2)	−122.265326(3)	0.0255048151649(5)
2.5	−0.6056587675478(2)	−1.139920844558(2)	−110.762090(3)	0.0285586762152(5)
2.6	−0.6026857185739(2)	−1.125349375691(2)	−94.705148(3)	0.0307777159451(5)
2.7	−0.5995256475229(3)	−1.111779250771(2)	−75.108016(3)	0.0323229793610(6)
2.8	−0.5962392764103(3)	−1.099174746713(2)	−52.773402(4)	0.0333227878958(6)
2.9	−0.5928758227881(3)	−1.087499799363(3)	−28.345228(5)	0.0338799469700(6)
3.0	−0.5894752668507(3)	−1.076718985643(3)	−2.357598(6)	0.0340771826860(7)
3.1	−0.5860701442826(4)	−1.066798410040(4)	24.712599(7)	0.0339812511371(8)
3.2	−0.5826869815349(4)	−1.057706698671(4)	52.376852(8)	0.0336460201245(10)
3.3	−0.5793474663804(5)	−1.049416418270(5)	80.024509(10)	0.033114701361(2)
3.4	−0.5760694353159(6)	−1.041906541149(6)	106.71430(2)	0.032421273377(2)
3.5	−0.5728677657488(7)	−1.035167384332(9)	130.73261(2)	0.031590899190(2)
3.6	−0.5697553045725(7)	−1.029211776440(8)	148.56136(2)	0.030638564640(2)
3.7	−0.5667441143017(6)	−1.024103794932(8)	152.20187(2)	0.029563360452(2)
3.8	−0.5638478402352(6)	−1.020045649000(9)	121.26837(2)	0.028328955650(3)
3.9	−0.5610881495529(6)	−1.01770277018(2)	−4.84731(2)	0.026788084341(3)
4.0	−0.5585193558056(8)	−1.01979097641(3)	−448.60916(2)	0.024311933799(6)
4.1	−0.556344784773(3)	−1.0380897102(2)	−2033.16429(3)	0.01819508765(3)
4.2	−0.554777269372(3)	−1.03911794016(7)	−4018(2)	0.01677061871(2)
4.3	−0.552433246118359(3)	−1.002979820660907(3)	104.036903499(3)	0.023694574785070(2)
4.4	−0.550118012898984(2)	−1.000745173189075(2)	114.364690716(2)	0.022611557411112(2)
4.5	−0.547910553943914(2)	−0.99889144476948(2)	125.766733882(2)	0.021539925137410(2)
4.6	−0.545809495672444(2)	−0.99739151721789(2)	138.398395939(3)	0.020484233505869(2)
4.7	−0.5438130492603691(10)	−0.99621928164518(2)	152.435434140(5)	0.019448258909693(3)
4.8	−0.541919082743901(2)	−0.99534970104188(3)	168.108114349(10)	0.018435096759567(5)
4.9	−0.540125188343350(2)	−0.99475934872619(8)	185.79930712(3)	0.01744714856337(2)
5.0	−0.538428773667737(5)	−0.9944307451160(5)	206.8159778(2)	0.01648536044390(9)

Table A36: Same as for Table A1, but for $11\,^3\Sigma_u^+$.

$11\,^3\Sigma_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46200186057(4)	−1.4449860448(2)	10.579265(3)	−0.5209823237(2)
1.1	−0.50662953154(2)	−1.4306648258(2)	12.4472461(6)	−0.37945978431(6)
1.2	−0.53919451706(2)	−1.41102119819(7)	14.5665210(2)	−0.27719347007(4)
1.3	−0.56296315991(2)	−1.38841445907(9)	16.963319646(2)	−0.20191395327(5)
1.4	−0.580208836770(6)	−1.36434944039(4)	19.6678205(5)	−0.14566554775(2)
1.5	−0.592551519253(6)	−1.33979626137(5)	22.7148479(5)	−0.10312881525(3)
1.6	−0.601168788533(4)	−1.31538270071(3)	26.1447233(6)	−0.07065320227(2)
1.7	−0.606931341517(3)	−1.29151331725(2)	30.0043193(3)	−0.045676843656(4)
1.8	−0.610492486441(4)	−1.268445018391(10)	34.34837066(9)	−0.026366691949(2)
1.9	−0.612348705173(3)	−1.24633598815(2)	39.2411040(4)	−0.011388725161(5)
2.0	−0.612881516440(2)	−1.225277916434(10)	44.7582892(3)	0.000242558223(3)
2.1	−0.612386960735(8)	−1.20531753686(4)	50.989839(2)	0.009264945053(10)
2.2	−0.611096715438(3)	−1.18647119210(2)	58.043139(3)	0.016237381260(5)
2.3	−0.609193442680(5)	−1.168734779056(7)	66.04734(2)	0.021587872299(7)
2.4	−0.606822095245(2)	−1.152090589400(10)	75.15902(2)	0.025647333785(6)
2.5	−0.604098346339(2)	−1.13651203962(3)	85.5695918(5)	0.028673861224(8)
2.6	−0.601114944144(2)	−1.121966953338(5)	97.5154159(2)	0.0308703595962(9)
2.7	−0.597946550353(2)	−1.108419843723(6)	111.2914625(2)	0.032397502586(2)
2.8	−0.5946534584539(9)	−1.095833504284(3)	127.2703890(3)	0.0333833616513(5)
2.9	−0.5912844757694(8)	−1.084170125774(3)	145.9295493(3)	0.0339306295740(6)
3.0	−0.5878791755942(5)	−1.073392097686(6)	167.8901194(4)	0.034122084501(2)
3.1	−0.5844696713272(6)	−1.063462619743(4)	193.9752147(2)	0.0340247493262(9)
3.2	−0.581082026088(2)	−1.05434623823(2)	225.29876581(4)	0.033693066857(3)
3.3	−0.577737384497(8)	−1.0460094430(4)	263.40614(4)	0.03317131094(8)
3.4	−0.574452895553(6)	−1.0384215406(6)	310.50635(6)	0.0324953678(2)
3.5	−0.5712424870721(9)	−1.03155625901(2)	369.8750662(4)	0.031693918609(3)
3.6	−0.5681175573460(6)	−1.025395239013(10)	446.6025036(5)	0.030788854355(3)
3.7	−0.565087690274(2)	−1.01993696731(3)	549.108049(2)	0.029794165739(7)
3.8	−0.562161666982(2)	−1.01522480941(5)	692.586090(2)	0.02871013804(2)
3.9	−0.559349839219(2)	−1.01146467680(8)	908.113217(3)	0.02749615427(2)
4.0	−0.556674398458(8)	−1.0098083296(6)	1268.15058(4)	0.0258851168(2)
4.1	−0.55425893497(4)	−1.021206833(3)	1714.9202(4)	0.0212953749(7)
4.2	−0.55238283366(2)	−1.024727847(2)	1859.0087(2)	0.0190566240(3)
4.3	−0.550345639855(8)	−1.0101765923(3)	2599.238596(10)	0.02104992730(6)
4.4	−0.54825382664(2)	−1.0060024269(4)	3523.26945(2)	0.02056936963(8)
4.5	−0.54626050059(2)	−1.0061703362(5)	5094.98373(5)	0.01918903665(9)
4.6	−0.54443315002(3)	−1.0092275524(5)	7236.14178(8)	0.01731277122(9)
4.7	−0.54278857314(3)	−1.0116306804(2)	8082.89736(6)	0.01573329062(3)
4.8	−0.54124843977(2)	−1.00945851992(6)	6270.44417(4)	0.01521632491(2)
4.9	−0.539733944829(10)	−1.00567232462(6)	3924.96568(4)	0.01506031939(2)
5.0	−0.53824426547(2)	−1.00305202942(9)	2327.6715(2)	0.01468730029(3)

Table A37: Same as for Table A1, but for $12\,^3\Sigma_u^+$.

$12\,^3\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46199256413(3)	−1.4449513536(2)	1.554523(2)	−0.5209662253(2)
1.1	−0.506618541225(2)	−1.43062327771(4)	1.8575985(6)	−0.37944199569(2)
1.2	−0.539181660899(6)	−1.41097203885(4)	2.1993189(3)	−0.27717393088(3)
1.3	−0.562948259400(3)	−1.38835688922(2)	2.5824575(2)	−0.20189259263(2)
1.4	−0.580191705736(3)	−1.36428260755(2)	3.0100308(2)	−0.145642282910(9)
1.5	−0.592531962568(4)	−1.33971924973(3)	3.4853226(2)	−0.103103549728(10)
1.6	−0.6011466006568(3)	−1.315294519395(2)	4.01191088(3)	−0.0706258238011(8)
1.7	−0.60690630478599(10)	−1.2914128862194(8)	4.59369776(2)	−0.0456472215573(4)
1.8	−0.61046436907594(5)	−1.2683311514065(4)	5.234944884(6)	−0.0263346740304(2)
1.9	−0.61231725894728(3)	−1.2462073723273(2)	5.940311912(3)	−0.01135413391196(8)
2.0	−0.61284647391702(2)	−1.22513308729561(10)	6.714900636(2)	0.00027993026922(4)
2.1	−0.612348031998278(6)	−1.20515484776261(5)	7.5643045647(4)	0.00930534106379(2)
2.2	−0.611053584190634(4)	−1.18628877652859(2)	8.4946648807(4)	0.016281087205762(3)
2.3	−0.609145761510125(3)	−1.16853050337189(2)	9.512733684(2)	0.021635225934067(8)
2.4	−0.606769479920857(2)	−1.15186199325423(4)	10.625945548(2)	0.02569873607812(2)
2.5	−0.604040368771410(3)	−1.13625625996895(8)	11.842498644(4)	0.02872979102954(4)
2.6	−0.601051123686375(2)	−1.12168062571424(2)	13.1714468744(10)	0.030931392945579(7)
2.7	−0.597876342856356(10)	−1.10809897195859(7)	14.622804714(8)	0.03246433842744(4)
2.8	−0.59457624232167(9)	−1.0954732856137(3)	16.20766685(2)	0.03345685679631(3)
2.9	−0.59119953387525(10)	−1.0837647103730(3)	17.938344924(9)	0.03401184737157(3)
3.0	−0.58778567136624(4)	−1.072934249565(2)	19.82852425(5)	0.0342123643893(4)
3.1	−0.58436661635495(3)	−1.0629432235370(9)	21.89344424(4)	0.0341258094106(3)
3.2	−0.58096823498450(2)	−1.0537535547606(6)	24.15010608(5)	0.0338071610026(2)
3.3	−0.577611409759664(10)	−1.04532793300879(6)	26.617513545(3)	0.033301480760769(10)
3.4	−0.57431292940037(9)	−1.0376298984302(4)	29.31695233(2)	0.03264587069721(5)
3.5	−0.57108620484437(8)	−1.0306238699510(3)	32.272316634(10)	0.03187101135364(3)
3.6	−0.56794184827393(6)	−1.0242751390868(2)	35.510491194(7)	0.03100237707252(2)
3.7	−0.56488814365494(5)	−1.0185498439272(2)	39.061800421(8)	0.03006120091425(2)
3.8	−0.56193143095598(5)	−1.0134149344109(2)	42.960530909(6)	0.029065244079232(7)
3.9	−0.55907642142119(3)	−1.00883813853601(9)	47.245485901(4)	0.028029411360609(8)
4.0	−0.55632645772783(2)	−1.00478795085792(5)	51.959922627(2)	0.026966241149437(4)
4.1	−0.55368373306217(2)	−1.0012342297504(2)	57.119859097(7)	0.02588615521316(3)
4.2	−0.551336900651(6)	−1.0076738020(3)	45.13191(2)	0.02261904744(6)
4.3	−0.549065902747(3)	−1.001731026984(6)	1316.62120(2)	0.0224187856999(4)
4.4	−0.546885956514(2)	−1.00096308775(4)	2494.45680(2)	0.021092914835(7)
4.5	−0.544861543555(8)	−1.0027039352(2)	4001.6662(2)	0.01933758932(4)
4.6	−0.543021623868(3)	−1.00545028234(5)	5091.24782(4)	0.017520209868(9)
4.7	−0.541328578195(3)	−1.005028765473(7)	4096.74636(3)	0.0165166789183(4)
4.8	−0.539697204294(2)	−1.001975780704(4)	2145.49193(3)	0.016128880808(2)
4.9	−0.5381084290856(9)	−0.999762879983(2)	878.98304(3)	0.0156028526908(7)
5.0	−0.53658415800(4)	−0.9988961914(7)	252.5650(3)	0.0148544249(2)

Table A38: Same as for Table A1, but for $13\,^3\Sigma_u^+$.

$13\,^3\Sigma_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.4601286468(3)	−1.441871444(2)	827.17863(9)	−0.5216141507(7)
1.1	−0.5048191520(2)	−1.4277274746(7)	700.3838(2)	−0.3800810641(4)
1.2	−0.53744489905(8)	−1.4082311765(5)	564.3287(3)	−0.2777844820(3)
1.3	−0.5612704849(2)	−1.385738701(2)	430.6961(10)	−0.2024597933(8)
1.4	−0.57856808222(5)	−1.3617560515(3)	308.5940(5)	−0.14615706216(10)
1.5	−0.59095702057(5)	−1.3372572841(5)	203.4523(6)	−0.1035621620(3)
1.6	−0.59961471342(6)	−1.3128752445(6)	117.3076(6)	−0.0710286361(3)
1.7	−0.60541202978(4)	−1.2890195200(4)	49.7547(5)	−0.0459973296(2)
1.8	−0.60900265886(4)	−1.2659513977(4)	−1.0108(5)	−0.0266367111(2)
1.9	−0.61088356872(2)	−1.2438326022(2)	−37.3803(3)	−0.01161340249(7)
2.0	−0.61143679826(2)	−1.2227575659(2)	−61.8189(3)	0.00005801531(6)
2.1	−0.61095889863(2)	−1.2027751036(2)	−76.5920(3)	0.00911556840(5)
2.2	−0.60968202504(2)	−1.1839031328(2)	−83.6531(2)	0.01611859875(4)
2.3	−0.60778927450(2)	−1.1661387586(2)	−84.6243(2)	0.02149556105(4)
2.4	−0.605425989755(10)	−1.14946522885(9)	−80.8198(2)	0.02557781278(3)
2.5	−0.602708191624(9)	−1.13385675664(8)	−73.2894(2)	0.02862385064(3)
2.6	−0.599728938576(5)	−1.11928187725(4)	−62.86422(8)	0.03083692304(2)
2.7	−0.596563171535(10)	−1.10570579687(9)	−50.2007(2)	0.03237798007(3)
2.8	−0.593271439215(7)	−1.09309205059(6)	−35.8180(2)	0.03337529566(2)
2.9	−0.589902787995(3)	−1.08140369984(3)	−20.13393(6)	0.033931681431(7)
3.0	−0.58649702322(2)	−1.0706042479(2)	−3.4976(4)	0.03412993286(5)
3.1	−0.583086495021(7)	−1.06065843462(7)	13.7774(2)	0.03403695336(2)
3.2	−0.579697524768(6)	−1.05153309919(6)	31.3582(2)	0.03370685948(2)
3.3	−0.576351563739(4)	−1.04319840462(5)	48.81364(9)	0.03318324935(2)
3.4	−0.573066164305(8)	−1.03563002406(9)	65.4461(2)	0.03250067781(3)
3.5	−0.569855850135(5)	−1.02881374029(6)	79.92193(9)	0.03168513142(2)
3.6	−0.566733019944(5)	−1.02275655872(6)	89.34706(6)	0.03075263366(2)
3.7	−0.563709195803(4)	−1.01751795155(6)	86.67000(7)	0.02970282164(2)
3.8	−0.560797616256(5)	−1.01331675299(8)	52.06741(6)	0.02849433672(2)
3.9	−0.558021518980(3)	−1.01101150363(6)	−83.13190(3)	0.02693116265(2)
4.0	−0.555454370126(5)	−1.0150969273(2)	−635.84365(4)	0.02395295324(5)
4.1	−0.55338040761(5)	−1.0333615219(2)	−2086.5740(2)	0.01790226663(5)
4.2	−0.55114943471080(4)	−0.9981450594076(6)	62.8475409(2)	0.0247985261938(2)
4.3	−0.5487239971102(3)	−0.995491987743(3)	69.2298373(4)	0.0237106991807(5)
4.4	−0.5464070907682(3)	−0.9932468908548(4)	76.265592(4)	0.02262892970028(5)
4.5	−0.5441978252236(3)	−0.991381459179(3)	84.0793589(5)	0.0215587091707(5)
4.6	−0.54209481181399(4)	−0.9898685698081(5)	92.78877020(8)	0.02050457691736(9)
4.7	−0.54009624702891(5)	−0.9886820576593(6)	102.54463168(10)	0.01947030561671(10)
4.8	−0.538199985956202(2)	−0.98779701381104(6)	113.57395584(3)	0.01845894960445(2)
4.9	−0.536403620060846(5)	−0.9871913552849(4)	126.3876216(2)	0.01747262955852(7)
5.0	−0.53470469224524(3)	−0.986871279434(5)	144.618721(2)	0.0165076210114(9)

Table A39: Same as for Table A1, but for $14\,^3\Sigma_u^+$.

		$14\,^3\Sigma_u$		
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.45960654850(3)	−1.4401888464(2)	7.15589547(7)	−0.5209757494(2)
1.1	−0.50423352836(2)	−1.42586484342(7)	8.4172318(2)	−0.37945253337(4)
1.2	−0.536797754173(10)	−1.40621813648(4)	9.8485345(2)	−0.27718552345(2)
1.3	−0.560565566657(7)	−1.38360800827(3)	11.46770824(10)	−0.201905288425(10)
1.4	−0.577810340039(4)	−1.35953927351(2)	13.2953881(4)	−0.145656138162(9)
1.5	−0.590152043050(4)	−1.33498203075(2)	15.3554281(4)	−0.103118629769(4)
1.6	−0.598768253498(4)	−1.31056403421(2)	17.67549738(9)	−0.070642204506(3)
1.7	−0.604529664345(2)	−1.286689813470(6)	20.28782293(7)	−0.045664991047(2)
1.8	−0.608089579228(2)	−1.263616241105(4)	23.2301130(2)	−0.0263539348053(8)
1.9	−0.609944474640(3)	−1.24150145959(3)	26.54671008(7)	−0.011375005429(9)
2.0	−0.610475863020(3)	−1.22043710915(2)	30.2900403(2)	0.000257308447(5)
2.1	−0.609979777503(2)	−1.200469863821(9)	34.52247167(8)	0.009280805326(3)
2.2	−0.6086878868520(8)	−1.181615994742(6)	39.31867510(7)	0.016254444983(2)
2.3	−0.6067828430410(5)	−1.163871312270(4)	44.76870931(9)	0.021606249483(2)
2.4	−0.6044095868898(4)	−1.147218002935(3)	50.98206408(10)	0.0256671545185(8)
2.5	−0.6016837774113(3)	−1.131629354850(2)	58.09304350(9)	0.0286952799890(6)
2.6	−0.5986981458941(2)	−1.117073033461(2)	66.26803625(9)	0.0308935608951(4)
2.7	−0.5955273337805(2)	−1.1035133551261(10)	75.71549268(9)	0.0324227083093(3)
2.8	−0.59223161010741(9)	−1.0909128659352(8)	86.69986409(9)	0.0334108408141(3)
2.9	−0.58885975240527(7)	−1.0792334412586(6)	99.56147073(8)	0.0339607115696(2)
3.0	−0.5854512972723(2)	−1.068437062079(2)	114.7454689(2)	0.0341551774885(4)
3.1	−0.58203831230316(10)	−1.058486388647(2)	132.8451948(2)	0.0340613664386(4)
3.2	−0.57864680252055(9)	−1.049345238051(2)	154.66901124(7)	0.0337338646843(4)
3.3	−0.57529783738563(9)	−1.040979086339(2)	181.34717147(4)	0.0332171480097(4)
3.4	−0.5720084663267(2)	−1.033355784434(3)	214.5102964(2)	0.0325473965350(7)
3.5	−0.5687924812956(2)	−1.026446888641(4)	256.6042732(4)	0.0317537354143(10)
3.6	−0.5656610888490(3)	−1.020230677984(7)	311.4868635(9)	0.030858749920(2)
3.7	−0.5626235936107(4)	−1.01470041184(2)	385.671342(2)	0.029877506861(3)
3.8	−0.5596883749262(7)	−1.00989302264(4)	491.277686(3)	0.028811507162(8)
3.9	−0.556865431260(3)	−1.0060318737(2)	654.192717(7)	0.02761512533(4)
4.0	−0.55418073285(2)	−1.004832343(2)	929.45918(2)	0.0258822807(3)
4.1	−0.55182359850(7)	−1.0188137478(2)	871.3625(5)	0.020691085179(8)
4.2	−0.549690711377(5)	−1.0055503975(2)	1244.48429(4)	0.02234072028(3)
4.3	−0.547441759221(5)	−0.9988242499(2)	1727.272235(5)	0.02233936477(4)
4.4	−0.545255458310(8)	−0.9968447773(3)	2528.17695(2)	0.02128775894(5)
4.5	−0.54320078425(2)	−0.9976083707(3)	3931.92911(4)	0.01973182173(6)
4.6	−0.54131638088(2)	−0.9998301661(2)	5288.94352(4)	0.01800056428(4)
4.7	−0.53957208676(2)	−0.99895567866(4)	4560.99445(3)	0.01706138187(2)
4.8	−0.537884089202(8)	−0.99554265332(8)	2760.15650(5)	0.01671365105(2)
4.9	−0.536234511760(5)	−0.99290075034(4)	1496.56447(5)	0.016238423094(10)
5.0	−0.534643314036(3)	−0.99148556924(3)	785.50796(5)	0.015560211764(6)

Table A40: Same as for Table A1, but for $1\,^1\Pi_g$ (I state) .

		$1\,^1\Pi_g$		
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.055620732852246(6)	–	249.3999921(1)	–
0.01	97.94464058640(2)	95.8897985410(2)	249.523(3)	−9999.948263184(8)
0.05	17.9504116140(3)	15.912232428(3)	252.367(2)	−399.77141603(5)
0.1	7.96614323261(8)	5.971361504(3)	260.412(2)	−99.60904962(2)
0.15	4.6553158497(2)	2.719322944(2)	272.618(3)	−43.942058368(5)
0.2	3.015754379264(7)	1.1467034992(4)	288.425(3)	−24.423926297(2)
0.3	1.4109876731(2)	−0.31676629408(5)	329.669(3)	−10.46240546760(10)
0.4	0.6435828674310(2)	−0.947599026340(5)	382.980(4)	−5.586861903004(9)
0.5	0.209322338243(4)	−1.2572025107527(7)	448.376(5)	−3.351654374485(2)
0.6	−0.060539402480564(4)	−1.4160157732823(2)	526.515(5)	−2.1581949472019(3)
0.7	−0.238393084120199(3)	−1.495929863340(4)	618.474(6)	−1.455948135860(7)
0.8	−0.360290592374370(4)	−1.531757474788(9)	725.6747(10)	−1.013995362548(9)
0.9	−0.4461288093169766(2)	−1.541950211832(2)	849.8240(10)	−0.721902881331(2)
1.0	−0.507698297532046(3)	−1.536925637121(7)	992.9701(6)	−0.521549042057(5)
1.1	−0.552383677344524(2)	−1.522842016503(6)	1157.4989(7)	−0.380086056195(4)
1.2	−0.585012709686148(3)	−1.503465896063(6)	1346.1899(2)	−0.277883730575(4)
1.3	−0.608852186979388(2)	−1.481159682383(6)	1562.2711(3)	−0.202673314172(4)
1.4	−0.626176016107194(4)	−1.457431948840(6)	1809.5006(3)	−0.146499940447(4)
1.5	−0.638604793189250(2)	−1.433257320895(2)	2092.2591(5)	−0.1040451563444(10)
1.6	−0.647316835137268(4)	−1.409269013823(2)	2415.6695(5)	−0.0716595897179(9)
1.7	−0.653183706517060(2)	−1.385878159319(9)	2785.74210(9)	−0.046782791932(5)
1.8	−0.656859740520023(5)	−1.363349631624(9)	3209.55351(10)	−0.027583416991(5)
1.9	−0.658842632362324(2)	−1.341851299313(9)	3695.4727(2)	−0.012729491888(4)
2.0	−0.659515340754017(6)	−1.32148666268(2)	4253.4349(2)	−0.001237990588(5)
2.1	−0.659175620023221(3)	−1.30231690829(2)	4895.2844(2)	0.007625872265(5)
2.2	−0.658057193711391(7)	−1.28437613052(2)	5635.1985(2)	0.014417389502(5)
2.3	−0.656345175033174(3)	−1.26768211147(2)	6490.2105(2)	0.019560103737(5)
2.4	−0.654187463248630(8)	−1.252244223916(5)	7480.8527(2)	0.023379459409(2)
2.5	−0.651703286081417(4)	−1.238069509824(5)	8631.9361(2)	0.026126824936(2)
2.6	−0.648989694529758(9)	−1.225167661976(5)	9973.4782(2)	0.027996818109(2)
2.7	−0.646126575090967(4)	−1.213555419303(5)	11541.7719(2)	0.029139900326(2)
2.8	−0.643180581113649(10)	−1.20326072123(2)	13380.5435(2)	0.029671586070(6)
2.9	−0.640208271512076(5)	−1.19432679988(2)	15542.0631(2)	0.029679221775(6)
3.0	−0.637258662449248(10)	−1.186816158137(9)	18087.9179(2)	0.029233722254(2)
3.1	−0.634375331677092(4)	−1.18081399722(3)	21088.8795(2)	0.028360214883(6)
3.2	−0.631598153855495(10)	−1.17642999892(3)	24622.8721(2)	0.027108221499(6)
3.3	−0.628964676764191(4)	−1.17379631274(3)	28769.4551(2)	0.025488800238(6)
3.4	−0.626511063061438(8)	−1.1730581475890(7)	33598.6320(7)	0.02351293486300(2)
3.5	−0.6242724190517674(3)	−1.1743519801153(7)	39151.7171(5)	0.021192245139593(9)
3.6	−0.622282235211503(7)	−1.1777665431815(6)	45413.5353(4)	0.018549424233847(9)
3.7	−0.6205706474226789(2)	−1.1832862801634(6)	52279.9757(3)	0.01563108504926(2)
3.8	−0.6191514231607989(2)	−1.1907285798419(6)	59533.0434(3)	0.01251954381048(2)
3.9	−0.61806809151767972(9)	−1.1997023807010(9)	66842.8232(2)	0.00933687239350(9)
4.0	−0.6172903557001000(2)	−1.209623294356(2)	73812.1075(2)	0.0062343542611(3)
4.1	−0.61680236035624(2)	−1.2198014186189(3)	80058.06987(8)	0.00336665904723(5)
4.2	−0.61659394644281(2)	−1.2295749041901(4)	85297.92785(4)	0.00086023540369(7)
4.3	−0.61661473822808(6)	−1.2384300938752(10)	89398.53653(2)	−0.00120944591128(9)
4.4	−0.61681964617742(5)	−1.2460600263929(8)	92373.1491(7)	−0.0028228940996(2)

4.5	−0.6171740315935651(2)	−1.252354957700(4)	94339.90681(2)	−0.0040059765584(6)
4.6	−0.61760738504809(5)	−1.2573517874(2)	95469.695(3)	−0.00481239510(7)
4.7	−0.61811525621423(2)	−1.261174570033(4)	95943.811062(4)	−0.0053072462988(7)
4.8	−0.618659769917686(6)	−1.2639857852(2)	95928.1752(10)	−0.00555546777(2)
4.9	−0.61921925170919(2)	−1.2659541495(3)	95562.0306(8)	−0.00561543796(3)
5.0	−0.6197874182528645(4)	−1.267236867755(3)	94955.857480(7)	−0.0055364062499(5)
5.1	−0.620322437421447(4)	−1.2679718288(4)	94194.0423(6)	−0.00535822624(5)
5.2	−0.620846026668478(6)	−1.2682756671(5)	93339.2962(6)	−0.00511223339(6)
5.3	−0.62134266489907(8)	−1.2682448430(6)	92437.2239(6)	−0.00482254964(7)
5.4	−0.621808939076557(7)	−1.2679580036(6)	91520.3617(7)	−0.00450743061(9)
5.5	−0.6222530198410015(3)	−1.2674786869(7)	90611.4664(8)	−0.00418048129(10)
5.6	−0.62264424934149(8)	−1.2668579106046(8)	89726.0792249(6)	−0.00385168070028(2)
5.7	−0.623012821742175(9)	−1.2661364598(10)	88874.4681(10)	−0.0035282133(2)
5.8	−0.62334953797260(4)	−1.265346811(2)	88063.085(2)	−0.0032151266(2)
5.9	−0.623655618866059(10)	−1.2645147281691(8)	87295.6319896(6)	−0.00291584583674(10)
6.0	−0.6239425636994983(7)	−1.26366056309(3)	86573.85020(4)	−0.002632572615(3)
6.5	−0.624950855257195(9)	−1.259507401581(5)	83634.613639(8)	−0.0014808755486(5)
7.0	−0.625488515522114(3)	−1.2561045375371(8)	81649.1164813(4)	−0.0007325009277(3)
7.5	−0.625733432092477(3)	−1.25362710222(3)	80354.852163(6)	−0.000288031739(5)
8.0	−0.625809393436053(2)	−1.2519515441(2)	79530.17202(9)	−0.00004159466(3)
8.5	−0.625795151273442(2)	−1.25088281746(2)	79013.262197(2)	0.000083233539(2)
9.0	−0.6257378199140553(8)	−1.250238427949(5)	78692.8532201(6)	0.0001374679863(8)
9.5	−0.6256640568552325(9)	−1.249874263060(5)	78495.2236093(2)	0.0001530369104(6)
10.0	−0.6255880139309715(6)	−1.2496864991391(6)	78372.9286996(5)	0.00014895287227(7)
11.0	−0.62545247254346736(9)	−1.249583860023(2)	78246.7110450(7)	0.0001200986421(2)
12.0	−0.62534812481753221(8)	−1.2496228004782(7)	78189.9762572(5)	0.00008945409639(7)
13.0	−0.62527125012850115(4)	−1.2496907379325(3)	78158.4589808(5)	0.00006552017880(3)
14.0	−0.625214829096054525(9)	−1.24975327550001(8)	78137.1353153(3)	0.000048313049432(9)
15.0	−0.625172937458233213(4)	−1.24980326081155(2)	78120.9282186(3)	0.000036174273659(4)
16.0	−0.625141309348841379(2)	−1.24984159110974(2)	78107.9681790(3)	0.0000275642242459(2)
17.0	−0.6251170092209620277(10)	−1.24987080184524(3)	78097.3996064(2)	0.0000213656821592(2)
18.0	−0.6250980286814565856(5)	−1.24989323672651(4)	78088.7079192(2)	0.0000168233686904(3)
19.0	−0.6250829796118870796(3)	−1.24991069220359(4)	78081.52089339(6)	0.0000134351063269(3)
20.0	−0.6250708868292175202(2)	−1.24992446796585(5)	78075.54818409(2)	0.0000108652846306(5)

Table A41: Same as for Table A1, but for $2\,^1\Pi_g$ (R state) .

R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
		$2\,^1\Pi_g$		
0.0	−2.031279846178687(7)	–	129.1751887(8)	–
0.01	97.96898149748(5)	95.9384804119(4)	129.20(2)	−9999.94825831(3)
0.05	17.974743084(3)	15.96091651(2)	130.67(2)	−399.7713932(3)
0.1	7.990476325(4)	6.02005190(3)	134.80(3)	−99.6090075(2)
0.15	4.679661482(3)	2.76802313(2)	141.07(3)	−43.94199892(8)
0.2	3.040093391(2)	1.195416640(9)	149.17(3)	−24.42385071(4)
0.3	1.4353357683(4)	−0.268018379(3)	170.29(3)	−10.462299719(6)
0.4	0.6679429860(2)	−0.8988049477(8)	197.56(3)	−5.586727299(2)
0.5	0.23369734525(5)	−1.2083509101(3)	230.98(3)	−3.3514912011(5)
0.6	−0.03614663925(2)	−1.3670950254(2)	270.86(3)	−2.1580029115(2)
0.7	−0.21396964720(8)	−1.4469278846(9)	316.5(6)	−1.4556979860(10)
0.8	−0.335843480423(7)	−1.48266156315(4)	372.39(5)	−1.01371825287(3)
0.9	−0.421654908186(5)	−1.49274689223(4)	435.64(8)	−0.721596750959(2)
1.0	−0.483194352338(4)	−1.487600491347(7)	508.68(4)	−0.5212117866713(5)
1.1	−0.527846263528(4)	−1.473379491779(8)	592.56(5)	−0.37971542247515(3)
1.2	−0.560438201388(4)	−1.45384908150(2)	688.78(5)	−0.277477232274(3)
1.3	−0.584236721495(7)	−1.43137004591(4)	798.90(9)	−0.20222815609(2)
1.4	−0.601515453262(4)	−1.407449024795(3)	925.20(4)	−0.146012941627(3)
1.5	−0.613894668415(4)	−1.383058338024(4)	1069.63(4)	−0.103512667467(3)
1.6	−0.622552304911(4)	−1.358828450219(3)	1234.96(4)	−0.071077400253(3)
1.7	−0.628359484639(2)	−1.335167209346(6)	1424.36(4)	−0.046146023571(2)
1.8	−0.631970023438(4)	−1.312335566114(9)	1641.57(3)	−0.0268863995767(5)
1.9	−0.633881011453(3)	−1.290496696858(8)	1891.03(3)	−0.0119656178701(2)
2.0	−0.634474699096(2)	−1.269748485726(8)	2178.03(3)	−0.0003995437677(4)
2.1	−0.634048010803(2)	−1.250145393312(10)	2508.95(3)	0.0085479182349(6)
2.2	−0.632833696942(5)	−1.23171345756(2)	2891.48(3)	0.015433607419(2)
2.3	−0.631015728869(2)	−1.21446081535(2)	3334.92(3)	0.020682887998(2)
2.4	−0.628740665838(3)	−1.19838530967(2)	3850.56(3)	0.024623342500(3)
2.5	−0.626126163784(2)	−1.18348024143(2)	4452.14(3)	0.027508834455(3)
2.6	−0.623267432745(3)	−1.16973901006(3)	5156.41(3)	0.029536867471(4)
2.7	−0.620242209025(2)	−1.15715918799(3)	5983.62(3)	0.030861196317(4)
2.8	−0.6171146462161(8)	−1.14574643036(3)	6958.07(3)	0.031601022170(5)
2.9	−0.613938417248(2)	−1.13551847539(3)	8108.32(3)	0.031847710038(5)
3.0	−0.6107592382490(3)	−1.12650924557(3)	9466.59(3)	0.031669743645(5)
3.1	−0.607616958029(6)	−1.11877254279(3)	11066.46(3)	0.031116572023(5)
3.2	−0.604547286532(4)	−1.11238372680(4)	12937.01(3)	0.030222139461(7)
3.3	−0.6015831388247(9)	−1.10743560675(5)	15090.430(6)	0.029009294213(9)
3.4	−0.598755419516(7)	−1.10402122711(5)	17499.1(2)	0.027496944682(10)
3.5	−0.596092853521(2)	−1.10219239180(7)	20060.64(2)	0.02571237578(2)
3.6	−0.593620257975(3)	−1.1018843390(3)	22552.5(2)	0.02371004917(6)
3.7	−0.59135474883(2)	−1.1028169415(3)	24610.17(6)	0.02159258274(5)
3.8	−0.58930033248(2)	−1.1044302537(4)	25768.1(2)	0.01951852929(7)
3.9	−0.587443305895(2)	−1.1059524040(5)	25610.29(8)	0.01767543792(6)
4.0	−0.585752331321(3)	−1.1066394141(5)	23965.67(3)	0.01621631218(8)
4.1	−0.584185223090(6)	−1.10605884822(8)	21012.8(10)	0.01519795072(2)
4.2	−0.582699683556(6)	−1.10420939855(8)	17201.1(10)	0.01456904013(2)
4.3	−0.581262361898(6)	−1.10141543864(7)	13048.4(9)	0.01421146166(2)
4.4	−0.579852676674(4)	−1.09812163741(5)	8980.7(10)	0.013996299078(9)

4.5	−0.578461827788(3)	−1.0947306592(4)	5267.75(4)	0.01382066587(6)
4.6	−0.577089453604(5)	−1.09153231092(5)	2029.9(9)	0.013618825279(9)
4.7	−0.575740073294(5)	−1.08870032059(5)	−704.6(9)	0.013357409786(9)
4.8	−0.574420336517(4)	−1.08631837819(3)	−2967.9(9)	0.013025478092(5)
4.9	−0.573137258629(4)	−1.08441040008(3)	−4813.3(3)	0.012625330036(5)
5.0	−0.571897247968(2)	−1.08296480632(7)	−6302.97(2)	0.012165937925(9)
5.1	−0.570705660189(4)	−1.08195103980(3)	−7494.1(3)	0.011658878544(5)
5.2	−0.569566662857(4)	−1.08132974701(3)	−8435.3(3)	0.011116072828(5)
5.3	−0.568483264306(4)	−1.08105861036(3)	−9168.7(3)	0.010548663820(5)
5.4	−0.567457418740(4)	−1.08109547131(3)	−9728.4(3)	0.009966549291(4)
5.5	−0.5664901587152(8)	−1.08139987277(9)	−10141.763(8)	0.00937826267(2)
5.6	−0.565581729976(4)	−1.08193373059(3)	−10431.9(3)	0.008791023100(4)
5.7	−0.564731717180(4)	−1.08266155588(3)	−10616.2(3)	0.008210855874(4)
5.8	−0.563939156335(4)	−1.08355046687(3)	−10709.5(3)	0.007642732035(4)
5.9	−0.563202633402(4)	−1.08457012074(3)	−10724.1(3)	0.007090702723(4)
6.0	−0.5625203701836(6)	−1.085692630102(10)	−10670.008(2)	0.006558018378(2)
6.5	−0.5598439170224(5)	−1.092036477110(7)	−9646.733(2)	0.0042540549132(7)
7.0	−0.5581563807460(4)	−1.098092696105(6)	−7889.0820(7)	0.0026028664840(5)
7.5	−0.5571442316310(4)	−1.102812526808(5)	−5897.17227(10)	0.0015301248606(4)
8.0	−0.5565555381049(3)	−1.106054491074(4)	−3964.8422(3)	0.0008820731421(3)
8.5	−0.5562164399864(3)	−1.108100153648(3)	−2235.7590(6)	0.0005097325089(2)
9.0	−0.5560185449046(3)	−1.109316439703(3)	−779.9190(7)	0.0003022944563(2)
9.5	−0.5558987748977(2)	−1.110011142256(2)	342.0609(7)	0.00018804289894(8)
10.0	−0.5558221945781(2)	−1.110401969994(2)	1033.0662(7)	0.00012424191619(10)
11.0	−0.5557335542238(2)	−1.110795088842(3)	149.9926(5)	0.0000610926914(2)
12.0	−0.5556957026404(4)	−1.111155764032(6)	920.4134(6)	0.0000196367708(4)
13.0	−0.55567702488107(7)	−1.1110967472276(8)	5349.58440(8)	0.00001979250266(4)
14.0	−0.5556565510545(2)	−1.111025483731(2)	6841.98756(7)	0.00002054416987(5)
15.0	−0.5556368480510(4)	−1.110995120281(3)	7750.579152(7)	0.00001857172142(10)
16.0	−0.5556197371646(2)	−1.110990183924(2)	8566.24287(9)	0.00001558065033(3)
17.0	−0.5556057060000(2)	−1.1109986676740(9)	9432.99453(3)	0.000012514372126(2)
18.0	−0.55559459594413(5)	−1.11101320824144(9)	10407.6213(3)	0.00000977686925(2)
19.0	−0.55558599811026(9)	−1.11102953652340(5)	11503.55681(3)	0.00000749787876(2)
20.0	−0.55557944576008(7)	−1.11104527987147(6)	12689.85889(2)	0.00000568058241(2)

Table A42: Same as for Table A1, but for $3\,^1\Pi_g$.

$3\,^1\Pi_g$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.020015836159984(4)	–	71.883131(6)	–
0.01	97.98024551692(8)	95.9610084699(6)	71.9085(10)	−9999.94825640(4)
0.05	17.986007318(5)	15.98344542(3)	72.4(2)	−399.7713843(4)
0.1	8.001741175(7)	6.04258320(5)	74.999(7)	−99.6089915(4)
0.15	4.690927296(7)	2.79055814(5)	78.473(6)	−43.9419764(3)
0.2	3.051360481(4)	1.21795653(3)	82.98(2)	−24.42382214(8)
0.3	1.446606285(2)	−0.245465395(8)	94.68(3)	−10.46225988(2)
0.4	0.6792180268(5)	−0.876234624(4)	109.764(2)	−5.586676693(6)
0.5	0.2449779797(2)	−1.185759006(2)	128.237(4)	−3.351429931(2)
0.6	−0.02485933989(8)	−1.3444771901(7)	150.278(3)	−2.1579308505(8)
0.7	−0.20267459095(3)	−1.4242795783(3)	176.191(4)	−1.4556148519(3)
0.8	−0.32453954069(3)	−1.4599779926(3)	206.32(4)	−1.0136236390(3)
0.9	−0.41034091172(5)	−1.4700229433(4)	241.20(6)	−0.7214901332(4)
1.0	−0.471869067616(3)	−1.464830657435(4)	281.56(2)	−0.521092522208(3)
1.1	−0.516508388425(2)	−1.45055778977(4)	327.854(8)	−0.379582739005(4)
1.2	−0.549086349362(4)	−1.43096895181(5)	380.63(8)	−0.2773302108956(4)
1.3	−0.5728694058654(6)	−1.4084242331(3)	441.41(9)	−0.20206570866(8)
1.4	−0.590131068915(4)	−1.38442943285(3)	510.99(10)	−0.14583378217(2)
1.5	−0.602491470290(2)	−1.35995585486(3)	590.55(9)	−0.10312564866(2)
1.6	−0.611128382454(2)	−1.33563273274(2)	682.1(2)	−0.07085997995(5)
1.7	−0.6169127315137(10)	−1.3118664196(4)	786.4(2)	−0.0459064450(2)
1.8	−0.6204981010747(10)	−1.28891604523(7)	906.3(2)	−0.02662213504(3)
1.9	−0.622381305268(2)	−1.26694256387(3)	1044.2(2)	−0.01167365972(8)
2.0	−0.6229442655573(9)	−1.24604113505(4)	1203.323(5)	−0.00007630199(4)
2.1	−0.622483513172(4)	−1.226262869473(9)	1386.517(5)	0.00890674135(2)
2.2	−0.621231326927(2)	−1.20762967126(8)	1598.535(6)	0.01583317391(3)
2.3	−0.6193711108282(9)	−1.19014455791(8)	1844.669(7)	0.02112941902(3)
2.4	−0.617048739210(3)	−1.173799014243(3)	2130.7(2)	0.025124360064(6)
2.5	−0.614381038582(2)	−1.158578427009(10)	2465.9(2)	0.0280734600628(2)
2.6	−0.6114622119373(7)	−1.144466336618(7)	2859.1(2)	0.0301761874070(7)
2.7	−0.608368770770(2)	−1.131448052442(4)	3322.1(2)	0.031588699659(5)
2.8	−0.605163378709(2)	−1.11951405305(3)	3869.71(6)	0.032433108703(7)
2.9	−0.6018979001210(10)	−1.1086634889(3)	4516.51(6)	0.03280424531(8)
3.0	−0.598615868329(2)	−1.09890792783(9)	5280.95(7)	0.03277460295(2)
3.1	−0.595354525705(5)	−1.09027506387(7)	6179.65(7)	0.03239806050(2)
3.2	−0.592146522881(2)	−1.0828110341(2)	7222.23(8)	0.03171312866(4)
3.3	−0.589021268989(5)	−1.0765775859(2)	8398.68(9)	0.03074695518(3)
3.4	−0.586005756797(6)	−1.0716357388(2)	9655.83(5)	0.02952228671(4)
3.5	−0.583124412319(9)	−1.0680018191(2)	10861.73(5)	0.02807057301(5)
3.6	−0.580397232006(7)	−1.0655638231(3)	11768.27(5)	0.02645295581(6)
3.7	−0.577835676195(8)	−1.0639798481(7)	12021.46(5)	0.0247814876(2)
3.8	−0.575437429020(10)	−1.0626576394(4)	11276.31(4)	0.02321505754(9)
3.9	−0.57318403156(2)	−1.0609406401(5)	9416.42(4)	0.0219044674(2)
4.0	−0.57104574559(2)	−1.0584379155(5)	6685.47(6)	0.0209133939(2)
4.1	−0.56899231280(3)	−1.0552002953(2)	3571.24(6)	0.02019130007(3)
4.2	−0.56700237369(3)	−1.05158882920(10)	544.93(7)	0.019622837660(10)
4.3	−0.56506641508(4)	−1.04802146416(6)	−2105.93(9)	0.0190956665120(6)
4.4	−0.56318441172(4)	−1.04481640217(9)	−4283.1(2)	0.018534641200(2)

4.5	−0.56136190667(3)	−1.0421657312(4)	−6006.3(2)	0.01790179603(5)
4.6	−0.55960694093(5)	−1.0401739306071(2)	−7345.3(2)	0.01718259806(2)
4.7	−0.55792843247(5)	−1.03890851432(4)	−8374.8(2)	0.01637198946(3)
4.8	−0.55633578677(3)	−1.03844559970(9)	−9156.6(3)	0.01546374453(3)
4.9	−0.55483945143(3)	−1.0389138705(2)	−9726.9(3)	0.01444184331(4)
5.0	−0.55345233874(2)	−1.0405481181(2)	−10084.7(3)	0.01327131183(5)
5.1	−0.55219227845(3)	−1.0437625960(2)	−10173.8(3)	0.01188665898(4)
5.2	−0.55108565805(3)	−1.0492289213(2)	−9837.3(3)	0.01018122975(5)
5.3	−0.55017123941(3)	−1.0578282696(3)	−8781.2(4)	0.00802154889(5)
5.4	−0.54949862426(2)	−1.0700841180(3)	−6630.6(3)	0.00535428342(6)
5.5	−0.549109438920(3)	−1.08485964803(7)	−3289.71(3)	0.00242895087(2)
5.6	−0.54900229322(2)	−1.0990459328(3)	645.1(3)	−0.00018595471(5)
5.7	−0.54912139941(3)	−1.1099878047(4)	4279.7(4)	−0.00206052737(8)
5.8	−0.54938911234(2)	−1.1172411649(3)	7144.2(4)	−0.00318326557(6)
5.9	−0.549739795756(6)	−1.12164884109(8)	9234.7(2)	−0.00375749993(2)
6.0	−0.5501291224359(10)	−1.124166740522(6)	10720.923(3)	−0.003984749276(2)
6.5	−0.5520136062840(6)	−1.125516912204(6)	13728.055(2)	−0.0033061076362(5)
7.0	−0.5533892069461(5)	−1.12237879354(3)	14251.9880(8)	−0.002228625664(3)
7.5	−0.5542897570472(5)	−1.11925454096(3)	14183.0897(8)	−0.001423336915(3)
8.0	−0.5548573111015(5)	−1.11679772493(2)	13929.2339(3)	−0.000885387841(2)
8.5	−0.5552072992737(5)	−1.11501171213(2)	13619.9237(3)	−0.000540836892(2)
9.0	−0.5554194618762(5)	−1.11376219641(2)	13334.6989(3)	−0.0003248080731(10)
9.5	−0.5555456677359(5)	−1.112902635467(10)	13165.5585(5)	−0.0001906631574(8)
10.0	−0.5556185277375(6)	−1.112310089186(10)	13246.8167(3)	−0.0001073033711(7)
11.0	−0.5556761340818(5)	−1.1115664330174(3)	15263.8056(5)	−0.0000194695325(2)
12.0	−0.55566779836772(4)	−1.110989841507(8)	15241.9217(2)	0.0000288129357(7)
13.0	−0.55563898013907(5)	−1.110943467126(2)	11306.9422(5)	0.0000257302424(2)
14.0	−0.55561711224048(3)	−1.1109776556118(4)	10138.68679(6)	0.00001832634780(2)
15.0	−0.55560160761690(2)	−1.1110080152956(3)	9440.55024(6)	0.000013013329216(10)
16.0	−0.55559052656376(2)	−1.1110309804546(3)	8760.0752(2)	0.000009379542059(8)
17.0	−0.555582469094821(7)	−1.11104781378529(7)	7979.4009(2)	0.000006889670846(2)
18.0	−0.555576494523461(6)	−1.11106007054241(7)	7059.2862(2)	0.000005162139140(2)
19.0	−0.555571976395343(8)	−1.11106904197475(6)	5997.8480(2)	0.0000039426745240(6)
20.0	−0.555568496600803(8)	−1.111075738449278(6)	4833.4858(2)	0.000003062737613(3)

Table A43: Same as for Table A1, but for $4\,^1\Pi_g$.

$4\,^1\Pi_g$				
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.02000071089858471(1)	–	1.4044136	–
0.01	97.980260650989(7)	95.96103875451(2)	1.4(2)	−9999.9482547467(3)
0.05	17.986022651915(9)	15.98347647195(3)	1.5(3)	−399.7713766376(2)
0.1	8.00175710873(2)	6.04261658202(4)	1.5(3)	−99.6089763544(2)
0.15	4.690944156554(10)	2.79059507758(4)	1.4(4)	−43.94195490354(8)
0.2	3.051378563840(9)	1.21799813423(3)	1.6(3)	−24.42379496724(5)
0.3	1.44662761337(2)	−0.24541146531(4)	1.6(6)	−10.46222230686(4)
0.4	0.67924360789(2)	−0.87616448791(5)	2.05(7)	−5.58662925921(4)
0.5	0.24500879223(2)	−1.18566877746(5)	2.62(6)	−3.35137272383(5)
0.6	−0.02482231207(2)	−1.34436284750(7)	3.34(8)	−2.15786370561(5)
0.7	−0.20263033837(3)	−1.42413687960(9)	4.16(9)	−1.45553743264(5)
0.8	−0.32448701317(3)	−1.45980240139(2)	5.13(10)	−1.01353546882(6)
0.9	−0.41027900492(3)	−1.4698095530(2)	6.3(2)	−0.72139060371(7)
1.0	−0.471796609452(7)	−1.46457410659(3)	8.22(10)	−0.52098088769(2)
1.1	−0.516424124807(7)	−1.4502521608(4)	9.8(2)	−0.3794581010(2)
1.2	−0.548988927859(2)	−1.43060765139(5)	11.60(8)	−0.27719149640(2)
1.3	−0.5727573568182(2)	−1.40799984609(2)	13.55(9)	−0.201911640352(4)
1.4	−0.5900027831365(3)	−1.383933541993(9)	15.86(6)	−0.145662839797(2)
1.5	−0.6023451724546(3)	−1.3593788177149(4)	18.2(2)	−0.1031256485379(7)
1.6	−0.61096209914(3)	−1.3349634047(3)	20.9(2)	−0.0706495040(2)
1.7	−0.616724252240(5)	−1.311091804780(2)	24.02(8)	−0.045672529599(7)
1.8	−0.620284930999(6)	−1.288020859716(3)	27.34(8)	−0.026361665410(8)
1.9	−0.622140606844(7)	−1.265908673843(2)	31.01(9)	−0.011382873779(8)
2.0	−0.62267278638(4)	−1.2448468421(5)	34.9(2)	0.0002493657(3)
2.1	−0.622177495806(2)	−1.224881980857(8)	39.4(2)	0.00927286224(2)
2.2	−0.6208863958439(4)	−1.206030292772(2)	44.3(2)	0.016246590410(6)
2.3	−0.618982128697(4)	−1.18828749956(7)	49.6(2)	0.02159859034(4)
2.4	−0.616609623343(3)	−1.17163567435(3)	55.7(2)	0.02565982179(3)
2.5	−0.613884524203(2)	−1.156047958225(8)	62.2(2)	0.02868843603(4)
2.6	−0.6108995443303(8)	−1.14149182228(2)	69.4(2)	0.03088741014(2)
2.7	−0.6077293020380(2)	−1.12793132212(5)	77.3(2)	0.032417511843(7)
2.8	−0.604434036573(5)	−1.11532864823(6)	85.7(3)	0.03340693744(4)
2.9	−0.6010624864(2)	−1.1036451813(9)	95.2(3)	0.0339585487(2)
3.0	−0.59765413634(2)	−1.09284220365(2)	105.7(3)	0.03415535626(6)
3.1	−0.594240983190(2)	−1.08288135807(3)	117.3(3)	0.03406471235(2)
3.2	−0.59084893391686(7)	−1.07372494609(3)	130.6(2)	0.033741538049(3)
3.3	−0.5874989179321(2)	−1.065336099839(7)	144.80(4)	0.033230829097(3)
3.4	−0.58420777795027(7)	−1.057678877310(8)	160.3(5)	0.032569611350(3)
3.5	−0.5809889871133(3)	−1.05071830470(3)	177.54(6)	0.031788477005(9)
3.6	−0.57785322934(2)	−1.0444203876(2)	196.0(4)	0.03091279748(7)
3.7	−0.5748088714682(2)	−1.038752104694(9)	215.3(7)	0.029963686006(8)
3.8	−0.57186234936291(9)	−1.03368140265(2)	241.2(2)	0.028958762119(10)
3.9	−0.5690184855323(2)	−1.02917719091(2)	264.8(7)	0.027912764142(5)
4.0	−0.56628075196476(2)	−1.025209356998(7)	293.8(7)	0.026838036733(2)
4.1	−0.56365148927456(8)	−1.0217488049730(5)	325.5(9)	0.02574492038443(7)
4.2	−0.56113209109228(8)	−1.0187675319700(6)	361.8(9)	0.02464205957489(9)
4.3	−0.55872316119001(9)	−1.0162387647427(7)	402.7(9)	0.0235366413110(2)
4.4	−0.556424650038(6)	−1.01413720247(4)	450.1(8)	0.02243456763(2)

4.5	−0.554235977807(2)	−1.01243948274(8)	502.2(8)	0.02134054952(3)
4.6	−0.552156154074(6)	−1.01112522422(4)	561.4(8)	0.02025806172(2)
4.7	−0.550183917496(6)	−1.01017995229(4)	629.1(8)	0.01918891121(2)
4.8	−0.548317979036(3)	−1.00960630645(3)	707.9(10)	0.018131177420(6)
4.9	−0.546557843250(3)	−1.00949288207(2)	800.4(4)	0.017065878454(5)
5.0	−0.544911255182(2)	−1.0111610506(4)	887.16(10)	0.01573229196(7)
5.1	−0.54368573246(2)	−1.0505036661(6)	1256.9(5)	0.0072289802(2)
5.2	−0.54320192046(3)	−1.0711463916(5)	6022.92(3)	0.00293412486(8)
5.3	−0.54302548727(3)	−1.0809108440(6)	9837.26(4)	0.00096983594(9)
5.4	−0.54293789782(3)	−1.0800525367(6)	11085.7(6)	0.00107838128(9)
5.5	−0.542766419283(7)	−1.07188955364(7)	9884.59(8)	0.002480597259(9)
5.6	−0.54243292422(3)	−1.0615650799(5)	7274.92(7)	0.00416085152(7)
5.7	−0.54194866213(3)	−1.0529511718(5)	4476.5(2)	0.00542914955(7)
5.8	−0.54136619133(3)	−1.0471591648(4)	2156.4(3)	0.00613331342(6)
5.9	−0.54073659844(3)	−1.0437145544(4)	434.0(3)	0.00639976992(5)
6.0	−0.540095497165(4)	−1.04187066192(3)	−790.24(7)	0.006386722063(9)
6.5	−0.537224683459(4)	−1.04246461933(3)	−3027.69(7)	0.004920730393(8)
7.0	−0.535182222692(4)	−1.04720328031(4)	−2822.00(6)	0.003308737863(8)
7.5	−0.533842859154(3)	−1.05176374318(5)	−1960.12(6)	0.002122930013(8)
8.0	−0.532992118107(3)	−1.05527884624(5)	−1043.45(5)	0.001338173744(8)
8.5	−0.532456202578(2)	−1.05773142774(5)	−340.98(4)	0.000844820870(7)
9.0	−0.532115776310(2)	−1.05935690349(5)	57.43(3)	0.000541627680(6)
9.5	−0.5318951269451(9)	−1.06040827828(4)	171.35(3)	0.000355997431(4)
10.0	−0.5317480709094(8)	−1.06108402680(2)	83.89(2)	0.000241211502(3)
11.0	−0.531575216531(2)	−1.061814827689(7)	−295.21(2)	0.0001214186704(2)
12.0	−0.531484073029(2)	−1.06215995175(3)	−575.80(2)	0.000067349526(2)
13.0	−0.531431848942(2)	−1.06234369567(3)	−718.50(2)	0.000040000171(2)
14.0	−0.531399894176(3)	−1.06244397330(3)	−766.94(2)	0.000025415361(2)
15.0	−0.531378768891(3)	−1.06249264579(3)	−727.43(2)	0.000017659466(2)
16.0	−0.531363355767(3)	−1.06250903107(3)	−621.98(2)	0.0000136050293(9)
17.0	−0.531350924558(2)	−1.06250670422(2)	−480.84(2)	0.0000114791118(7)
18.0	−0.531340086370(2)	−1.06249475025(2)	−326.31(2)	0.0000103012497(5)
19.0	−0.531330184557(2)	−1.06247903310(2)	−171.79(2)	0.0000095440008(4)
20.0	−0.531320951017(2)	−1.062463234414(10)	−24.71(2)	0.0000089333810(2)

Table A44: Same as for Table A1, but for $1\,^3\Pi_g$ (i state) .

		$1\,^3\Pi_g$		
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.055620732852246(6)	–	−25.322839(1)	–
0.01	97.94462500300(2)	95.8897673608(2)	−25.347(6)	−9999.948264525(9)
0.05	17.9503858791(3)	15.912200652(2)	−25.6986(4)	−399.77142213(3)
0.1	7.96612707339(9)	5.971328111(2)	−26.676(5)	−99.609060363(10)
0.15	4.6552990567(4)	2.719287184(2)	−28.083(5)	−43.942072865(8)
0.2	3.015736780386(7)	1.1466647710(3)	−29.847(5)	−24.4239439487(8)
0.3	1.410958041133(9)	−0.31681240027(5)	−34.267(9)	−10.46242827513(10)
0.4	0.643550737713(5)	−0.947654097237(9)	−39.751(3)	−5.5869389314(3)
0.5	0.2092873205590(5)	−1.25726786806(3)	−46.369(3)	−3.35172501810(4)
0.6	−0.060577644443435(3)	−1.4160925136660(3)	−54.230(3)	−2.1582287079955(3)
0.7	−0.238424837235351(3)	−1.4960188312820(2)	−63.515(3)	−1.455984509733(2)
0.8	−0.360326089847806(4)	−1.5318591958253(6)	−74.452(3)	−1.0140337701622(4)
0.9	−0.4461682204850169(8)	−1.542064796361(2)	−87.318(2)	−0.7219426171005(7)
1.0	−0.5077417129942512(10)	−1.537052655548(2)	−102.438(2)	−0.5215892295590(10)
1.1	−0.5524310896822232(8)	−1.522980343681(2)	−120.195(2)	−0.3801256039240(4)
1.2	−0.585063989615279(7)	−1.5036135204861(5)	−141.042(2)	−0.2779212843796(2)
1.3	−0.608907054468511(2)	−1.48131347386(7)	−165.57(6)	−0.20270720375(3)
1.4	−0.626234005739364(2)	−1.45758737555(2)	−194.31(6)	−0.146528117186(6)
1.5	−0.638665212798672(2)	−1.433408106498(3)	−228.0418(9)	−0.1040651206001(10)
1.6	−0.647378716476691(2)	−1.409406718892(2)	−267.7908(10)	−0.0716683037118(8)
1.7	−0.653245746384718(2)	−1.385991670694(3)	−314.6310(9)	−0.046776575250(2)
1.8	−0.656920230372685(2)	−1.363424536754(3)	−369.9339(9)	−0.027557820005(2)
1.9	−0.658899373938490(3)	−1.341869116725(3)	−435.3778(10)	−0.0126791414987(10)
2.0	−0.659565544600868(3)	−1.321423891691(4)	−513.0275(8)	−0.001156401245(2)
2.1	−0.659215783031648(3)	−1.302143850859(4)	−605.4372(8)	0.007746531050(2)
2.2	−0.658082950784804(3)	−1.284055425623(4)	−715.7780(9)	0.014586579976(2)
2.3	−0.656351118823734(4)	−1.267166907248(4)	−848.0092(9)	0.019789274087(2)
2.4	−0.654166924488570(4)	−1.251475896218(5)	−1007.0977(10)	0.023682480316(2)
2.5	−0.651648065471791(4)	−1.236974819644(5)	−1199.306(2)	0.026520524520(2)
2.6	−0.648889735599453(5)	−1.223655234290(5)	−1432.570(2)	0.028501629580(2)
2.7	−0.645969566320446(5)	−1.211511434369(5)	−1716.998(2)	0.029780628990(2)
2.8	−0.642951475809495(5)	−1.200543760788(6)	−2065.5268(9)	0.030478282440(2)
2.9	−0.639888717148283(5)	−1.190761932048(6)	−2494.7824(9)	0.030688104224(2)
3.0	−0.636826340677847(5)	−1.182188660866(6)	−3026.2001(9)	0.030481340163(2)
3.1	−0.633803231604719(5)	−1.174863753226(6)	−3687.4565(9)	0.029910551608(2)
3.2	−0.630853843666905(6)	−1.168848756461(6)	−4514.2367(8)	0.029012165898(2)
3.3	−0.628009715485452(5)	−1.164231936802(6)	−5552.2761(8)	0.0278083315665(10)
3.4	−0.625300819501107(5)	−1.161132760547(8)	−6859.4165(9)	0.026308493663(2)
3.5	−0.622756742501709(5)	−1.159703871803(8)	−8506.9953(8)	0.024511318057(2)
3.6	−0.620407616136948(4)	−1.160126516766(7)	−10579.1322(8)	0.022407976530(2)
3.7	−0.618284589996605(4)	−1.162592469710(6)	−13167.3473(7)	0.0199883000767(10)
3.8	−0.6164194715688430(5)	−1.1672630132324(3)	−16356.8482(2)	0.0172515605012(3)
3.9	−0.6148430127018683(3)	−1.1741975019997(5)	−20201.21857(9)	0.0142226983086(3)
4.0	−0.6135813920642892(2)	−1.1832578210603(2)	−24686.92266(6)	0.01097624076700(8)
4.1	−0.61264102319971(2)	−1.19402450549040(5)	−29699.8796058(8)	0.00762379046560(3)
4.2	−0.61204300455725(2)	−1.205788604580563(8)	−35017.685123(2)	0.004356524889018(9)
4.3	−0.61175967360714(2)	−1.21766771029289(8)	−40346.995929(2)	0.00136084579567(2)
4.4	−0.61175550977433(2)	−1.2288150325516(3)	−45397.230859(2)	−0.00120545750057(4)

4.5	−0.6119925392460975(2)	−1.238612312751(2)	−49951.73927(3)	−0.0032549409463(2)
4.6	−0.612387969721989(5)	−1.246751130078(2)	−53900.338960(10)	−0.0047772153551(4)
4.7	−0.612921095686271(6)	−1.253196032447(3)	−57228.8354510(10)	−0.0058199661861(5)
4.8	−0.613537719915784(4)	−1.258089013289(2)	−59986.173653(5)	−0.0064611611369(4)
4.9	−0.6142019566093(2)	−1.261655155612(3)	−62251.048607(9)	−0.0067859678354(4)
5.0	−0.6148961836067952(3)	−1.264137041445(3)	−64108.43754(2)	−0.0068729348463(5)
5.1	−0.615570031381760(6)	−1.265759260899(3)	−65636.86120(2)	−0.0067880780657(5)
5.2	−0.61623904916449(3)	−1.266714068969(4)	−66903.26601(2)	−0.0065838405077(5)
5.3	−0.616883401355604(9)	−1.267158926281(4)	−67962.20188(2)	−0.0063004006735(6)
5.4	−0.617496744203276(9)	−1.267219536365(4)	−68856.97913(2)	−0.0059677866589(6)
5.5	−0.6180853196896611(4)	−1.266994774604(4)	−69621.493243(10)	−0.0056080245862(6)
5.6	−0.61861725175936(8)	−1.2665617579874(8)	−70282.0815747(3)	−0.0052370097265(2)
5.7	−0.61912201191664(8)	−1.2659803415671(8)	−70859.1559792(3)	−0.0048660206551(2)
5.8	−0.61959001904326(8)	−1.2652968411745(8)	−71368.5422729(2)	−0.0045028970841(2)
5.9	−0.62002234241467(9)	−1.2645470073349(8)	−71822.5397140(2)	−0.00415293601788(10)
6.0	−0.6204304827255747(5)	−1.263758359(3)	−72230.89(8)	−0.0038162323(5)
6.5	−0.62197421146385(3)	−1.2598165566(10)	−73799.2527(5)	−0.0024412514(2)
7.0	−0.62294868122491(2)	−1.2565668374(5)	−74882.642(2)	−0.00152421072(8)
7.5	−0.62355517660007(2)	−1.2542213627(3)	−75675.0084(5)	−0.00094813461(5)
8.0	−0.623934198222452(9)	−1.2526481546(2)	−76263.5451(3)	−0.00059746978(3)
8.5	−0.624175920351951(6)	−1.251644951966(5)	−76700.1251(3)	−0.0003874248547(9)
9.0	−0.624335617890345(5)	−1.251029658832(4)	−77022.11251(2)	−0.0002620470059(7)
9.5	−0.624446191820649(10)	−1.250663874871(7)	−77258.445184(9)	−0.0001885780243(9)
10.0	−0.624526858556839(2)	−1.250451608377(3)	−77431.645411(5)	−0.0001397891264(4)
11.0	−0.6246382508422657(3)	−1.25026097210325(2)	−77653.0312283(2)	−0.000089497310795(3)
12.0	−0.62471380189591186(10)	−1.25019536682094(9)	−77776.64663864(4)	−0.000063980252425(5)
13.0	−0.624769358751530723(10)	−1.25016520828807(10)	−77849.6363596(2)	−0.000048191598845(6)
14.0	−0.624811753081569110(6)	−1.25014420717773(3)	−77895.65769984(6)	−0.000037192929615(3)
15.0	−0.6248447073495333346(4)	−1.250126062678238(3)	−77926.55327888(9)	−0.0000291098652784(5)
16.0	−0.624870637584202693(2)	−1.250109782346086(2)	−77948.41483907(9)	−0.0000230316986052(3)
17.0	−0.6248912526172034632(10)	−1.250095383081320(2)	−77964.53144884(7)	−0.0000184045792303(3)
18.0	−0.624907802583200445(2)	−1.250082877226923(8)	−77976.7884072(6)	−0.000014848447808(2)
19.0	−0.6249212147302255493(4)	−1.2500721469967913(3)	−77986.33463603(5)	−0.0000120903966496(2)
20.0	−0.6249321825437318401(2)	−1.2500629969621513(6)	−77993.91014723(6)	−0.00000993159373442(6)

Table A45: Same as for Table A1, but for $2\,^3\Pi_g$ (r state) .

$2\,^3\Pi_g$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.031279846178687(7)	–	−29.442651(2)	–
0.01	97.96897249229(5)	95.9384623939(3)	−29.58(4)	−9999.94825907(3)
0.05	17.974733993(3)	15.96089816(2)	−29.95(4)	−399.7713966(3)
0.1	7.990466994(4)	6.02003263(3)	−30.96(4)	−99.6090136(2)
0.15	4.679651792(3)	2.76800251(2)	−32.47(4)	−43.94200712(9)
0.2	3.040083244(2)	1.195394350(8)	−34.36(4)	−24.42386069(3)
0.3	1.4353244743(5)	−0.268044819(3)	−39.341(5)	−10.462312558(7)
0.4	0.6679302897(2)	−0.898836393(2)	−45.516(6)	−5.586742432(2)
0.5	0.23368303745(7)	−1.2083880467(5)	−52.96(2)	−3.3515082433(7)
0.6	−0.036162732986(10)	−1.36713838656(7)	−61.75(2)	−2.15802153431(7)
0.7	−0.21398766828(2)	−1.44697783131(8)	−71.84(8)	−1.45571784965(7)
0.8	−0.335863533943(8)	−1.48271824072(4)	−83.53(5)	−1.01373896604(3)
0.9	−0.42167705612(4)	−1.4928101672(2)	−97.53(7)	−0.72161783887(10)
1.0	−0.483218603955(4)	−1.48766987222(6)	−112.90(7)	−0.52123266430(2)
1.1	−0.527872562920(4)	−1.47345402934(2)	−130.82(5)	−0.379735366815(4)
1.2	−0.560466412202(2)	−1.453927246952(10)	−151.46(5)	−0.277495352111(4)
1.3	−0.584266608433(5)	−1.43144958156(2)	−175.09(5)	−0.202243357455(3)
1.4	−0.601546659844(5)	−1.40752676236(2)	−202.17(4)	−0.146023887623(6)
1.5	−0.613926690353(5)	−1.383129975964(8)	−233.25(5)	−0.1035177301723(5)
1.6	−0.622584458218(5)	−1.35888828103(2)	−268.93(4)	−0.071074602872(2)
1.7	−0.628390867321(5)	−1.33520778332(2)	−310.00(4)	−0.046132969810(3)
1.8	−0.631999469354(2)	−1.312347274881(10)	−357.37(4)	−0.026860186750(3)
1.9	−0.6339070344882(10)	−1.29046725435(2)	−412.18(4)	−0.011922729142(4)
2.0	−0.634495425267(6)	−1.26966227753(2)	−475.81(4)	−0.000335713500(4)
2.1	−0.6340610952283(10)	−1.24998265547(3)	−549.98(4)	0.008637873804(5)
2.2	−0.6328362217667(9)	−1.23144923436(2)	−636.83(4)	0.015556004171(2)
2.3	−0.631004077017(3)	−1.21406362994(2)	−739.05(4)	0.020845445252(3)
2.4	−0.6287103641287(10)	−1.19781546324(2)	−860.05(5)	0.024835527092(2)
2.5	−0.626071687315(2)	−1.18268763655(2)	−1004.14(4)	0.0277822952317(7)
2.6	−0.623181960512(2)	−1.16866037939(4)	−1176.98(5)	0.029885977557(8)
2.7	−0.620117319480(9)	−1.15571461300(5)	−1385.82(5)	0.031303713318(10)
2.8	−0.616939941277(2)	−1.14383509553(3)	−1640.34(5)	0.032158852512(2)
2.9	−0.613701067412(2)	−1.13301379787(3)	−1953.35(4)	0.032547702403(2)
3.0	−0.610443454976(10)	−1.12325402413(6)	−2342.13(5)	0.03254429527(2)
3.1	−0.6072034345004(8)	−1.11457593274(3)	−2830.23(5)	0.0322035278307(8)
3.2	−0.6040127274893(4)	−1.10702433055(6)	−3450.05(5)	0.031562851390(10)
3.3	−0.60090016421(5)	−1.1006798295(2)	−4246.34(9)	0.03064257542(3)
3.4	−0.597893438122(2)	−1.0956743553(2)	−5280.6(2)	0.02944485912(2)
3.5	−0.5950210111332(9)	−1.09221049207(5)	−6635.36(10)	0.027951865773(7)
3.6	−0.5923141735452(10)	−1.09057810870(8)	−8415.19(9)	0.026125066233(6)
3.7	−0.58980888806(5)	−1.0911438734(3)	−10731.78(10)	0.02391186561(4)
3.8	−0.587546038389(4)	−1.09425014963(7)	−13650.69(9)	0.02127419135(2)
3.9	−0.585566812893(2)	−1.0999184816(2)	−17069.24(5)	0.01826029340(3)
4.0	−0.58389875797(7)	−1.1073512504(9)	−20551.8(2)	0.0151115664(2)
4.1	−0.582533615723(10)	−1.1146761090(3)	−23320.32(10)	0.01229051766(5)
4.2	−0.58141345036(2)	−1.1196745366(3)	−24626.08(8)	0.01027437242(6)
4.3	−0.58044545601(2)	−1.1211438305(3)	−24239.72(6)	0.00924350733(6)
4.4	−0.579537736090(4)	−1.119396887738(10)	−22509.4(2)	0.0090178601005(7)

4.5	−0.578626447785(2)	−1.11559560495(4)	−20018.1(2)	0.00925717569(2)
4.6	−0.577681007509(4)	−1.11092911352(3)	−17273.2(2)	0.009659326412(4)
4.7	−0.576695637475(4)	−1.10623517270(3)	−14597.80(10)	0.010033213245(5)
4.8	−0.575678431733(2)	−1.101978327294(8)	−12153.1(2)	0.0102871950359(10)
4.9	−0.574643151342(2)	−1.098357357808(9)	−9994.61(10)	0.010393662220(2)
5.0	−0.5736044316392(6)	−1.09541587003(5)	−8121.37(4)	0.010358598656(2)
5.1	−0.572575477973(2)	−1.093119471736(10)	−6507.09(8)	0.010202251806(2)
5.2	−0.571567218809(2)	−1.091401019259(10)	−5116.86(8)	0.009948734300(2)
5.3	−0.570588196543(2)	−1.090184287824(10)	−3916.27(7)	0.009621151936(2)
5.4	−0.569644779897(2)	−1.08939511668(2)	−2874.52(7)	0.009239711688(2)
5.5	−0.5687414837363(4)	−1.088965929463(6)	−1965.4156(7)	0.0088212796383(7)
5.6	−0.567881296888(2)	−1.08883701003(2)	−1167.72(6)	0.008379568525(2)
5.7	−0.567065977772(2)	−1.08895632656(2)	−463.71(6)	0.007925548944(2)
5.8	−0.566296306044(2)	−1.08927880037(2)	160.57(6)	0.007467898573(2)
5.9	−0.565572290847(2)	−1.089765440700(2)	716.38(6)	0.007013413728(2)
6.0	−0.5648933409067(3)	−1.090382525557(5)	1212.8604(2)	0.0065673593761(5)
6.5	−0.5621272672658(3)	−1.094533119681(5)	3016.4348(2)	0.0045725253617(5)
7.0	−0.5602367585114(3)	−1.098954993884(4)	4014.6310(4)	0.0030740747342(4)
7.5	−0.5589750788789(3)	−1.102634972097(5)	4448.0180(5)	0.0020420247548(4)
8.0	−0.5581352901404(3)	−1.105336010159(5)	4443.1333(7)	0.0013668212652(5)
8.5	−0.5575673021790(3)	−1.107159388805(6)	4076.9943(6)	0.0009382606533(5)
9.0	−0.5571703362076(4)	−1.108304198224(6)	3420.5415(6)	0.0006707193546(5)
9.5	−0.5568799100018(3)	−1.108973060378(5)	2568.2339(7)	0.0005038694343(4)
10.0	−0.5566565205232(3)	−1.109341170137(5)	1630.4671(7)	0.0003971870909(4)
11.0	−0.5563284005582(3)	−1.109664801141(5)	−152.0813(5)	0.0002719999978(3)
12.0	−0.5560970777438(3)	−1.109850331165(4)	−1552.6811(2)	0.0001953186935(2)
13.0	−0.5559309645041(3)	−1.110047299406(3)	−2548.6089(2)	0.0001395868925(2)
14.0	−0.5558132331397(4)	−1.110255059114(2)	−3220.975(2)	0.00009795765466(6)
15.0	−0.5557313019435(3)	−1.1104489609929(8)	−3651.0238(2)	0.00006757619293(3)
16.0	−0.5556751333245(2)	−1.1106135897104(10)	−3898.9277(2)	0.00004604230867(3)
17.0	−0.5556370122850(2)	−1.1107447155183(9)	−4005.5948(2)	0.00003113582657(2)
18.0	−0.55561128066310(9)	−1.1108447965701(4)	−3998.8046(2)	0.000020986930896(4)
19.0	−0.55559393894908(7)	−1.1109190340775(3)	−3899.0180(3)	0.0000141496747722(4)
20.0	−0.55558223232900(9)	−1.1109730671575(3)	−3723.7860(3)	0.000009569875012(8)

Table A46: Same as for Table A1, but for $3\,^3\Pi_g$ (w state) .

$3\,^3\Pi_g$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.020015836159984(4)	–	−19.56885(1)	–
0.01	97.980260651(4)	95.96103869(4)	−20(4)	−9999.948255(3)
0.05	17.986002072(4)	15.98343482(3)	−20(2)	−399.7713865(5)
0.1	8.001735794(5)	6.04257208(4)	−20.5(5)	−99.6089950(3)
0.15	4.690921725(9)	2.79054636(4)	−22.2(3)	−43.9419806(2)
0.2	3.051354635(3)	1.21794370(2)	−23.2(3)	−24.42382784(7)
0.3	1.4465997850(10)	−0.245480588(7)	−25.95(3)	−10.46226719(2)
0.4	0.6792107298(4)	−0.876252655(3)	−30.01(4)	−5.586685287(5)
0.5	0.2449697690(2)	−1.185780251(2)	−34.87(4)	−3.351439577(2)
0.6	−0.02486855955(7)	−1.3445019281(5)	−40.59(4)	−2.1579413483(7)
0.7	−0.20263033853(6)	−1.4241368802(3)	4.39(10)	−1.4555374331(3)
0.8	−0.32455098042(3)	−1.4600101054(2)	−54.96(5)	−1.0136351807(2)
0.9	−0.410353513774(8)	−1.4700586337(2)	−63.80(6)	−0.7215017846(2)
1.0	−0.47188282573(2)	−1.46486957680(10)	−73.799(7)	−0.52110392535(7)
1.1	−0.516523256428(4)	−1.4505993106(2)	−85.340(6)	−0.3795934525(2)
1.2	−0.54910223210(3)	−1.4310120949(7)	−99.3(4)	−0.27733969195(3)
1.3	−0.57288614798(3)	−1.4084675779(5)	−114.9(7)	−0.202073296(2)
1.4	−0.59014844149(3)	−1.3844710060(10)	−132.4(9)	−0.145838659(2)
1.5	−0.602509154775(7)	−1.3599929961(2)	−150.5(2)	−0.10331645769(2)
1.6	−0.611145951413(5)	−1.33566193194(2)	−172.8(2)	−0.070856268284(8)
1.7	−0.6169296252958(7)	−1.31188310842(3)	−198.3(2)	−0.04589638701(5)
1.8	−0.62051359977(3)	−1.28891434255(3)	−227.6(2)	−0.02660396840(5)
1.9	−0.6223944944604(9)	−1.26691495310(4)	−261.4(2)	−0.01164524421(2)
2.0	−0.6229539945173(2)	−1.24597805894(7)	−300.134(8)	−0.00003503495(3)
2.1	−0.6224883432629(8)	−1.2261522122(2)	−345.459(8)	0.00896403544(6)
2.2	−0.621229467652(4)	−1.207456092(2)	−398.351(8)	0.0159103834(5)
2.3	−0.61936033985(6)	−1.189888630(2)	−460.433(8)	0.0212313261(5)
2.4	−0.617026301867(2)	−1.17343610673(8)	−534.5(3)	0.02525687375(3)
2.5	−0.614343520731(3)	−1.15807724838(9)	−621.9(3)	0.02824391723(4)
2.6	−0.611405378735(2)	−1.14378704185(7)	−726.7(3)	0.03039373677(3)
2.7	−0.6082873623758(4)	−1.1305398186(3)	−853.6(3)	0.03186478007(9)
2.8	−0.605050853566(3)	−1.1183120624(2)	−1008.168(6)	0.03278201599(4)
2.9	−0.601746119221(9)	−1.1070854301(2)	−1200.612(7)	0.03324372701(4)
3.0	−0.598414725798(3)	−1.0968505922(2)	−1442.244(8)	0.03332628648(4)
3.1	−0.595091564382(2)	−1.08761282686(8)	−1750.299(10)	0.03308719416(3)
3.2	−0.591806657791(4)	−1.0794009100(2)	−2149.82(2)	0.03256637675(4)
3.3	−0.5885869362907(6)	−1.0722819623(2)	−2677.85(2)	0.03178542734(4)
3.4	−0.585458221540(4)	−1.06638669579(8)	−3389.80(9)	0.03074404332(2)
3.5	−0.582447749429(4)	−1.06195117164(8)	−4367.19(3)	0.02941266491(2)
3.6	−0.57958761710(2)	−1.0593766634(4)	−5723.83(7)	0.02772182520(10)
3.7	−0.576919104957(5)	−1.0592697080(5)	−7582.34(5)	0.0255590545(2)
3.8	−0.574495127752(4)	−1.0622605937(3)	−9948.09(5)	0.02282359521(6)
3.9	−0.572369539222(8)	−1.0680827644(5)	−12362.49(6)	0.0196554651(2)
4.0	−0.57055501751(2)	−1.0740251841(7)	−13626.20(8)	0.0167712127(2)
4.1	−0.56897296524(3)	−1.0759441729(4)	−12670.7(7)	0.01512237989(8)
4.2	−0.56748417402(6)	−1.0726675837(7)	−9907.2(2)	0.0148335153(2)
4.3	−0.56598403102(4)	−1.0665364737(3)	−6639.6(2)	0.01521664844(6)
4.4	−0.56444044335(7)	−1.0601283091(6)	−3760.6(3)	0.01562558581(9)

4.5	−0.56286778313(3)	−1.0547427949(4)	−1527.7(3)	0.01577617139(5)
4.6	−0.56129549183(6)	−1.050735469356(5)	116.6(4)	0.01562076394(3)
4.7	−0.55975257539(6)	−1.04807832298(6)	1309.9(4)	0.01519719736(4)
4.8	−0.55826333472(4)	−1.04666443702(9)	2171.7(4)	0.01455463173(4)
4.9	−0.55684774996(4)	−1.0464265137(2)	2782.6(5)	0.01372836450(4)
5.0	−0.55552324180(2)	−1.0473762498(2)	3184.0(3)	0.01273404670(6)
5.1	−0.55430664336(4)	−1.0496159443(2)	3377.2(5)	0.01156810633(5)
5.2	−0.55321596915(4)	−1.0533322512(2)	3328.7(5)	0.01021147827(5)
5.3	−0.55227153165(3)	−1.0587517540(3)	2964.7(5)	0.00863986966(6)
5.4	−0.55149542065(3)	−1.0660148397(3)	2186.7(5)	0.00684740768(6)
5.5	−0.550907811175(6)	−1.07494668362(2)	916.66(2)	0.004885261579(7)
5.6	−0.55051950127(3)	−1.0848470408(3)	−831.0(4)	0.00289142173(6)
5.7	−0.55032397818(2)	−1.0945893051(3)	−2893.6(4)	0.00106292127(5)
5.8	−0.55029573584(2)	−1.1031081937(3)	−5023.7(3)	−0.00043391761(5)
5.9	−0.55039743388(2)	−1.1098469381(2)	−7005.2(3)	−0.00153424922(4)
6.0	−0.5505903149951(10)	−1.11478798400(4)	−8722.89(2)	−0.002267892337(8)
6.5	−0.5520226931304(9)	−1.123041986567(10)	−13687.530(2)	−0.0029225538931(5)
7.0	−0.5533069724790(5)	−1.121814783512(5)	−15610.0224(10)	−0.0021715483647(3)
7.5	−0.5542013958060(5)	−1.119168153365(5)	−16500.8104(7)	−0.0014353815670(3)
8.0	−0.5547756733757(3)	−1.116708047518(2)	−16924.8499(7)	−0.00089458759575(6)
8.5	−0.5551256323114(3)	−1.1147661795338(8)	−17039.5989(5)	−0.00053116646017(4)
9.0	−0.5553289651888(2)	−1.113364025742446(3)	−16903.4812(4)	−0.00030067726291(9)
9.5	−0.55544159127004(10)	−1.1124237919690(4)	−16580.1317(3)	−0.00016216941367(10)
10.0	−0.55550099498568(7)	−1.1118333062833(4)	−16152.6728(2)	−0.00008313163125(7)
11.0	−0.55554449337938(3)	−1.11128329348558(3)	−15268.13578(9)	−0.00001766424792(2)
12.0	−0.55555197077828(2)	−1.1111193407869(2)	−14561.53445(4)	−0.000001283269190(3)
13.0	−0.555551319952593(10)	−1.1110820304889(2)	−14065.32844(4)	0.000001585339715(4)
14.0	−0.555549771540706(8)	−1.1110809890510(2)	−13735.94614(4)	0.000001325287891(6)
15.0	−0.555548790654518(6)	−1.1110879318886(2)	−13533.42264(6)	0.000000643294695(5)
16.0	−0.555548427064753(7)	−1.1110949209489(2)	−13432.75693(2)	0.000000120823788(7)
17.0	−0.555548479071485(8)	−1.1111002615034(2)	−13419.64225(7)	−0.000000194315322(7)
18.0	−0.555548765560403(7)	−1.1111039897134(2)	−13485.07562(5)	−0.000000358810701(5)
19.0	−0.555549165800166(6)	−1.11110650159334(7)	−13621.264652(3)	−0.000000429999631(2)
20.0	−0.555549608016373(6)	−1.11110817701461(8)	−13818.942931(10)	−0.000000448049093(3)

Table A47: Same as for Table A1, but for $4\,^3\Pi_g$ (wa state).

$4\,^3\Pi_g$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.02000071089858471(1)	–	1.4040013	–
0.01	97.98026065107(3)	95.9610387553(2)	1.403(3)	−9999.948254680(8)
0.05	17.9860226531(9)	15.983476480(7)	1.22(5)	−399.77137652(9)
0.1	8.001757107(3)	6.04261657(3)	1.30(5)	−99.6089764(2)
0.15	4.6909441566(4)	2.790595078(3)	1.38(6)	−43.94195490(2)
0.2	3.05137856388(8)	1.2179981347(7)	1.55(3)	−24.423794965(3)
0.3	1.44662761328(8)	−0.2454114657(7)	1.93(4)	−10.462222308(2)
0.4	0.6792436074(10)	−0.876164494(4)	2.42(6)	−5.586629266(4)
0.5	0.2450087920(3)	−1.185668779(3)	3.04(7)	−3.351372725(3)
0.6	−0.0248223122(2)	−1.3443628483(10)	3.79(7)	−2.157863706(2)
0.7	−0.20263033850(7)	−1.4241368802(4)	4.68(7)	−1.4555374331(4)
0.8	−0.32448701335(3)	−1.4598024023(5)	5.75(7)	−1.0135354694(5)
0.9	−0.41027900504(2)	−1.4698095539(3)	6.95(7)	−0.7213906042(3)
1.0	−0.47179660964(3)	−1.4645741074(2)	8.31(8)	−0.5209808881(2)
1.1	−0.51642412504(5)	−1.4502521619(7)	9.81(10)	−0.3794581014(2)
1.2	−0.548988928116(7)	−1.43060765248(6)	11.64(8)	−0.27719149692(2)
1.3	−0.572757357129(4)	−1.40799986(2)	12.2(2)	−0.201911651(10)
1.4	−0.5900027835016(10)	−1.38393354355(3)	14.3(2)	−0.145662840390(5)
1.5	−0.60234517289(3)	−1.3593788198(3)	18.2(2)	−0.1031256493(2)
1.6	−0.61096209962(2)	−1.3349634068(3)	20.9(2)	−0.0706495047(2)
1.7	−0.61672425280(2)	−1.3110918072(2)	22.4(3)	−0.04567253034(4)
1.8	−0.62028493151(9)	−1.2880208618(6)	25.6(3)	−0.0263616662(2)
1.9	−0.622140607553(5)	−1.2659086763(8)	30.52(5)	−0.0113828746(3)
2.0	−0.622672787129(2)	−1.2448468447(3)	34.9(2)	0.00024936486(6)
2.1	−0.622177496641(7)	−1.224881983630(10)	39.3(2)	0.00927286169(4)
2.2	−0.620886396721(5)	−1.20603029524(2)	44.2(2)	0.01624659006(3)
2.3	−0.6189821295875(8)	−1.18828750130(9)	49.6(2)	0.021598590407(10)
2.4	−0.616609624211(3)	−1.17163567500(3)	55.7(2)	0.02565982224(3)
2.5	−0.613884524997(2)	−1.156047957185(4)	62.2(2)	0.02868843709(4)
2.6	−0.61089954498231(3)	−1.141491818822(4)	69.3(2)	0.0308874119783(7)
2.7	−0.607729302462(3)	−1.12793132(2)	77.2(2)	0.032417512(4)
2.8	−0.604434036660(3)	−1.115328643(7)	85.7(3)	0.033406940(2)
2.9	−0.601062486082(2)	−1.10364516529(4)	95.6(2)	0.03395855408(2)
3.0	−0.5976541353407(3)	−1.092842180552(9)	105.7(3)	0.034155363373(5)
3.1	−0.594240981408(2)	−1.08288132760(5)	117.7(2)	0.03406472103(3)
3.2	−0.5908489311837(2)	−1.073724907610(7)	130.62(4)	0.033741548360(3)
3.3	−0.5874989141010(2)	−1.065336054083(8)	144.70(4)	0.033230840641(4)
3.4	−0.584207772941(2)	−1.05767882736(3)	161(5)	0.03256962303(5)
3.5	−0.5809889809831(8)	−1.05071825695(5)	176.4(5)	0.03178848714(2)
3.6	−0.577853222423(10)	−1.0444203562(2)	195.9(4)	0.03091280236(7)
3.7	−0.5748088645768(2)	−1.03875211641(3)	216.5(5)	0.02996367911(2)
3.8	−0.57186234419821(8)	−1.033681506919(9)	241.21(3)	0.028958731967(3)
3.9	−0.5690184853498(2)	−1.02917747912(3)	265.3(7)	0.02791269014(2)
4.0	−0.5662807628308(5)	−1.02520999997(4)	294.5(7)	0.02683788142(2)
4.1	−0.563651522477(2)	−1.02175013198(2)	326.3(9)	0.025744612919(4)
4.2	−0.561132168078(2)	−1.01877021099(2)	363.0(9)	0.024641458372(4)
4.3	−0.558723324592(2)	−1.01624425782(2)	404.4(9)	0.023535439850(4)
4.4	−0.556424991325(2)	−1.01414909522(2)	451.2(10)	0.022432019869(4)

4.5	−0.5542367194623(6)	−1.01246826453(5)	506.2(10)	0.02133448319(3)
4.6	−0.552157969677(3)	−1.01121240352(2)	574.0(10)	0.020239899094(2)
4.7	−0.550190044063(4)	−1.0106378188(3)	686.2(9)	0.01909409986(5)
4.8	−0.54837960546(5)	−1.017610257(6)	1392.26(7)	0.016489365(2)
4.9	−0.54685717563(2)	−1.02378502053(6)	846.7(5)	0.014271291994(2)
5.0	−0.545520491245(7)	−1.0289855764(2)	435.19(3)	0.01241108119(4)
5.1	−0.544388163498(8)	−1.03693940053(8)	−1039.98(5)	0.01016410323(2)
5.2	−0.543499875982(9)	−1.0476614273(2)	−3279.21(7)	0.00756506244(3)
5.3	−0.54287304482(2)	−1.0590340778(3)	−6009.89(9)	0.00504000224(4)
5.4	−0.54246677276(2)	−1.0673568701(3)	−8456.4(2)	0.00325493989(5)
5.5	−0.542185330424(5)	−1.07033736098(2)	−9900.58(7)	0.0025515090648(9)
5.6	−0.54192653397(2)	−1.0685181911(3)	−10165.6(2)	0.00273837086(4)
5.7	−0.54162260302(4)	−1.0639831237(3)	−9516.4(2)	0.00337931268(3)
5.8	−0.54124859050(4)	−1.0587813124(2)	−8370.8(3)	0.00408894286(2)
5.9	−0.54080986750(4)	−1.05417180394(8)	−7084.3(3)	0.0046521916946(10)
6.0	−0.540325255086(7)	−1.05062065262(2)	−5867.44(10)	0.005004976249(8)
6.5	−0.537801898946(7)	−1.04500542947(6)	−2098.31(10)	0.00470744129(2)
7.0	−0.535754064289(6)	−1.04719492291(5)	−654.20(8)	0.00347331509(2)
7.5	−0.534299142806(5)	−1.05065086308(4)	−46.79(9)	0.002392989665(9)
8.0	−0.533312900075(6)	−1.05384794035(2)	260.97(6)	0.001597232469(5)
8.5	−0.532663314686(6)	−1.056566944634(3)	589.56(8)	0.001030551140(4)
9.0	−0.532275678755(6)	−1.06024179869(3)	1947.0(2)	0.000478839863(7)
9.5	−0.532172897818(8)	−1.06365363957(7)	3129.6(2)	0.000072858527(10)
10.0	−0.532138695503(4)	−1.063530098533(5)	2861.22(6)	0.000074729244(3)
11.0	−0.532048285349(3)	−1.062997143635(2)	2405.53(5)	0.000099947913(2)
12.0	−0.531948458311(2)	−1.062733482675(3)	2089.68(3)	0.0000969528277(9)
13.0	−0.531856907345(2)	−1.062597356958(4)	1828.93(2)	0.0000858813635(3)
14.0	−0.531776339041(2)	−1.062493684751(4)	1578.87(2)	0.0000756423803(3)
15.0	−0.531704840705(3)	−1.062394393909(9)	1325.79(4)	0.000067685832(2)
16.0	−0.531640485492(2)	−1.06230210568(2)	1072.39(4)	0.000061179080(2)
17.0	−0.531582305099(2)	−1.062225845513(10)	826.26(3)	0.000055221451(2)
18.0	−0.531530015278(2)	−1.062171584740(4)	594.610(9)	0.00004935810078(4)
19.0	−0.5314835893486(10)	−1.062140689325(4)	382.36(2)	0.0000434994402(5)
20.0	−0.5314429823395(10)	−1.062131071774(6)	192.165(8)	0.00003774464524(8)

Table A48: Same as for Table A1, but for $1\,{}^1\Pi_u$ (C state) .

$1\,{}^1\Pi_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.123843086498093(2)	–	−46044.524937(1)	–
0.01	97.87641882002(3)	95.7533561775(2)	−46051.813(3)	−9999.94814625(2)
0.05	17.878(3)	15.775843794(3)	−46211.3428(4)	−399.77086138(3)
0.1	7.89797526705(6)	5.835130023(6)	−46644.3052(5)	−99.60820512(4)
0.15	4.58721127140(5)	2.5833363154(4)	−47262.6289(3)	−43.940574849(2)
0.2	2.94772409428(2)	1.0110393618(2)	−48007.6518346(10)	−24.4220441337(4)
0.3	1.3431916946396(7)	−0.45158265945(2)	−49719.15865(3)	−10.45982016243(5)
0.4	0.5760763831697(2)	−1.081335952969(6)	−51558.11223(2)	−5.583671798272(10)
0.5	0.1421617432877(2)	−1.389665929514(9)	−53404.707(5)	−3.34793883218(2)
0.6	−0.12730504535678(7)	−1.547043344283(4)	−55193.346(7)	−2.154022089283(5)
0.7	−0.30472111986125(2)	−1.6253871098818(10)	−56889.031(2)	−1.451349814518(4)
0.8	−0.426144098149866(8)	−1.6595347035215(5)	−58474.737(2)	−1.009058134031(3)
0.9	−0.511476040894782(4)	−1.667959773943(3)	−59944.217(3)	−0.716675213508(7)
1.0	−0.5725122002500037(6)	−1.661099371730(4)	−61297.808(4)	−0.516074971233(7)
1.1	−0.6166414355384560(5)	−1.645128821106(3)	−62539.821(3)	−0.374405409119(4)
1.2	−0.6486953222788965(4)	−1.623829401961(2)	−63676.895(2)	−0.272032297837(2)
1.3	−0.6719440628717529(2)	−1.5995760188437(9)	−64716.9283(10)	−0.196682994693(2)
1.4	−0.6886645852543717(2)	−1.5738875749463(5)	−65668.3886(7)	−0.1403988603129(7)
1.5	−0.70048012973757201(7)	−1.5477468953045(3)	−66539.8629(5)	−0.0978577572198(4)
1.6	−0.70857128863671537(7)	−1.5217932622403(2)	−67339.7667(4)	−0.0654066781045(3)
1.7	−0.71381153642099093(7)	−1.49644168780805(4)	−68076.1598(3)	−0.0404815382154(2)
1.8	−0.71685674809695454(7)	−1.47195862051467(4)	−68756.6349(2)	−0.02124729128935(5)
1.9	−0.71820578281118996(10)	−1.44851099645105(10)	−69388.2535(2)	−0.006368121488745(3)
2.0	−0.71824236670036556(7)	−1.42619857507619(9)	−69977.51475(8)	0.005143079162299(4)
2.1	−0.71726459560211364(9)	−1.4050755662359(2)	−70530.34526(6)	0.01402553569922(4)
2.2	−0.71550606600699063(8)	−1.3851652666310(2)	−71052.10228(4)	0.02083948426503(5)
2.3	−0.71315123661799040(10)	−1.3664700568044(3)	−71547.58484(4)	0.02601409410072(6)
2.4	−0.71034674581405077(9)	−1.3489782734655(3)	−72021.04919(3)	0.02988134090111(7)
2.5	−0.7072098505635767(2)	−1.3326689496068(4)	−72476.22621(2)	0.0327003006082(2)
2.6	−0.7038347876834872(2)	−1.3175150823969(4)	−72916.33900(2)	0.03467480498851(10)
2.7	−0.7002976163305326(2)	−1.3034858736413(4)	−73344.11968(2)	0.03596642926661(10)
2.8	−0.6966599372605290(2)	−1.2905482462189(5)	−73761.82521(2)	0.0367041529651(2)
2.9	−0.6929717724196934(2)	−1.2786678457900(5)	−74171.251766(9)	0.0369916203619(2)
3.0	−0.6892738105894307(2)	−1.2678096737223(6)	−74573.748307(9)	0.0369126491522(2)
3.1	−0.6855991699852617(2)	−1.2579384541750(7)	−74970.229575(7)	0.0365354470308(2)
3.2	−0.6819747896432710(2)	−1.2490188089329(8)	−75361.18954(2)	0.0359158657355(2)
3.3	−0.6784225332837652(2)	−1.2410152935379(9)	−75746.716048(9)	0.0350999312211(2)
3.4	−0.6749500688674244(3)	−1.23389233468(7)	−76126.50807(4)	0.03412582443(2)
3.5	−0.6716015720323385(3)	−1.227614099682(2)	−76499.896608(10)	0.0330254412521(3)
3.6	−0.6683582904851809(3)	−1.222144323209(2)	−76865.87056(2)	0.0318256271560(3)
3.7	−0.6652389981417824(3)	−1.217446112362(2)	−77223.109145(8)	0.0305491578168(3)
3.8	−0.6622503616102817(3)	−1.213481749661(2)	−77570.021556(2)	0.0292155193578(3)
3.9	−0.6593972369372506(3)	−1.210212511924(2)	−77904.794961(9)	0.0278415287054(3)
4.0	−0.6566829109953528(4)	−1.207598522484(2)	−78225.45115(2)	0.0264418248767(4)
4.1	−0.654099299184826(4)	−1.20559865337372(3)	−78529.91142295(5)	0.025024376828276(6)
4.2	−0.651667109027330(2)	−1.20417049276955(2)	−78816.069067695(6)	0.023610410782170(3)
4.3	−0.649375977578229(2)	−1.20327039079930(2)	−79081.866994670(6)	0.022205014966780(3)
4.4	−0.64722458923940(2)	−1.20285359342066(9)	−79325.3783950(2)	0.02081717842230(2)

4.5	−0.645220779416894(4)	−1.202874469363(8)	−79544.886531(6)	0.019459353216(2)
4.6	−0.64333162846020(3)	−1.2032868292099(2)	−79738.95969890(10)	0.01812531037184(3)
4.7	−0.641583549389955(10)	−1.20404432901620(8)	−79906.5170664(2)	0.01683463186462(2)
4.8	−0.639962372040222(5)	−1.20510094370474(4)	−80046.88111079(5)	0.015588291744939(5)
4.9	−0.638463425400578(5)	−1.20641148920627(4)	−80159.81319833(5)	0.014390890121405(5)
5.0	−0.6370916191536998(10)	−1.207932167067(4)	−80245.52976(3)	0.0132502142482(5)
5.1	−0.635811524688255(5)	−1.20962110234689(4)	−80304.6977420516(5)	0.012157244515612(5)
5.2	−0.634647455255780(5)	−1.21143884533120(3)	−80338.41035424(3)	0.011126166380839(4)
5.3	−0.633583544463294(5)	−1.21334880994012(3)	−80348.14407516(3)	0.010154392261598(4)
5.4	−0.632613821972769(5)	−1.21531762680567(3)	−80335.70120869(2)	0.009242595766643(4)
5.5	−0.6317422851233830(9)	−1.217315395743(6)	−80303.14167(3)	0.0083907590010(6)
5.6	−0.630932965196095(5)	−1.21931583019345(3)	−80252.708736439(4)	0.007598232178347(3)
5.7	−0.630209987181096(5)	−1.22129629421567(3)	−80186.75407951(2)	0.006863803534477(3)
5.8	−0.629557622154015(5)	−1.22323773935119(3)	−80107.66535146(3)	0.006185776716697(3)
5.9	−0.628970331676965(5)	−1.22512455456054(3)	−80017.800857694(6)	0.005562052337862(3)
6.0	−0.628452803975520(2)	−1.22694434582(2)	−79919.43326(2)	0.004990210357(2)
6.5	−0.6265344615036(9)	−1.234792805325(4)	−79368.7821037(10)	0.0028117104127(4)
7.0	−0.6254830758624(10)	−1.240434316360(4)	−78846.9515496(10)	0.0015045479093(3)
7.5	−0.6249345126910(2)	−1.244200333827(10)	−78438.3159(7)	0.000758492207(2)
8.0	−0.624679211501909(7)	−1.246601880059(7)	−78153.76591(3)	0.000344567868(2)
8.5	−0.624568123253735(5)	−1.248086820078(6)	−77972.71109(2)	0.0001234619326(10)
9.0	−0.624537960784432(2)	−1.248983581122(5)	−77867.575707(9)	0.0000102600494(8)
9.5	−0.6245481466282422(8)	−1.249513834665(4)	−77813.945687(6)	−0.0000439517273(6)
10.0	−0.6245767350901419(3)	−1.249820500254(3)	−77793.254095(4)	−0.0000667030075(4)
11.0	−0.6246486388186960(2)	−1.25008649610831(4)	−77802.9074258(2)	−0.000071747133719(2)
12.0	−0.62471513973456472(10)	−1.25015485752458(10)	−77837.4046086(2)	−0.000060381504619(6)
13.0	−0.62476909754281706(2)	−1.25015927265955(10)	−77873.8851086(3)	−0.000047775197993(6)
14.0	−0.62481143329763644(2)	−1.25014525348072(10)	−77905.2293572(2)	−0.000037313348959(6)
15.0	−0.624844524351388597(4)	−1.25012757382227(10)	−77930.3020114(2)	−0.000029235007965(6)
16.0	−0.624870551390126816(2)	−1.2501107229993(2)	−77949.87476202(4)	−0.000023101263688(6)
17.0	−0.6248912155003121249(7)	−1.2500958590476(2)	−77965.09763516(6)	−0.000018436943939(7)
18.0	−0.6249077873851430764(5)	−1.2500830959983(2)	−77977.0072788(2)	−0.000014862290444(9)
19.0	−0.6249212086986736248(3)	−1.2500722421742(3)	−77986.4190265(3)	−0.000012096040887(10)
20.0	−0.6249321801986659208(2)	−1.2500630369473(3)	−77993.9426143(4)	−0.00000993382749(2)

Table A49: Same as for Table A1, but for $2\,^1\Pi_u$ (D state) .

$2\,^1\Pi_u$				
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.05514636209194(3)	–	−14548.047097(1)	–
0.01	97.94511517135(10)	95.8907481378(4)	−14550.6(3)	−9999.94822049(2)
0.05	17.950881130(2)	15.913201507(7)	−14596.8(3)	−399.77121507(10)
0.1	7.966627265(2)	5.972387177(10)	−14720.25(8)	−99.60867352(8)
0.15	4.6558326467(8)	2.720436298(6)	−14897.19(9)	−43.94152664(3)
0.2	3.0162913325(5)	1.147931870(4)	−15109.80(9)	−24.42325398(2)
0.3	1.4116045615(2)	−0.315236556(2)	−15595.7(2)	−10.461485595(3)
0.4	0.64430269414(8)	−0.9456857053(6)	−16113.49(5)	−5.585727734(2)
0.5	0.21016522518(8)	−1.2548350840(3)	−16629.6(3)	−3.3503310688(3)
0.6	−0.0595555925(2)	−1.4131329195(3)	−17125.5(5)	−2.1567028917(8)
0.7	−0.237242357038(7)	−1.49247785835(2)	−17589.48(4)	−1.454275920391(8)
0.8	−0.358968543370(6)	−1.52768895743(3)	−18020.62(3)	−1.01218983836(2)
0.9	−0.444622398405(8)	−1.53722309917(3)	−18416.56(4)	−0.719975891513(10)
1.0	−0.505995654029(7)	−1.531502113127(10)	−18777.89(4)	−0.519510805078(5)
1.1	−0.550473919665(7)	−1.51668754663(2)	−19106.24(4)	−0.377945188456(3)
1.2	−0.582885772892(7)	−1.496548241043(9)	−19403.79(4)	−0.275647246058(5)
1.3	−0.606498653130(6)	−1.47344788730(2)	−19672.94(3)	−0.200346600797(3)
1.4	−0.623586943478(6)	−1.44889528142(2)	−19916.19(3)	−0.1440867103279(8)
1.5	−0.635771540644(6)	−1.42386412860(2)	−20135.97(2)	−0.101547364875(5)
1.6	−0.644230877691(6)	−1.39898546239(2)	−20334.57(2)	−0.069077316879(6)
1.7	−0.649836437571(8)	−1.37466680677(2)	−20514.17(4)	−0.04411407745(2)
1.8	−0.653242255418(7)	−1.35116778045(2)	−20676.64(3)	−0.0248240386788(7)
1.9	−0.654945486842(6)	−1.32864905535(2)	−20823.80(2)	−0.009872674561(4)
2.0	−0.655328276407(8)	−1.307204609756(10)	−20957.27(3)	0.001725971524(3)
2.1	−0.654687247073(6)	−1.28688328429(3)	−21078.33(2)	0.010710099932(5)
2.2	−0.653254619118(5)	−1.26770335866(2)	−21188.26(2)	0.0176390361724(2)
2.3	−0.651213560945(7)	−1.249662501071(5)	−21288.06(3)	0.022941139479(4)
2.4	−0.648709497184(6)	−1.23274460533(3)	−21378.559(8)	0.026947662098(8)
2.5	−0.645858539690(6)	−1.21692450850(2)	−21460.51(2)	0.029917028351(2)
2.6	−0.642753842361(5)	−1.202171249781(10)	−21534.43(2)	0.0320524749773(2)
2.7	−0.639470438773(6)	−1.18845031572(3)	−21600.726(10)	0.033515022897(6)
2.8	−0.636068958176(7)	−1.17572517599(4)	−21659.717(10)	0.034433121558(7)
2.9	−0.632598503520(6)	−1.16395831943(2)	−21711.57(2)	0.034909892279(2)
3.0	−0.629098897264(6)	−1.153111936916(6)	−21756.33(2)	0.035028619200(2)
3.1	−0.625602445941(6)	−1.14314835406(2)	−21793.95(2)	0.034856947686(2)
3.2	−0.622135335353(6)	−1.13403028727(2)	−21824.33(2)	0.034450119824(3)
3.3	−0.618718740083(8)	−1.12572097592(6)	−21847.260(5)	0.03385348613(2)
3.4	−0.615369710545(6)	−1.11818422886(2)	−21862.51(2)	0.03310446830378(10)
3.5	−0.612101885658(6)	−1.111384413670(9)	−21869.74(2)	0.0322341021831(8)
3.6	−0.608926068091(6)	−1.10528640950(2)	−21868.62(2)	0.0312682574118(4)
3.7	−0.605850690616(6)	−1.09985553953(2)	−21858.82(2)	0.0302286058649(3)
3.8	−0.602882195833(7)	−1.09505749537(2)	−21839.99(2)	0.0291333937609(3)
3.9	−0.600025346725(7)	−1.09085826292(2)	−21811.82(2)	0.0279980591102(3)
4.0	−0.597283481822(7)	−1.08722405734(2)	−21774.04(2)	0.02683572657513(2)
4.1	−0.594658725960(6)	−1.08412127333(3)	−21726.455(6)	0.025657604533(3)
4.2	−0.592152165391(4)	−1.081516455297(7)	−21668.98(2)	0.024473303683(4)
4.3	−0.589763994311(7)	−1.07937629126(2)	−21601.58(2)	0.02329109240965(5)
4.4	−0.587493638503(5)	−1.07766763303(3)	−21524.381(5)	0.022118100903(3)

4.5	−0.585339860710(6)	−1.07635754385(2)	−21437.679(10)	0.0209604839049(2)
4.6	−0.583300851470(4)	−1.075413374016(2)	−21341.844(7)	0.019823549764(2)
4.7	−0.581374308459(6)	−1.07480286326(3)	−21237.443(2)	0.018711862481(4)
4.8	−0.579557506745(6)	−1.074494267433(3)	−21125.203(9)	0.017629322092(2)
4.9	−0.577847361884(3)	−1.074456506058(2)	−21005.927(6)	0.016579228102(2)
5.0	−0.576240487369(5)	−1.074659325367(3)	−20880.604(7)	0.015564329870(2)
5.1	−0.5747332477(3)	−1.0750734719(8)	−20750.5(2)	0.01458686733(8)
5.2	−0.5733218068(3)	−1.0756708651(10)	−20616.3(2)	0.01364860550(10)
5.3	−0.5720021754(3)	−1.076424772(2)	−20479.5(2)	0.0127508639(2)
5.4	−0.5707702529(3)	−1.077309963(2)	−20341.2(2)	0.0118945449(2)
5.5	−0.569621868018(4)	−1.07830285189(2)	−20202.32(2)	0.011080160751(5)
5.7	−0.5675588990(4)	−1.080526260(3)	−19928.6(2)	0.0095774629(4)
5.8	−0.5666359442(4)	−1.081718693(4)	−19795.2(2)	0.0088884820(6)
5.9	−0.5657798469(5)	−1.082942727(5)	−19665.2(2)	0.0082401638(7)
6.0	−0.5649865882492(2)	−1.084184057324(5)	−19538.938(3)	0.0076315198622(9)
6.5	−0.56183080960121(4)	−1.090273456485(2)	−18976.6363(4)	0.0051366404181(2)
7.0	−0.55972210610446(5)	−1.09558524074(2)	−18505.163(3)	0.003408424495(2)
7.5	−0.5583288376230(4)	−1.09983725612(2)	−18039.6654(3)	0.002242722550(2)
8.0	−0.5574145446368(2)	−1.103088169639(7)	−17463.9949(3)	0.0014676149544(8)
8.5	−0.55681752585672(6)	−1.1055089749790(10)	−16656.7985(3)	0.00095600902760(8)
9.0	−0.5564294172808(10)	−1.10727807955(3)	−15509.5462(4)	0.000620083891(3)
9.5	−0.5561780284343(7)	−1.10854370615(2)	−13972.5310(2)	0.000401300075(2)
10.0	−0.5560150859946(9)	−1.10941910879(2)	−12134.7702(4)	0.000261106320(2)
11.0	−0.5558361283483(2)	−1.110358904788(3)	−8553.38701(4)	0.0001193956281(2)
12.0	−0.5557479986964(7)	−1.110715426413(9)	−6203.63848(3)	0.0000650475817(5)
13.0	−0.5556961115907(5)	−1.110851220285(5)	−4962.1459(3)	0.0000416156074(2)
14.0	−0.55566111306376(7)	−1.1109090270975(6)	−4334.1179(2)	0.00002951421644(2)
15.0	−0.55563556713766(5)	−1.1109399002889(3)	−4008.50164(8)	0.0000220822657683(9)
16.0	−0.55561622332729(3)	−1.11096252165040(10)	−3821.87530(6)	0.000016870312755(6)
17.0	−0.55560140904228(3)	−1.11098305464362(2)	−3688.95179(2)	0.000012927261221(8)
18.0	−0.55559008007670(2)	−1.11100274834615(8)	−3564.92879(3)	0.000009856211504(10)
19.0	−0.55558147283856(2)	−1.11102123499783(3)	−3426.99262(2)	0.000007458456797(6)
20.0	−0.555574982611434(10)	−1.11103790313518(5)	−3265.135147(3)	0.000005603104379(6)

Table A50: Same as for Table A1, but for $3\,^1\Pi_u$ (V state) .

		$3\,^1\Pi_u$		
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.031255144381749(1)	–	10.0242694(2)	–
0.01	97.96900621343(6)	95.9385298721(4)	10.026(3)	−9999.94825548(3)
0.05	17.974768118(3)	15.96096722(2)	10.161(7)	−399.7713804(3)
0.1	7.990502276(3)	6.02010615(2)	10.51(2)	−99.6089840(2)
0.15	4.6796888490(6)	2.768082789(4)	10.94(8)	−43.94196606(2)
0.2	3.040122617(3)	1.19548336(2)	11.70(9)	−24.42380937(5)
0.3	1.4353699121(3)	−0.267933052(2)	13.937(4)	−10.462242921(4)
0.4	0.66798354391(9)	−0.8986952649(7)	16.629(8)	−5.586655882(2)
0.5	0.23374576882(4)	−1.2082111053(3)	19.9735(8)	−3.3514052859(4)
0.6	−0.03608888848(2)	−1.36691910203(10)	23.9937(6)	−2.1579022085(2)
0.7	−0.213901063874(2)	−1.4467094737(3)	28.48(2)	−1.4555819226(2)
0.8	−0.335762490242(9)	−1.48239380155(4)	34.19(2)	−1.01358602633(3)
0.9	−0.421559845534(7)	−1.49242229645(4)	40.51(2)	−0.72144733932(3)
1.0	−0.4830834382166(2)	−1.48721081710(2)	47.721(7)	−0.52104394066(2)
1.1	−0.52771758166707(8)	−1.472915568114(8)	55.876(6)	−0.379527640708(6)
1.2	−0.5602896712967(2)	−1.453300612159(10)	65.070(5)	−0.277267724636(4)
1.3	−0.5840660672443(4)	−1.43072536750(2)	75.396(5)	−0.201994794627(8)
1.4	−0.6013201666894(2)	−1.406694810571(10)	86.955(5)	−0.145753197993(6)
1.5	−0.61367196530083(10)	−1.382179232022(8)	99.862(5)	−0.103223534280(5)
1.6	−0.62229907235362(6)	−1.357806613543(7)	114.245(5)	−0.070755293022(4)
1.7	−0.62807221744024(5)	−1.333981753549(5)	130.25211(7)	−0.045786658040(3)
1.8	−0.63164474672497(8)	−1.310961841547(4)	148.023(5)	−0.026484637832(2)
1.9	−0.63351318598876(4)	−1.288905393145(3)	167.76002(10)	−0.011515274299(2)
2.0	−0.63405910469922(8)	−1.267904487228(4)	189.64406(5)	0.000106861085(2)
2.1	−0.63357860189655(7)	−1.248006312896(5)	213.90473(4)	0.009119471856(2)
2.2	−0.63230342242578(4)	−1.229227745287(4)	240.79371(4)	0.016081408893(2)
2.3	−0.63041630601095(7)	−1.211565302295(3)	270.59474(4)	0.0214205694467(10)
2.4	−0.62806229459085(7)	−1.195001998137(6)	303.628453(5)	0.025467746269(2)
2.5	−0.62535716359586(3)	−1.179512087631(4)	340.24(2)	0.028480895824(2)
2.6	−0.62239377820286(4)	−1.165064362910(4)	380.893(2)	0.030662766729(2)
2.7	−0.61924693362574(5)	−1.151624449532(4)	426.00871(2)	0.032173858415(2)
2.8	−0.6159770751770(2)	−1.1391564080602(3)	476.1317(7)	0.0331420508181(10)
2.9	−0.61263318190023(4)	−1.127623853581(5)	531.88119(2)	0.033669831110(2)
3.0	−0.60925501978092(6)	−1.116990742842(6)	593.950(2)	0.033839765574(2)
3.1	−0.60587491575974(7)	−1.107221936474(10)	663.14947(7)	0.033718675821(3)
3.2	−0.60251916477657(8)	−1.098283615007(8)	740.400(2)	0.033360848296(2)
3.3	−0.59920915398249(3)	−1.09014360839(2)	826.775008(6)	0.032810515025(3)
3.4	−0.59596226786315(7)	−1.08277168615(2)	923.50533(2)	0.032103779288(4)
3.5	−0.59279262307761(6)	−1.076139847821(7)	1032.01979(2)	0.031270113810(2)
3.6	−0.58971167080997(7)	−1.070222648863(7)	1153.9694(4)	0.030333525766(2)
3.7	−0.58672869628358(7)	−1.064997596083(2)	1291.24(2)	0.0293134585088(5)
3.8	−0.58385123904255(7)	−1.060445646756(9)	1446.099(2)	0.028225481929(2)
3.9	−0.58108545310471(8)	−1.056551846253(6)	1620.996(3)	0.027081810245(2)
4.0	−0.57843642270569(9)	−1.05330613846(2)	1818.8164(9)	0.025891676738(3)
4.1	−0.5759084467052(8)	−1.05070437618(2)	2042.746(2)	0.024661589569(3)
4.2	−0.5735053023974(10)	−1.04874953849(2)	2296.2556(6)	0.023395491978(4)
4.3	−0.571230496915(5)	−1.047453115(2)	2581.2(8)	0.0220948552(6)
4.4	−0.569087510704(2)	−1.04683648738(4)	2906.221(2)	0.020758757733(7)

4.5	−0.5670800314725(3)	−1.0469320172(2)	3268.79(2)	0.01938401017(3)
4.6	−0.565212165924(3)	−1.04778301555(7)	3671.720(2)	0.01796550354(2)
4.7	−0.563488598378(4)	−1.04944140503(8)	4112.864(3)	0.01649697696(2)
4.8	−0.561914636653(5)	−1.05196096510(10)	4584.85(2)	0.01497256421(2)
4.9	−0.560496048521(5)	−1.0553835663(2)	5072.445(4)	0.01338949607(3)
5.0	−0.5592385599918(7)	−1.0597163384(4)	5549.84(5)	0.01175215632(6)
5.5	−0.555416132802(2)	−1.08968313657(7)	6362.383(8)	0.00384529619(2)
6.0	−0.554668430236(2)	−1.10964769596(3)	3550.674(6)	−0.000051805914(3)
6.5	−0.554932208220(2)	−1.11458878863(6)	432.42041(10)	−0.00072682650(2)
7.0	−0.5552660307472(4)	−1.114487170634(5)	−1647.2922(5)	−0.0005650155912(4)
7.5	−0.5554874525832(3)	−1.113433000190(3)	−2919.0298(3)	−0.0003277460031(2)
8.0	−0.5556053571365(3)	−1.112462195983(2)	−3771.2760(7)	−0.00015643521369(7)
8.5	−0.5556551702212(3)	−1.111755460336(2)	−4526.5582(5)	−0.000052367046307(10)
9.0	−0.5556654965765(2)	−1.1112869171620(4)	−5430.4476(4)	0.00000489733220(9)
9.5	−0.5556551596727(2)	−1.1110003941295(5)	−6624.8485(5)	0.0000326237068(2)
10.0	−0.5556359044567(2)	−1.110851459399(2)	−8081.5902(2)	0.0000420349513(3)
11.0	−0.55559625780807(5)	−1.110821829684(2)	−10924.41678(5)	0.0000336987211(2)
12.0	−0.55557051756912(4)	−1.110920828423(2)	−12669.1260(2)	0.0000183505596(2)
13.0	−0.555557556335343(10)	−1.1110033781885(2)	−13464.7135(2)	0.00000859496016(3)
14.0	−0.555551692841503(6)	−1.11105115476994(7)	−13784.1981(2)	0.000003730779506(2)
15.0	−0.55554924751854(2)	−1.1110767936785(2)	−13905.2087(2)	0.00000144675723(2)
16.0	−0.555548402978363(8)	−1.111090799347596(4)	−13960.3639(2)	0.000000375413066(3)
17.0	−0.555548311291048(7)	−1.111098811867588(4)	−14010.9171(2)	−0.000000128781503(3)
18.0	−0.55554857089486(2)	−1.1111036080589(2)	−14084.4411(2)	−0.000000359237173(5)
19.0	−0.555548984947825(9)	−1.1111065785693(2)	−14192.02608(10)	−0.00000045308809(2)
20.0	−0.555549454309680(8)	−1.1111084613651(2)	−14335.99101(9)	−0.00000047763729(2)

Table A51: Same as for Table A1, but for $4\,^1\Pi_u$ (D' state).

$4\,^1\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.03106965045024(3)	–	−6254.9235543(1)	–
0.01	97.96919178520(6)	95.9389011706(4)	−6255.859(9)	−9999.94823998(3)
0.05	17.974955488(2)	15.96134562(2)	−6274.951(2)	−399.7713070(2)
0.1	7.990694954(4)	6.02050527(3)	−6326.740(5)	−99.6088464(3)
0.15	4.679889863(2)	2.76851403(2)	−6403(2)	−43.94177128(6)
0.2	3.0403346762(8)	1.195956722(7)	−6489.7(3)	−24.42356315(3)
0.3	1.4356112125(3)	−0.267349651(3)	−6691.37678(9)	−10.461906918(6)
0.4	0.6682623581(3)	−0.897972708(3)	−6906.67(2)	−5.586243561(5)
0.5	0.23406918181(4)	−1.2073252509(3)	−7120.619(3)	−3.3509272290(5)
0.6	−0.03571475804(4)	−1.3658498886(4)	−7325.72(3)	−2.1573672875(5)
0.7	−0.21347092383(2)	−1.44544035045(9)	−7518.078(8)	−1.45499786113(10)
0.8	−0.335271776213(6)	−1.48091130513(5)	−7696.067(7)	−1.01295969088(5)
0.9	−0.421004643982(4)	−1.49071569864(4)	−7859.23(2)	−0.72078490076(3)
1.0	−0.482460422266(3)	−1.48527181946(4)	−8007.87(2)	−0.52035097492(3)
1.1	−0.527023955252(4)	−1.47073802835(3)	−8142.70(2)	−0.37880919804(3)
1.2	−0.559523119342(4)	−1.45088029758(3)	−8264.60(3)	−0.27652838242(2)
1.3	−0.583224710587(4)	−1.42805973147(3)	−8374.59(3)	−0.20123870023(2)
1.4	−0.600402520940(4)	−1.40378278899(3)	−8473.68(3)	−0.14498410508(2)
1.5	−0.612676903060(4)	−1.37902105684(3)	−8562.84(4)	−0.10244483381(2)
1.6	−0.621225788304(5)	−1.35440364006(4)	−8643.02(4)	−0.06997003966(2)
1.7	−0.626920195845(5)	−1.33033629813(3)	−8715.01(4)	−0.044997592024(10)
1.8	−0.630413730895(6)	−1.30707702612(3)	−8779.64(5)	−0.025694202406(8)
1.9	−0.632203149262(6)	−1.28478499264(4)	−8837.59(5)	−0.01072562849(2)
2.0	−0.632670222456(6)	−1.26355277577(5)	−8889.42(5)	0.00089383457(2)
2.1	−0.632111224111(7)	−1.24342790420(5)	−8935.67(6)	0.00990216381(2)
2.2	−0.630758046230(9)	−1.22442742240(5)	−8976.79(6)	0.01685848639(2)
2.3	−0.628793547669(7)	−1.20654783089(3)	−9013.08(6)	0.022190984542(2)
2.4	−0.626362860314(8)	−1.18977191740(3)	−9044.94(6)	0.0262307513462(6)
2.5	−0.623581818423(9)	−1.17407347105(5)	−9072.64(7)	0.029236066315(10)
2.6	−0.620543312213(8)	−1.15942054060(2)	−9096.12(6)	0.0314100322442(3)
2.7	−0.617322124591(9)	−1.14577768231(6)	−9115.84(7)	0.032913543285(8)
2.8	−0.613978646581(9)	−1.13310750028(3)	−9131.45(6)	0.0338749260328(4)
2.9	−0.610561755163(10)	−1.12137169105(3)	−9143.32(6)	0.034397179063(2)
3.0	−0.60711105923(2)	−1.11053173672(6)	−9151.17(4)	0.034563460575(8)
3.1	−0.60365866464(2)	−1.10054935104(8)	−9155.22(4)	0.03444128330(2)
3.2	−0.60023057028(2)	−1.09138675154(6)	−9155.24(4)	0.034085746563(7)
3.3	−0.59684777871(2)	−1.08300680946(6)	−9151.110(3)	0.033542044836(5)
3.4	−0.59352718475(2)	−1.07537311580(4)	−9142.69(2)	0.032847427561(4)
3.5	−0.59028228983(2)	−1.06844999151(7)	−9129.822(3)	0.032032739469(6)
3.6	−0.58712377929(2)	−1.06220246042(7)	−9112.374(6)	0.031123638375(6)
3.7	−0.58405999085(2)	−1.05659620211(7)	−9090.180(8)	0.030141562048(5)
3.8	−0.58109729660(2)	−1.05159749355(7)	−9063.092(4)	0.029104499910(6)
3.9	−0.57824041584(2)	−1.04717314892(10)	−9030.97884(2)	0.02802761097(2)
4.0	−0.57549267233(2)	−1.04329046377(2)	−8993.91(7)	0.026923720211(10)
4.1	−0.57285620704(2)	−1.03991716734(2)	−8951.49(7)	0.025803718673(2)
4.2	−0.57033215480(4)	−1.0370213886(2)	−8903.71(2)	0.024676885945(9)
4.3	−0.56792079200(2)	−1.034571636684(7)	−8850.98(6)	0.023551150480(3)
4.4	−0.56562166080(3)	−1.03253680390(3)	−8793.13(8)	0.022433299424(2)

4.5	−0.563433674549(10)	−1.030886186793(4)	−8730.12(4)	0.021329147173(4)
4.6	−0.56135520807(2)	−1.02958953703(2)	−8662.68(8)	0.02024366934(2)
4.7	−0.55938417602(2)	−1.02861713785(2)	−8590.72(6)	0.01918110942(2)
4.8	−0.55751810183(2)	−1.027939913574(8)	−8514.794(5)	0.01814506040(2)
4.9	−0.55575417941(4)	−1.02752956681(3)	−8435.84(7)	0.017138529015(3)
5.0	−0.554089329273(10)	−1.02735874132(7)	−8353.933(6)	0.016163983447(10)
5.5	−0.547130494300(7)	−1.02922781957(8)	−7936.90(9)	0.01182421254(3)
6.0	−0.542110507075(9)	−1.033783152(4)	−7591.85(4)	0.0084063103(7)
6.5	−0.5385829807664(5)	−1.03924597591(2)	−7382.925(7)	0.005833843942(2)
7.0	−0.5361589831596(6)	−1.04454759093(2)	−7279.964(8)	0.003967196485(2)
7.5	−0.534523275932(8)	−1.04912705530(8)	−7215.00(8)	0.00265593287(2)
8.0	−0.533434102274(5)	−1.05279525231(5)	−7134.77(6)	0.001759119026(8)
8.5	−0.532715078128(5)	−1.05558966628(5)	−7012.82(6)	0.001157704698(8)
9.0	−0.532242655247(4)	−1.05764888576(4)	−6837.67(5)	0.000759602746(6)
9.5	−0.531932821972(2)	−1.05913365382(3)	−6600.445(10)	0.000498104224(2)
10.0	−0.531729575482(2)	−1.06018961805(3)	−6287.512(9)	0.000326953291(2)
11.0	−0.5315091958367(8)	−1.06153320476(7)	−5234.371(7)	0.000135016991(7)
12.0	−0.531444947891(2)	−1.06245559262(5)	−1615.23(2)	0.000036191930(3)
13.0	−0.531414787611(3)	−1.06249922172(5)	−1420.78(2)	0.000025411808(3)
14.0	−0.531392772851(3)	−1.06251852662(5)	−1347.81(2)	0.000019072792(3)
15.0	−0.531375882969(3)	−1.06252638105(5)	−1255.64(3)	0.000015025659(2)
16.0	−0.531362195352(3)	−1.06252343116(4)	−1145.97(3)	0.000012559972(2)
17.0	−0.531350434205(3)	−1.06251240472(4)	−1035.33(2)	0.000011086100(2)
18.0	−0.531339840773(3)	−1.06249672282(3)	−935.07(2)	0.0000101643735(9)
19.0	−0.531330020045(2)	−1.06247948779(3)	−850.73(2)	0.0000095027525(7)
20.0	−0.531320808096(2)	−1.06246310788(2)	−784.12(2)	0.0000089254159(5)

Table A52: Same as for Table A1, but for $5\,^1\Pi_u$ (kb state).

$5\,^1\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.471811425816(8)	−1.46462818692(5)	26.15(6)	−0.52100533532(7)
1.1	−0.516441514314(6)	−1.45031667543(5)	30.61(5)	−0.37948513347(5)
1.2	−0.549009154422(5)	−1.43068377893(4)	35.62(4)	−0.27722122509(4)
1.3	−0.572780696376(2)	−1.408088846068(5)	41.27(2)	−0.2019441948589(7)
1.4	−0.590029525616(2)	−1.384036770148(4)	47.55(2)	−0.1456983706547(3)
1.5	−0.602375623985(2)	−1.359497742779(3)	54.57(2)	−0.1031643298742(8)
1.6	−0.610996584584(2)	−1.335099628324(8)	62.392(10)	−0.070691536973(4)
1.7	−0.616763118146(2)	−1.311247086486(10)	71.09(2)	−0.045718147173(5)
1.8	−0.620328548926(2)	−1.28819714327(2)	80.76(2)	−0.026411136344(5)
1.9	−0.622189377299(2)	−1.26610812191(2)	91.48(2)	−0.011436509111(9)
2.0	−0.622727143343(2)	−1.24507187527(2)	103.40(2)	0.000191205707(5)
2.1	−0.622237912141(2)	−1.225135327446(9)	116.62(3)	0.009209760398(3)
2.2	−0.620953389358(3)	−1.20631504308(2)	131.22(5)	0.016178061654(4)
2.3	−0.619056269571(3)	−1.18860717680(2)	147.47(3)	0.021524070590(2)
2.4	−0.616691542730(3)	−1.171994318163(9)	165.46(3)	0.0255786530452(3)
2.5	−0.613974924450(4)	−1.156450226125(8)	185.39(6)	0.0285998491150(3)
2.6	−0.610999211152(4)	−1.141943114233(5)	207.57(4)	0.030790503102(2)
2.62	−0.610379825292(4)	−1.139163082852(4)	212.28(4)	0.031143728139(2)
2.64	−0.609753632556(4)	−1.136422843008(4)	217.10(4)	0.031471372007(2)
2.66	−0.609121133850(3)	−1.133722101655(4)	222.00(3)	0.0317744985117(8)
2.68	−0.608482809274(3)	−1.131060563965(4)	227.02(3)	0.0320541248423(9)
2.7	−0.607839119029(3)	−1.128437933650(3)	232.15(3)	0.0323112238530(10)
2.72	−0.607190504288(3)	−1.125853913294(3)	237.39(3)	0.032546726205(2)
2.74	−0.606537388013(3)	−1.123308204648(3)	242.74(3)	0.032761522399(2)
2.76	−0.605880175735(5)	−1.12080050891(3)	248.16(3)	0.032956464694(6)
2.78	−0.605219256330(5)	−1.11833052697(3)	253.75(3)	0.033132368954(6)
2.8	−0.604555002682(5)	−1.115897959600(9)	259.45(3)	0.033290016338(6)
2.82	−0.603887772394(5)	−1.11350250794(3)	265.28(3)	0.033430154911(6)
2.84	−0.603217908426(5)	−1.11114387321(3)	271.23(3)	0.033553501282(6)
2.86	−0.6025457397144(2)	−1.1088217573590(5)	277.600(6)	0.0336607419822(3)
2.88	−0.6018715817332(2)	−1.1065358630846(5)	283.816(6)	0.0337525348546(3)
2.9	−0.6011957370963(2)	−1.1042858939400(5)	290.168(6)	0.0338295104318(3)
2.92	−0.6005184960629(2)	−1.1020715545632(5)	296.658(6)	0.0338922731377(3)
2.94	−0.5998401370546(2)	−1.0998925508059(5)	303.291(6)	0.0339414024839(3)
2.96	−0.599160927135(5)	−1.09774858989(3)	309.83(4)	0.033977454181(6)
2.98	−0.598481122505(5)	−1.09563938047(3)	316.76(5)	0.034000961256(6)
3.0	−0.597800968889(4)	−1.09356463284(3)	323.83(5)	0.034012434988(6)
3.1	−0.594402888388(6)	−1.08369780804(3)	361.65(5)	0.033905796367(6)
3.2	−0.591027634146(6)	−1.07465018026(3)	403.89(5)	0.033564090009(6)
3.3	−0.587696414792(7)	−1.06638794572(2)	451.15(5)	0.033031782991(2)
3.4	−0.584426411432(7)	−1.05887900522(3)	504.07(10)	0.0323452404907(4)
3.5	−0.581231509841(8)	−1.05209323902(4)	563.55(6)	0.031534223045(6)
3.6	−0.578122900397(8)	−1.04600283020(4)	630.38(6)	0.030623047382(5)
3.7	−0.575109575846(9)	−1.040582681169(7)	705.62(6)	0.029631478523(3)
3.8	−0.572198751217(9)	−1.035810977604(10)	790.40(7)	0.028575401272(4)
3.9	−0.569396226170(10)	−1.03166996461(4)	885.98(7)	0.027467304538(4)
4.0	−0.566706707370(10)	−1.02814701784(5)	993.67(7)	0.026316599217(4)
4.1	−0.56413410685(2)	−1.02523610728(5)	1114.7(2)	0.025129782055(4)

4.2	−0.56168183132(2)	−1.022939755934(3)	1250.06(8)	0.023910453974(6)
4.3	−0.55935307638(2)	−1.02127155361(6)	1399.90(8)	0.022659209106(8)
4.4	−0.55715113640(2)	−1.02025911522(7)	1562.84(8)	0.021373444905(9)
4.5	−0.55507973196(2)	−1.01994688880(3)	1734.38(9)	0.020047238921(3)
4.6	−0.55314333250(2)	−1.02039704262(5)	1904.6(2)	0.018671657048(2)
4.7	−0.55134739565(2)	−1.02168420011(8)	2053.25(10)	0.017236296008(8)
4.8	−0.54969833195(2)	−1.0238756632(2)	2146.4(2)	0.01573354181(2)
4.9	−0.54820282532(3)	−1.0269848897(2)	2129.9(2)	0.01416750223(2)
5.0	−0.54686598972(3)	−1.0308915696(2)	1932.5(2)	0.01256808197(2)

Table A53: Same as for Table A1, but for $6\,^1\Pi_u$.

$6\,^1\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.471489776137(6)	−1.46362897108(4)	−4123.28(2)	−0.52064941881(3)
1.1	−0.516083592385(5)	−1.44919479574(3)	−4191.96(2)	−0.37911600997(2)
1.2	−0.548613757173(5)	−1.42943696497(3)	−4254.07(2)	−0.27684120886(2)
1.3	−0.572346840994(5)	−1.40671567605(3)	−4310.08(2)	−0.20155538005(2)
1.4	−0.589556428468(6)	−1.38253656638(3)	−4360.53(3)	−0.14530264960(2)
1.5	−0.601862681247(6)	−1.35787047554(3)	−4405.87(3)	−0.10276340869(2)
1.6	−0.610443354275(4)	−1.33334582587(2)	−4446.56(2)	−0.070286948326(5)
1.7	−0.616169303324(8)	−1.30936774976(4)	−4483.09(3)	−0.04531126066(2)
1.8	−0.619693981780(10)	−1.28619366270(6)	−4515.77(4)	−0.02600316619(2)
1.9	−0.62151400390(2)	−1.26398219455(8)	−4544.93(4)	−0.01102851934(3)
2.0	−0.62201100878(2)	−1.2428254197(2)	−4570.86(4)	0.00059829894(4)
2.1	−0.62148114568(3)	−1.2227703934(2)	−4593.82(4)	0.00961518953(6)
2.2	−0.62015618947(3)	−1.2038337132(3)	−4614.02(4)	0.01658121168(7)
2.3	−0.61821888828(4)	−1.1860114569(3)	−4631.61(5)	0.02192448679(9)
2.4	−0.61581426904(6)	−1.1692860114(4)	−4646.75(5)	0.0259760528(2)
2.5	−0.61305806636(7)	−1.1536307862(6)	−4659.53(5)	0.0289941386(2)
2.6	−0.61004307569(10)	−1.1390134727(8)	−4670.03(5)	0.0311817995(3)
2.62	−0.60941586956(9)	−1.1362114526(8)	−4671.86(5)	0.0315344605(3)
2.64	−0.60878186769(9)	−1.1334492260(7)	−4673.60(5)	0.0318615566(2)
2.66	−0.6081415706(2)	−1.1307264924(10)	−4675.25(5)	0.0321641537(3)
2.68	−0.6074954581(2)	−1.1280429493(9)	−4676.81(5)	0.0324432712(3)
2.7	−0.6068439898(2)	−1.1253982920(9)	−4678.29(5)	0.0326998843(3)
2.72	−0.6061876065(2)	−1.1227922144(10)	−4679.68(5)	0.0329349259(3)
2.74	−0.6055267306(2)	−1.1202244092(10)	−4680.97(5)	0.0331492890(3)
2.76	−0.6048617671(2)	−1.1176945678(10)	−4682.18(5)	0.0333438284(3)
2.78	−0.6041931042(2)	−1.115202381(2)	−4683.30(5)	0.0335193624(3)
2.8	−0.6035211141(2)	−1.112747538(2)	−4684.33(4)	0.0336766749(3)
2.82	−0.6028461536(2)	−1.110329730(2)	−4685.28(4)	0.0338165167(3)
2.84	−0.6021685651(2)	−1.107948645(2)	−4686.13(4)	0.0339396073(4)
2.86	−0.6014886764(2)	−1.105603973(2)	−4686.89(4)	0.0340466361(4)
2.88	−0.6008068023(2)	−1.103295404(2)	−4687.57(4)	0.0341382641(4)
2.9	−0.6001232443(2)	−1.101022626(2)	−4688.16(4)	0.0342151249(4)
2.92	−0.5994382917(2)	−1.098785331(2)	−4688.65(4)	0.0342778261(4)
2.94	−0.5987522217(2)	−1.096583208(2)	−4689.06(4)	0.0343269508(4)
2.96	−0.5980653004(2)	−1.094415949(2)	−4689.38(4)	0.0343630581(4)
2.98	−0.5973777826(2)	−1.092283245(2)	−4689.60(4)	0.0343866847(4)
3.0	−0.5966899128(2)	−1.090184789(2)	−4689.73(4)	0.0343983456(4)
3.1	−0.5932531537(2)	−1.080195526(2)	−4689.03(4)	0.0342938003(4)
3.2	−0.5898388991(2)	−1.071016888(2)	−4685.97(4)	0.0339565346(4)
3.3	−0.5864680908(2)	−1.062611623(2)	−4680.50(4)	0.0334316843(4)
3.4	−0.5831575685(2)	−1.054943262(2)	−4672.54(4)	0.0327564338(4)
3.5	−0.5799207859(2)	−1.047976127(2)	−4661.99(3)	0.0319615557(4)
3.6	−0.5767683877(2)	−1.041675316(2)	−4648.78(3)	0.0310726276(4)
3.7	−0.5737086799(2)	−1.036006666(2)	−4632.82(3)	0.0301109982(4)
3.8	−0.5707480119(3)	−1.030936701(2)	−4614.02(3)	0.0290945586(4)
3.9	−0.5678910909(3)	−1.026432579(2)	−4592.30(3)	0.0280383596(3)
4.0	−0.5651412396(3)	−1.022462045(2)	−4567.61(3)	0.0269551086(3)
4.1	−0.5625006103(2)	−1.018993386(2)	−4539.90(3)	0.0258555695(3)

4.2	−0.5599703623(2)	−1.015995402(2)	−4509.13(3)	0.0247488863(3)
4.3	−0.5575508104(3)	−1.013437391(2)	−4475.29(3)	0.0236428441(3)
4.4	−0.5552415498(3)	−1.011289141(2)	−4438.42(3)	0.0225440814(3)
4.5	−0.5530415618(3)	−1.009520954(2)	−4398.57(3)	0.0214582599(3)
4.6	−0.5509493049(2)	−1.008103681(2)	−4355.82(3)	0.0203902019(2)
4.7	−0.5489627922(2)	−1.007008788(2)	−4310.34(3)	0.0193439992(2)
4.8	−0.54707966093(5)	−1.0062084479(2)	−4262.35(5)	0.018323098752(7)
4.9	−0.5452972329(2)	−1.0056756590(8)	−4211.98(3)	0.01733036872(10)
5.0	−0.5436125696(2)	−1.0053843905(9)	−4159.65(3)	0.01636814975(10)

Table A54: Same as for Table A1, but for $7\,^1\Pi_u$.

$7\,^1\Pi_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.465690043530(5)	−1.45236764754(2)	15.76(2)	−0.52098756036(2)
1.1	−0.510318264439(6)	−1.438048631078(7)	18.41(2)	−0.37946554747(2)
1.2	−0.542883853380(6)	−1.4184074412639(4)	21.39(2)	−0.27719977878(2)
1.3	−0.566653155304(5)	−1.39580338962(2)	24.74(2)	−0.20192083001(2)
1.4	−0.583899549321(5)	−1.37174132490(4)	28.50(2)	−0.14567301875(3)
1.5	−0.596243009858(5)	−1.34719138585(3)	32.69(2)	−0.10313691076(2)
1.6	−0.604861121352(4)	−1.32278137429(3)	37.36(2)	−0.070661957239(9)
1.7	−0.610624584452(2)	−1.29891587580(2)	42.56(2)	−0.045686298175(7)
1.8	−0.614186711690(3)	−1.27585182880(2)	48.34(2)	−0.026376891899(7)
1.9	−0.616043989841(3)	−1.25374745311(2)	54.76(2)	−0.011399722855(5)
2.0	−0.616577943209(2)	−1.232694479570(2)	61.87(3)	0.000230703421(3)
2.1	−0.616084618592(2)	−1.212739688184(2)	69.78(2)	0.00925216619328(4)
2.2	−0.614795700477(2)	−1.193899473574(2)	39.26(2)	0.016223603352(3)
2.3	−0.612893858888(3)	−1.176169789549(3)	88.19(3)	0.021573012273(3)
2.4	−0.610524055314(2)	−1.15953298839(2)	98.94(3)	0.025631300931(3)
2.5	−0.607801972355(2)	−1.14396254831(2)	110.86(3)	0.028656558556(2)
2.6	−0.604820368094(3)	−1.12942635043(2)	124.09(3)	0.030851686830(2)
2.62	−0.604199749091(3)	−1.12664013981(2)	126.90(3)	0.031205861974(2)
2.64	−0.603572304014(3)	−1.12389359218(2)	129.78(3)	0.031534475698(2)
2.66	−0.602938533366(3)	−1.12118641093(4)	132.60(7)	0.03183859240(2)
2.68	−0.602298916835(3)	−1.11851829741(2)	135.71(3)	0.032119229947(2)
2.7	−0.601653914198(2)	−1.11588895154(2)	138.78(3)	0.032377361796(2)
2.72	−0.601003966184(3)	−1.11329807188(2)	141.91(3)	0.032613919293(2)
2.74	−0.600349495301(5)	−1.11074535604(2)	145.10(4)	0.032829793635(2)
2.76	−0.599690906635(4)	−1.1082305011(2)	148.28(5)	0.03302583781(4)
2.78	−0.599028588539(5)	−1.10575320298(2)	151.70(4)	0.033202868382(2)
2.8	−0.598362913429(5)	−1.10331315842(2)	155.11(4)	0.033361667298(2)
2.82	−0.597694238391(5)	−1.100910063485(8)	158.59(4)	0.0335029834376(4)
2.84	−0.597022905854(5)	−1.09854361461(2)	162.14(4)	0.033627534189(2)
2.86	−0.596349244202(6)	−1.09621350860(2)	165.68(6)	0.033736006926(2)
2.88	−0.595673568366(5)	−1.09391944275(2)	169.49(4)	0.033829060409(2)
2.9	−0.594996180367(5)	−1.091661115243(8)	173.28(4)	0.0339073260298(6)
2.92	−0.594317369868(5)	−1.08943822494(2)	177.16(4)	0.0339714091761(6)
2.94	−0.593637414674(5)	−1.087250471879(9)	181.12(4)	0.0340218902943(5)
2.96	−0.592956581219(5)	−1.085097557092(8)	185.06(7)	0.0340593261289(8)
2.98	−0.592275125032(6)	−1.08297918296(2)	189.30(4)	0.03408425070583(10)
3.0	−0.5915932911807(10)	−1.080895053170(9)	193.53(4)	0.0340971763930(10)
3.1	−0.5881863537271(10)	−1.070977809356(10)	216.12(4)	0.0339983542208(7)
3.2	−0.584801410083(2)	−1.06187319306(2)	241.35(4)	0.0336655084696(5)
3.3	−0.581459555601(4)	−1.05354625945(2)	269.58(4)	0.0331432884068(5)
3.4	−0.578177838239(7)	−1.045963539454(6)	301.22(4)	0.0324682756004(3)
3.5	−0.57496998703087(2)	−1.039093268314(3)	336.72(5)	0.0316704873454(7)
3.6	−0.571847007633(8)	−1.032905656729(10)	376.61(5)	0.030774544044(2)
3.7	−0.568817675113(6)	−1.02737325120(2)	421.48(5)	0.029800567300(2)
3.8	−0.56588894832867(8)	−1.022471447011(2)	471.96(5)	0.0287648551701(6)
3.9	−0.563066326697(6)	−1.018179234306(9)	528.70(5)	0.027680363863(3)
4.0	−0.5603541677539(5)	−1.014480295289(9)	592.30(5)	0.026557010050(3)
4.1	−0.5577559835232(5)	−1.011364619328(10)	663.14(5)	0.025401792122(3)

4.2	−0.5552747343222(5)	−1.00883086259(2)	741.09(6)	0.024218715711(2)
4.3	−0.5529131407997(5)	−1.006889728957(10)	824.92(6)	0.023008500600(2)
4.4	−0.5506740365522(4)	−1.005568581031(6)	911.17(6)	0.0217680663662(3)
4.5	−0.5485607797348(5)	−1.004916995595(8)	992.02(6)	0.020489903069(2)
4.6	−0.5465777165616(6)	−1.00501117204(2)	1051.50(6)	0.019161795888(3)
4.7	−0.5447306011234(8)	−1.00594996581(2)	1059.32(6)	0.017768348177(4)
4.8	−0.5430266389667(7)	−1.00782388303(2)	963.10(6)	0.016297790604(5)
4.9	−0.5414733490509(6)	−1.01062378962(2)	685.55(6)	0.014759777241(3)
5.0	−0.5400749910519(6)	−1.014074535172(2)	145.39(6)	0.0132150893864(2)

Table A55: Same as for Table A1, but for $8\,^1\Pi_u$.

$8\,^1\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46567830347(5)	−1.4523245629(7)	2.06(3)	−0.5209679560(6)
1.1	−0.51030446184(3)	−1.4379972039(4)	2.47(5)	−0.3794438911(3)
1.2	−0.54286777927(2)	−1.4183467477(3)	2.96(3)	−0.2771759910(2)
1.3	−0.56663459201(2)	−1.3957324469(2)	3.49(3)	−0.20189481759(7)
1.4	−0.58387826910(3)	−1.3716590807(2)	4.02(2)	−0.14564467320(9)
1.5	−0.59621877325(5)	−1.3470967057(2)	4.66(2)	−0.10310610610(8)
1.6	−0.60483367532(4)	−1.3226730266(2)	5.39(2)	−0.07062854745(6)
1.7	−0.61059366024(3)	−1.2987925145(2)	6.19(2)	−0.04565011413(4)
1.8	−0.61415202231(3)	−1.27571197251(10)	7.06(4)	−0.02633773771(4)
1.9	−0.61600522722(2)	−1.25358946035(10)	8.05(2)	−0.01135737153(3)
2.0	−0.61653477479(2)	−1.23251651925(9)	9.13(3)	0.00027651516(3)
2.1	−0.61603668343(2)	−1.21253970428(9)	10.32(3)	0.00930174409(3)
2.2	−0.61474260463(2)	−1.19367514259(8)	11.61(3)	0.01627730303(3)
2.3	−0.61283516999(2)	−1.17591846931(8)	13.03(4)	0.02163124812(3)
2.4	−0.61045929617(2)	−1.15925165574(8)	14.58(4)	0.02569455692(2)
2.5	−0.60773061337(2)	−1.14364772326(8)	16.27(4)	0.02872540139(2)
2.6	−0.60474181821(2)	−1.12907400305(8)	18.12(4)	0.03092678207(2)
2.62	−0.60411968395(2)	−1.12627974818(8)	18.51(4)	0.03128229760(2)
2.64	−0.60349069649(2)	−1.12352496304(8)	18.91(4)	0.03161228407(2)
2.66	−0.60285535567(2)	−1.12080934478(8)	19.32(4)	0.03191780698(2)
2.68	−0.60221414050(2)	−1.11813258843(9)	19.73(4)	0.03219988529(2)
2.7	−0.60156751005(2)	−1.11549438714(9)	20.15(4)	0.03245949369(2)
2.72	−0.60091590435(5)	−1.1128944327(3)	20.54(8)	0.03269756471(6)
2.74	−0.60025974508(2)	−1.11033241499(9)	21.01(4)	0.03291499094(2)
2.76	−0.59959943661(2)	−1.10780802388(9)	21.45(4)	0.03311262657(2)
2.78	−0.59893536649(2)	−1.10532094780(9)	21.90(4)	0.03329128963(2)
2.8	−0.59826790628(2)	−1.10287087482(9)	22.36(5)	0.03345176348(2)
2.82	−0.59759741220(2)	−1.10045749264(9)	22.83(5)	0.03359479850(2)
2.84	−0.59692422579(2)	−1.09808048883(9)	23.30(5)	0.03372111365(2)
2.86	−0.59624867452(2)	−1.09573955096(10)	23.78(5)	0.03383139793(2)
2.88	−0.59557107234(2)	−1.09343436675(10)	24.27(5)	0.03392631178(2)
2.9	−0.59489172029(2)	−1.09116462425(10)	24.77(5)	0.03400648839(2)
2.92	−0.59421090700(2)	−1.08893001192(10)	25.28(5)	0.03407253495(2)
2.94	−0.59352890920(2)	−1.08673021881(10)	25.80(5)	0.03412503387(2)
2.96	−0.59284599223(3)	−1.08456493461(10)	26.33(5)	0.03416454387(2)
2.98	−0.59216241046(3)	−1.08243384976(10)	26.87(5)	0.03419160106(3)
3.0	−0.59147840777(3)	−1.08033665556(2)	27.41(5)	0.03420671999(3)
3.1	−0.58805993239(3)	−1.0703483086(2)	30.29(6)	0.03411985684(4)
3.2	−0.58466216273(3)	−1.0611615281(2)	33.41(5)	0.03380087418(3)
3.3	−0.58130598412(3)	−1.0527390299(2)	36.85(5)	0.03329482980(3)
3.4	−0.57800818845(3)	−1.0450443836(2)	40.63(4)	0.03263882156(4)
3.5	−0.57478219031(6)	−1.0380420422(8)	44.74(3)	0.0318635253(2)
3.6	−0.57163860600(7)	−1.031697335(2)	49.27(4)	0.0309944103(3)
3.7	−0.56858572411(4)	−1.0259764417(2)	54.26(7)	0.03005270446(3)
3.8	−0.56562988983(4)	−1.0208463617(2)	59.70(8)	0.02905616263(3)
3.9	−0.5627758203(2)	−1.016274873(3)	65.6(2)	0.0280196839(5)
4.0	−0.56002686403(5)	−1.0122304968(3)	72.17(8)	0.02695580782(5)
4.1	−0.55738521751(5)	−1.0086824876(3)	79.36(8)	0.02587510913(5)

4.2	−0.55485210355(5)	−1.0056008055(4)	87.30(8)	0.02478652418(5)
4.3	−0.55242792236(6)	−1.0029561239(4)	96.04(8)	0.02369760949(6)
4.4	−0.55011237856(6)	−1.0007198410(4)	105.62(7)	0.02261475367(6)
4.5	−0.54790458895(6)	−0.9988641071(4)	116.35(9)	0.02154334908(7)
4.6	−0.54580317501(7)	−0.9973618651(5)	128.18(9)	0.02048793150(7)
4.7	−0.54380634259(7)	−0.9961869048(5)	141.29(9)	0.01945229371(8)
4.8	−0.54191195154(7)	−0.9953139296(5)	155.85(9)	0.01843957782(8)
4.9	−0.54011757683(8)	−0.9947186375(6)	172.08(10)	0.01745235024(8)
5.0	−0.53842056299(8)	−0.9943778175(6)	190.19(10)	0.01649266170(8)

Table A56: Same as for Table A1, but for $9\,^1\Pi_u$.

		$9\,^1\Pi_u$		
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46550306650(2)	−1.4517872991(2)	−2396.3(8)	−0.5207811661(2)
1.1	−0.51011025087(2)	−1.4373970917(2)	−2434.60(2)	−0.37925144539(9)
1.2	−0.54265410020(2)	−1.4176833597(2)	−2470.6(10)	−0.27697929940(8)
1.3	−0.56640108601(4)	−1.4(9)	−2503.15(2)	−0.2(7)
1.4	−0.58362470168(2)	−1.3708699925(2)	−2533.4(6)	−0.14544327795(6)
1.5	−0.59594502498(2)	−1.3462461422(2)	−2558.75(3)	−0.10290406152(6)
1.6	−0.60453973313(2)	−1.3217624708(2)	−2582.40(2)	−0.07042687786(8)
1.7	−0.61027960981(6)	−1.2978238321(5)	−2603.60(2)	−0.0454497720(3)
1.8	−0.61381804133(2)	−1.2746873834(2)	−2622.513(8)	−0.02613961154(5)
1.9	−0.61565157927(2)	−1.2525115141(2)	−2639.383(5)	−0.01116229242(5)
2.0	−0.61616180398(2)	−1.2313880731(2)	−2654.37(2)	0.00046776745(6)
2.1	−0.61564480947(2)	−1.2113639030(2)	−2667.572(5)	0.00948843616(5)
2.2	−0.61433231845(2)	−1.1924554008(2)	−2679.134(4)	0.01645874367(5)
2.3	−0.61240702966(3)	−1.8(7)	−2689.15(2)	−0.3(3)
2.4	−0.61001392314(2)	−1.1579552679(2)	−2697.655(3)	0.02586357432(5)
2.5	−0.6072686890(2)	−1.142319083(2)	−2704.76(2)	0.0288873180(4)
2.6	−0.6042640801(2)	−1.127717427(2)	−2710.45(2)	0.0310810511(4)
2.62	−0.60363887629(5)	−1.1249181188(4)	−2711.415(6)	0.0314349747(2)
2.64	−0.60300685138(5)	−1.1221584620(4)	−2712.3325(5)	0.0317633488(2)
2.66	−0.60236850556(2)	−1.1194381547(2)	−2713.189(2)	0.03206723926(5)
2.68	−0.60172431827(7)	−1.1167568933(6)	−2714.004(7)	0.0323476654(2)
2.7	−0.6010747488(5)	−1.114114371(4)	−2714.77(2)	0.0326056026(10)
2.72	−0.60042023784(3)	−1.1115102825(2)	−2715.4509(10)	0.03284198279(5)
2.74	−0.59976120730(3)	−1.1089443180(2)	−2716.095(2)	0.03305769949(6)
2.76	−0.59909806191(3)	−1.1064161683(2)	−2716.6848(10)	0.03325360707(6)
2.78	−0.59843118961(3)	−1.1039255230(2)	−2717.2195(10)	0.03343052380(6)
2.8	−0.59776096233(3)	−1.1014720713(2)	−2717.6991(10)	0.03358923335(6)
2.82	−0.59708773665(3)	−1.0990555017(3)	−2718.1238(10)	0.03373048639(6)
2.84	−0.59641185445(3)	−1.0966755027(3)	−2718.4933(10)	0.03385500218(6)
2.86	−0.59573364354(3)	−1.0943317628(3)	−2718.8075(10)	0.03396347003(6)
2.88	−0.59505341823(6)	−1.0920239705(5)	−2719.071(5)	0.0340565507(2)
2.9	−0.59437147987(3)	−1.0897518145(3)	−2719.2693(10)	0.03413487766(6)
2.92	−0.59368811742(3)	−1.0875149841(3)	−2719.417(2)	0.03419905846(7)
2.94	−0.59300360795(3)	−1.0853131690(3)	−2719.508(2)	0.03424967582(7)
2.96	−0.59231821708(3)	−1.0831460594(3)	−2719.543(2)	0.03428728877(7)
2.98	−0.59163219951(4)	−1.0810133463(3)	−2719.522(2)	0.03431243380(7)
3.0	−0.59094579941(4)	−1.0789147215(3)	−2719.443(2)	0.03432562577(8)
3.1	−0.5875159230(2)	−1.068922200(2)	−2718.207(10)	0.0342289182(4)
3.2	−0.58410775259(6)	−1.0597362187(5)	−2715.49(2)	0.0338997770(2)
3.3	−0.58074220283(6)	−1.0513194801(5)	−2711.260(5)	0.0333833108(2)
3.4	−0.5774360890(3)	−1.043635484(3)	−2705.66(9)	0.0327166746(5)
3.5	−0.5742028431(5)	−1.036648558(4)	−2698.097(9)	0.0319306082(8)
3.6	−0.5710530923(4)	−1.030323836(4)	−2689.041(8)	0.0310506523(7)
3.7	−0.5679951287(9)	−1.024627235(7)	−2678.5(2)	0.030098114(2)
3.8	−0.5650352908(4)	−1.019525387(4)	−2665.716(8)	0.0290908406(6)
3.9	−0.5621782821(4)	−1.014985627(3)	−2651.46(6)	0.0280438302(6)
4.0	−0.5594274255(4)	−1.010975914(3)	−2635.1(5)	0.0269697343(6)
4.1	−0.5567848796(4)	−1.007464814(3)	−2616.95(2)	0.0258792548(5)

4.2	−0.5542518166(4)	−1.004421471(3)	−2596.874(6)	0.0247814672(5)
4.3	−0.5518285714(4)	−1.001815588(3)	−2574.813(3)	0.0236840824(5)
4.4	−0.5495147670(4)	−0.999617439(3)	−2550.78(2)	0.0225936579(4)
4.5	−0.5473094211(4)	−0.997797885(3)	−2524.76(4)	0.0215157683(4)
4.6	−0.5452110376(9)	−0.996328426(8)	−2496.81(3)	0.020455141(2)
4.7	−0.5432176835(4)	−0.995181250(2)	−2466.8(2)	0.0194157695(3)
4.8	−0.5413270630(4)	−0.994329397(2)	−2434.879(8)	0.0184009851(3)
4.9	−0.5395365750(4)	−0.993746873(2)	−2400.947(9)	0.0174135258(3)
5.0	−0.5378433740(3)	−0.993408947(2)	−2364.894(9)	0.0164555602(2)

Table A57: Same as for Table A1, but for $10\,^1\Pi_u$.

$10\,^1\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.461999858085(3)	−1.444978033902(5)	10.15(2)	−0.520978317734(2)
1.1	−0.506627107566(2)	−1.430655109869(4)	11.857(3)	−0.3794553588519(3)
1.2	−0.5391916292234(9)	−1.411009598434(4)	13.770(4)	−0.277188616656(2)
1.3	−0.5629597649249(8)	−1.388400790097(5)	15.920(4)	−0.201908661728(3)
1.4	−0.5802048902330(8)	−1.364333508731(6)	18.332(4)	−0.145659805903(4)
1.5	−0.5925469754198(8)	−1.339777863607(7)	21.020(6)	−0.103122608511(4)
1.6	−0.6011636000736(10)	−1.315361621393(7)	24.017(8)	−0.070646513278(4)
1.7	−0.606925459196(2)	−1.291489326192(7)	27.351(10)	−0.045669651647(3)
1.8	−0.610485858752(2)	−1.268417867275(7)	31.05(2)	−0.026358972095(3)
1.9	−0.612341277888(2)	−1.246305406269(5)	35.16(3)	−0.011380447627(2)
2.0	−0.6128732320463(5)	−1.225243605129(5)	39.7840(3)	0.000251429482(2)
2.1	−0.612377757731(2)	−1.205279162255(6)	44.767(8)	0.009274453908(2)
2.2	−0.61108652748106(6)	−1.186428375531(2)	50.438(4)	0.0162475815594(9)
2.3	−0.6091821974003(10)	−1.168687083879(4)	56.63(2)	0.021598830834(3)
2.4	−0.6068097127908(2)	−1.1520375029451(3)	63.543(4)	0.0256591344316(3)
2.5	−0.604084737385(2)	−1.136452948211(4)	71.16(2)	0.028686610621(3)
2.6	−0.60110000723287(10)	−1.1219011063026(10)	79.680(2)	0.0308841954474(3)
2.62	−0.60047873284324(10)	−1.1191115636368(9)	81.486(2)	0.0312388939121(3)
2.64	−0.59985062179842(9)	−1.1163616115596(9)	83.330(2)	0.0315680424383(3)
2.66	−0.59921617436969(9)	−1.1136509512760(9)	85.213(2)	0.0318727058133(3)
2.68	−0.59857587000232(8)	−1.1109792819896(9)	87.136(2)	0.0321539022444(3)
2.7	−0.59793016822415(8)	−1.1083463012384(8)	89.100(2)	0.0324126056333(3)
2.72	−0.59727950951004(8)	−1.1057517052052(8)	91.106(2)	0.0326497477260(3)
2.74	−0.59662431610443(8)	−1.1031951890064(8)	93.155(2)	0.0328662201469(3)
2.76	−0.59596499280437(7)	−1.1006764469580(8)	95.248(2)	0.0330628763227(3)
2.78	−0.59530192770510(7)	−1.0981951728236(8)	97.3865(10)	0.0332405333045(3)
2.8	−0.5946354929102(3)	−1.095751060045(5)	99.565(4)	0.033399973491(2)
2.82	−0.59396604520785(7)	−1.0933438019450(8)	101.8016(9)	0.0335419462564(2)
2.84	−0.59329392671614(5)	−1.0909730919418(6)	104.071(8)	0.0336671695389(2)
2.86	−0.59261946549723(6)	−1.0886386237141(8)	106.4097(8)	0.0337763312169(3)
2.88	−0.59194297614342(6)	−1.0863400913749(8)	108.7890(7)	0.0338700905944(3)
2.9	−0.591264760335(4)	−1.084077189646(10)	111.14(3)	0.0339490796632(7)
2.92	−0.59058510738006(6)	−1.0818496139159(8)	113.7043(6)	0.0340139043987(3)
2.94	−0.58990429471008(5)	−1.0796570605419(6)	116.241(2)	0.0340651458769(2)
2.96	−0.589222588379(3)	−1.07749922684(2)	118.836(2)	0.034103361456(8)
2.98	−0.58854024352105(6)	−1.0753758111187(8)	121.4880(5)	0.0341290858803(3)
3.0	−0.587857504793(4)	−1.07328651311343(10)	124.13(3)	0.034142832153(3)
3.1	−0.58444578460337(10)	−1.063341371517(2)	138.659(2)	0.0340484508678(6)
3.2	−0.581055583036(2)	−1.05420496865(2)	154.80(2)	0.033720686692(5)
3.3	−0.5777079253614(3)	−1.045841616915(4)	172.915(3)	0.033204313275(2)
3.4	−0.5744197756790(3)	−1.038216931874(5)	193.178(3)	0.032536064554(2)
3.5	−0.5712047622179(3)	−1.031298015430(6)	215.907(4)	0.031746145430(2)
3.6	−0.5680737689576(4)	−1.025053668743(7)	241.432(4)	0.030859408103(2)
3.7	−0.56503542351(9)	−1.0194546805(2)	270.09(2)	0.02989626120(2)
3.8	−0.5620965049904(5)	−1.01447424917(2)	302.313(3)	0.028873358108(3)
3.9	−0.5592622939741(6)	−1.01008862626(2)	338.408(4)	0.027804092740(4)
4.0	−0.5565368804416(5)	−1.00627810396(2)	378.652(3)	0.026698914230(3)
4.1	−0.5539234507250(9)	−1.00302854958(3)	423.080(5)	0.025565451681(5)

4.2	−0.551424572216(2)	−1.00033379092(3)	471.162(5)	0.024408417502(6)
4.3	−0.5490425012002(6)	−0.99819930629(5)	521.221(5)	0.02322923165(2)
4.4	−0.546779545213(3)	−0.99664778457(8)	569.216(4)	0.02202529678(2)
4.5	−0.544638516025(10)	−0.9957268564(3)	606.340(5)	0.02078892792(5)
4.6	−0.54262329335(2)	−0.9955173750(3)	614.497(3)	0.01950635036(5)
4.7	−0.54073941775(3)	−0.9961331081(7)	558.608(6)	0.0181586654(2)
4.8	−0.53899426835(4)	−0.9976812629(8)	377.503(6)	0.0167306821(2)
4.9	−0.53739549288(4)	−1.000119314(3)	−12.382(6)	0.0152391167(5)
5.0	−0.53594547592(10)	−1.002990923(2)	−663.270(10)	0.0137800058(2)

Table A58: Same as for Table A1, but for $1\,^3\Pi_u$ (c state) .

$1\,^3\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.123843086498093(2)	–	64572.425024(4)	–
0.01	97.86709492124(2)	95.73470285376(9)	64585.06318(3)	−9999.948698872(7)
0.05	17.8728183563(2)	15.756952570(2)	64860.67829(6)	−399.77328286(3)
0.1	7.88842353645(6)	5.8156116724(9)	65603.91522(5)	−99.612154006(7)
0.15	4.5774293771(5)	2.562944028(4)	66657.392(2)	−43.94609817(2)
0.2	2.937639120191(10)	0.98961256543(9)	67915.9848(10)	−24.4283283748(4)
0.3	1.3324174365043(7)	−0.47534337084(2)	70761.19780(2)	−10.46719414615(5)
0.4	0.5645364079553(2)	−1.107561169738(7)	73733.01047(2)	−5.59153496412(2)
0.5	0.1298272808145(2)	−1.418323094452(5)	76602.419188(10)	−3.355915312162(7)
0.6	−0.14043207358477(8)	−1.578002013033(3)	79239.842496(7)	−2.161863109772(4)
0.7	−0.318618175318982(10)	−1.658456709946(6)	81575.610(2)	−1.458886227582(4)
0.8	−0.440774586238020(4)	−1.69448898162579(5)	83578.02105(7)	−1.016174761442(4)
0.9	−0.5267938790676480(2)	−1.704553656081(4)	85239.9819(2)	−0.723295442164(5)
1.0	−0.5884651352607144(2)	−1.6990808718222(9)	86570.3074(3)	−0.522150601302(2)
1.1	−0.63317350636365122(7)	−1.6842474227727(10)	87587.771077(7)	−0.379909463678(2)
1.2	−0.66574870265886954(10)	−1.6638418158373(3)	88316.97630(3)	−0.2769536754333(5)
1.3	−0.68946043541486091(6)	−1.6402499598424(2)	88785.47514(3)	−0.2010223761637(3)
1.4	−0.70658615416404380(6)	−1.61500405128016(2)	89021.78568(4)	−0.14416553068014(7)
1.5	−0.71875035217035077(7)	−1.58910139498553(5)	89054.06279(2)	−0.10106712709657(3)
1.6	−0.72713538673373312(6)	−1.56319614059885(5)	88909.244594(8)	−0.068078354457113(7)
1.7	−0.73261683909347919(6)	−1.53771799311280(8)	88612.541423(6)	−0.04263783230930(2)
1.8	−0.73585290173154405(8)	−1.5129475405081(2)	88187.167435(5)	−0.02291207613610(7)
1.9	−0.73734486220859607(7)	−1.4890650647139(2)	87654.240729(4)	−0.00756596857721(6)
2.0	−0.73747891123618292(5)	−1.4661827411580(2)	87032.796807(2)	0.00438754065720(5)
2.1	−0.73655559047517172(8)	−1.4443662061127(2)	86339.875093(3)	0.01368808325602(7)
2.2	−0.73481088429473340(6)	−1.4236491890151(2)	85590.649687(3)	0.02089662707928(7)
2.3	−0.73243155451833786(9)	−1.4040435449615(3)	84798.5838315(9)	0.02644328872833(9)
2.4	−0.72956644077963539(8)	−1.3855461904592(3)	83975.594054(2)	0.03066112129173(9)
2.5	−0.72633488990980888(10)	−1.3681439263878(4)	83132.2143823(8)	0.03381034137273(10)
2.6	−0.72283311357693170(7)	−1.3518168021408(3)	82277.754425(2)	0.03609593269734(8)
2.7	−0.71913903175379168(9)	−1.3365404615788(4)	81420.447444(3)	0.03768059330696(10)
2.8	−0.7153159965322639(2)	−1.3222877713946(6)	80567.5860983(7)	0.0386943648821(2)
2.9	−0.7114156790624591(2)	−1.3090299392872(6)	79725.644681(2)	0.0392418685648(2)
3.0	−0.7074803247316160(2)	−1.2967372665477(6)	78900.387381(4)	0.0394077943052(2)
3.1	−0.7035445270119220(2)	−1.2853796368801(7)	78096.962483(3)	0.0392611023045(2)
3.2	−0.6996366314351171(2)	−1.2749268138770(7)	77319.982743(5)	0.0388582653104(2)
3.3	−0.6957798530696988(2)	−1.2653485992047(8)	76573.592347(5)	0.0382457899802(2)
3.4	−0.6919931704330150(2)	−1.2566148893943(9)	75861.520798(9)	0.0374621916094(2)
3.5	−0.6882920437468887(2)	−1.248695659282(2)	75187.124362(9)	0.0365395509176(3)
3.6	−0.6846889943089719(3)	−1.241560893329(2)	74553.415471(7)	0.0355047486914(3)
3.7	−0.6811940734319673(3)	−1.235180481387(2)	73963.080832(7)	0.0343804501291(3)
3.8	−0.6778152431428819(3)	−1.229524092390(2)	73418.48894(2)	0.0331858931305(3)
3.9	−0.6745586860948836(3)	−1.224561037471(2)	72921.687934(5)	0.0319375217227(4)
4.0	−0.6714290585358247(3)	−1.220260132796(2)	72474.394808(7)	0.0306494960689(3)
4.1	−0.668419697416228(2)	−1.216589571777470(10)	72077.977748200(5)	0.029329225135362(2)
4.2	−0.665552790595878(2)	−1.213516815938344(10)	71733.432921185(5)	0.027997325060336(2)
4.3	−0.662819517465230(2)	−1.211008513393224(10)	71441.358223023(6)	0.026658260822613(2)
4.4	−0.660220166016223(2)	−1.20903045352423(2)	71201.92614520(2)	0.025320426933686(3)

4.5	−0.6577642313845241(4)	−1.207547565652(3)	71014.85859(2)	0.0239957549149(4)
4.6	−0.655420500069249(2)	−1.20652396828002(2)	70879.40653889(2)	0.022677615621408(3)
4.7	−0.653217123359737(2)	−1.20592307366320(2)	70794.33710810(2)	0.021385355969420(3)
4.8	−0.651141682917086(3)	−1.20570774991040(2)	70757.93112519(2)	0.020119919984119(3)
4.9	−0.649191250937030(3)	−1.20584053977854(2)	70767.99287316(2)	0.018886114713372(3)
5.0	−0.6473724468364923(6)	−1.206283931723(4)	70821.87377(2)	0.0176921923901(5)
5.1	−0.645651491944746(3)	−1.20700067505292(2)	70916.51063896(2)	0.016529864477760(3)
5.2	−0.644054263236758(3)	−1.20795412753332(2)	71048.47768681(2)	0.015414307488499(3)
5.3	−0.642566346724458(3)	−1.20910862073727(2)	71214.05152150(2)	0.014344164662575(3)
5.4	−0.641183090731343(3)	−1.21042982656531(2)	71409.28595620(2)	0.013321547203217(3)
5.5	−0.6399096589310119(7)	−1.2118851076(2)	71630.09374(8)	0.01235167459(2)
5.6	−0.638711082746008(3)	−1.21344383419598(2)	71872.33190288(2)	0.011424702017150(2)
5.7	−0.637612312492567(3)	−1.21507765497993(2)	72131.88489906(2)	0.010552100000914(2)
5.8	−0.636598266527892(3)	−1.21676070722305(2)	72404.74485478(2)	0.009730314798748(2)
5.9	−0.635663877610870(3)	−1.21846976189146(2)	72687.08246249(2)	0.008958981920386(2)
6.0	−0.6348141357193404(9)	−1.22018429918(7)	72975.30770(6)	0.008240662047(8)
6.5	−0.631458245403886(10)	−1.22830667405602(5)	74400.83955026(2)	0.005324587192577(4)
7.0	−0.629313556242347(5)	−1.234912514982(2)	75621.69638(3)	0.003390656784(2)
7.5	−0.627950934798369(6)	−1.239758606917(7)	76540.66137(2)	0.002155101689(3)
8.0	−0.627091405366481(8)	−1.243109576993(6)	77176.083217(10)	0.001384154217(2)
8.5	−0.626528240798876(7)	−1.245351849010(2)	77589.876500(8)	0.000906427363(2)
9.0	−0.626155135224279(5)	−1.24682787628977(10)	77846.947399(3)	0.00060915490650(4)
9.5	−0.625900908966620(2)	−1.247794296651(4)	77999.899097(7)	0.0004218443453(5)
10.0	−0.6257222116757563(9)	−1.248428790364(3)	78086.602799(6)	0.0003015632987(4)
11.0	−0.6254955149381342(2)	−1.249132170440(2)	78154.103490(4)	0.0001689872214(2)
12.0	−0.62536199674893989(4)	−1.2494628008583(7)	78161.053116(2)	0.00010509938661(7)
13.0	−0.62527576869255419(4)	−1.249634289924639(7)	78149.6506828(2)	0.0000690190354204(8)
14.0	−0.62521632296272500(2)	−1.24973329021444(9)	78134.4901374(5)	0.00004995397935(2)
15.0	−0.625173439941072551(5)	−1.24979612121462(7)	78120.1333767(3)	0.000036717244498(7)
16.0	−0.625141481419891787(3)	−1.249839008982235(5)	78107.7245893(2)	0.000027747116094(3)
17.0	−0.625117069157575256(2)	−1.249869855226915(10)	78097.3217796(2)	0.000021428416954(2)
18.0	−0.6250980498764705517(6)	−1.24989288510072(3)	78088.68150160(10)	0.0000168452584580(3)
19.0	−0.6250829872020891020(4)	−1.24991056007342(4)	78081.51129363(9)	0.00001344285951499(9)
20.0	−0.6250708895747465466(2)	−1.24992441784911(4)	78075.54447619(5)	0.00001086806502036(6)

Table A59: Same as for Table A1, but for $2\,^3\Pi_u$ (d state) .

$2\,^3\Pi_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.05514636209194(3)	–	18369.001636(2)	–
0.01	97.9421796391(3)	95.884875471(3)	18371.511(10)	−9999.9483807(2)
0.05	17.947927878(2)	15.907259954(9)	18426.39(2)	−399.7719160(2)
0.1	7.963625847(2)	5.966264626(9)	18572.43(2)	−99.60987068(7)
0.15	4.6527620903(7)	2.714062972(6)	18774.768(9)	−43.94307473(3)
0.2	3.0131368395(4)	1.141263959(4)	19009.168(9)	−24.42504860(2)
0.3	1.4082545724(2)	−0.3225595998(7)	19507.1(2)	−10.463562482(2)
0.4	0.6407387542(2)	−0.953685282(2)	19974.5(2)	−5.587906975(3)
0.5	0.20638302081(8)	−1.2634853360(5)	20363.3(2)	−3.3525027553(6)
0.6	−0.06355156071(9)	−1.4223814891(6)	20652.1(2)	−2.1587972795(6)
0.7	−0.241441962005(9)	−1.50225782108(2)	20835.2(3)	−1.4562484246(2)
0.8	−0.363358090254(4)	−1.53792628057(7)	20916.121(4)	−1.01401262507(7)
0.9	−0.449186022790(5)	−1.54784148556(4)	20902.508(2)	−0.72163271109(3)
1.0	−0.510716296965(4)	−1.54242613630(3)	20805.785(5)	−0.52099354237(2)
1.1	−0.555334013438(3)	−1.52784461499(3)	20637.955(4)	−0.37925144375(2)
1.2	−0.587867720451(3)	−1.50786974158(3)	20410.911(4)	−0.2767785838816(10)
1.3	−0.611585156943(3)	−1.48486975727(3)	20135.845(4)	−0.20130726414(2)
1.4	−0.628761223602(5)	−1.46035818963(3)	19822.905(10)	−0.14488267316(2)
1.5	−0.641017471263(3)	−1.43531339906(3)	19481.089(9)	−0.10218563769(2)
1.6	−0.649533064212(4)	−1.41037083700(3)	19118.167(6)	−0.06956544286(2)
1.7	−0.655180250875(3)	−1.38594211596(3)	18740.769(5)	−0.04445977306(2)
1.8	−0.658613835899(3)	−1.36229057004(3)	18354.478(7)	−0.02503494347(2)
1.9	−0.660331727693(3)	−1.33958020240(3)	17963.955(7)	−0.009956182640(10)
2.0	−0.660716793295(3)	−1.31790794973(3)	17573.029(7)	0.001762818430(10)
2.1	−0.660066339495(3)	−1.29732526324(3)	17184.837(5)	0.010860674168(10)
2.2	−0.658613227342(3)	−1.27785271948(3)	16801.908(7)	0.017897152365(8)
2.3	−0.656541221424(3)	−1.25949000883(3)	16426.294(8)	0.023301058268(5)
2.4	−0.653996298535(5)	−1.24222281450(2)	16059.623(9)	0.027404076072(3)
2.5	−0.651095080745(3)	−1.22602757356(2)	15703.193(9)	0.030465035174(3)
2.6	−0.647931193414(5)	−1.21087477967(2)	15358.025(10)	0.032687541214(3)
2.7	−0.644580106774(5)	−1.19673127239(2)	15024.936(8)	0.034232941168(4)
2.8	−0.641102856483(3)	−1.18356181693(2)	14704.56(2)	0.0352299628710(10)
2.9	−0.637548926592(5)	−1.17133018410(2)	14397.424(3)	0.035781954855(2)
3.0	−0.633958500603(3)	−1.15999987694(2)	14103.939(10)	0.035972374757(2)
3.1	−0.630364231516(3)	−1.14953460686(2)	13824.493(4)	0.035868985863(2)
3.2	−0.626792642633(3)	−1.13989859276(4)	13559.395(7)	0.035527091410(6)
3.3	−0.623265242795(3)	−1.13105673520(2)	13308.978(4)	0.034992045573(2)
3.4	−0.619799419190(3)	−1.12297470366(2)	13073.549(9)	0.034301216094(3)
3.5	−0.616409155765(2)	−1.11561896398(2)	12853.473(9)	0.033485527871(3)
3.6	−0.613105614109(2)	−1.10895676609(2)	12649.127(3)	0.032570683924(3)
3.7	−0.609897605264(2)	−1.10295610648(2)	12460.921(9)	0.031578136229(2)
3.8	−0.606791974614(2)	−1.09758567601(2)	12289.368(3)	0.030525861374(3)
3.9	−0.6037939171736(4)	−1.09281480077(3)	12134.982(9)	0.029428982970(4)
4.0	−0.6009072369177(4)	−1.08861338155(3)	11998.403(9)	0.028300273072(4)
4.1	−0.598134560958(5)	−1.08495183581(2)	11880.307(7)	0.027150557586(2)
4.2	−0.595477517142(6)	−1.08180104482(2)	11781.438(9)	0.025989045111(2)
4.3	−0.592936881957(8)	−1.07913230780(4)	11702.624(7)	0.024823594445(6)
4.4	−0.590512704231(5)	−1.07691730425(2)	11644.732(7)	0.023660932776(2)

4.5	−0.5882044090772(3)	−1.075128065163(6)	11608.686(9)	0.022506834000(2)
4.6	−0.586010885686(5)	−1.07373695361(3)	11595.461(3)	0.021366264730(4)
4.7	−0.583930561864(5)	−1.07271665528(3)	11606.014(3)	0.020243503924(4)
4.8	−0.581961467746(6)	−1.07204017934(3)	11641.326(7)	0.019142240864(2)
4.9	−0.580101290618(5)	−1.07168087052(2)	11702.365(5)	0.018065655247(2)
5.0	−0.5783474225041(2)	−1.07161243331(2)	11790.020(7)	0.01701648233984(8)
5.1	−0.5766970020(3)	−1.071808970(2)	11904.9(2)	0.0159970654(2)
5.2	−0.575146950730(3)	−1.07224503070(2)	12048.412(2)	0.015009398221(4)
5.3	−0.5736940079(3)	−1.072895688(2)	12220.2(2)	0.0140551562(2)
5.4	−0.5723347590(3)	−1.073736612(2)	12421.5(2)	0.0131357234(3)
5.5	−0.5710656654584(8)	−1.074744182712(5)	12652.4334(9)	0.0122522087647(2)
5.6	−0.5698830916(4)	−1.075895615(3)	12912.4(2)	0.0114054585(4)
5.7	−0.5687833285(4)	−1.077169076(4)	13201.9(2)	0.0105960667(4)
5.8	−0.5677626212(5)	−1.078543853(4)	13520.3(2)	0.0098243775(5)
5.9	−0.5668171927(6)	−1.080000495(5)	13867.0(2)	0.0090904898(7)
6.0	−0.5659432672059(5)	−1.081520967019(5)	14241.0570(3)	0.008394261231(2)
6.5	−0.5625171794935(2)	−1.089563721276(6)	16454.7661(3)	0.0054570211863(7)
7.0	−0.5603514813976(4)	−1.09740673438(5)	18803.359(7)	0.003328032631(6)
7.5	−0.5590726874112(7)	−1.1038588192(2)	19665.851(6)	0.00190487409(2)
8.0	−0.558329991536(3)	−1.10731794567(7)	17728.1280(2)	0.001167754676(8)
8.5	−0.5578334410802(8)	−1.10834942525(2)	14765.12633(5)	0.000860877284(2)
9.0	−0.557445192242(3)	−1.10855139169(5)	12217.848(3)	0.000704332533(4)
9.5	−0.5571221417933(3)	−1.108621328762(4)	10285.5101(2)	0.0005918899816(3)
10.0	−0.5568504344795(4)	−1.108728792292(6)	8857.6821(2)	0.0004972076667(4)
11.0	−0.55575951572416(3)	−1.109081112783(3)	7055.1736(9)	0.0003441795112(2)
12.0	−0.5561478551589(2)	−1.109491690365(2)	6152.0789(2)	0.00023366832943(7)
13.0	−0.5559548564812(4)	−1.109866277174(4)	5790.69692(4)	0.0001571873683(2)
14.0	−0.5558252887067(5)	−1.110175681974(4)	5772.8904(2)	0.0001053496742(2)
15.0	−0.5557385144044(2)	−1.110419311221(2)	5990.66169(10)	0.00007051450585(5)
16.0	−0.55568044084928(10)	−1.1106057930895(7)	6393.39937(8)	0.00004719303807(2)
17.0	−0.5556415610819(2)	−1.1107456970544(6)	6970.89257(2)	0.000031613241735(5)
18.0	−0.55561549531781(8)	−1.1108490692914(4)	7742.87643(6)	0.00002121785245928(7)
19.0	−0.55559797845052(8)	−1.1109246018733(3)	8747.82147(9)	0.000014281843561(3)
20.0	−0.55558616842347(5)	−1.11097937283242(7)	10019.95581(10)	0.000009648200715(7)

Table A60: Same as for Table A1, but for $3\,^3\Pi_u$ (k state) .

$3\,^3\Pi_u$				
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.03106965045024(3)	–	7555.17898(1)	–
0.01	97.96793674552(8)	95.9363904275(5)	7555.99(2)	−9999.94830635(3)
0.05	17.973693112(8)	15.95880640(5)	7575.14(10)	−399.7715965(7)
0.1	7.989412601(3)	6.01789097(2)	7625.3(4)	−99.6093424(2)
0.15	4.678578887(4)	2.76579601(3)	7695.50(8)	−43.9424117(2)
0.2	3.038989001(3)	1.19311713(2)	7774.85(7)	−24.42430437(5)
0.3	1.43418496(3)	−0.2704585(3)	7937.72(3)	−10.4627612(8)
0.4	0.6667482922(4)	−0.901357764(3)	8081.459(9)	−5.587135871(5)
0.5	0.23246596(2)	−1.21097412(7)	8187.7(6)	−3.35181209(8)
0.6	−0.03740485663(8)	−1.3697395064(6)	8252.89(2)	−2.1582163219(7)
0.7	−0.215243361937(5)	−1.4495420539(3)	8274.00(2)	−1.4557933285(3)
0.8	−0.337120612874(7)	−1.48519391168(5)	8254.68(3)	−1.01369085741(5)
0.9	−0.422923118196(5)	−1.49514745837(5)	8199.43(4)	−0.72144580220(4)
1.0	−0.484441351024(6)	−1.48982163393(4)	8113.53(4)	−0.52093893188(3)
1.1	−0.529060007460(6)	−1.47537617796(4)	8002.32(5)	−0.37932378458(3)
1.2	−0.561607002378(2)	−1.45557883354(4)	7870.89(5)	−0.27697069064(2)
1.3	−0.585349294188(8)	−1.43279264146(4)	7723.83(6)	−0.20161081006(2)
1.4	−0.602560915761(8)	−1.40852601416(4)	7565.20(6)	−0.14528870189(2)
1.5	−0.614862506795(9)	−1.38375241545(4)	7398.50(7)	−0.102684934569(9)
1.6	−0.623432308595(10)	−1.35910269664(3)	7226.62(7)	−0.070148799656(6)
1.7	−0.62914165701(2)	−1.33498420529(3)	7052.02(7)	−0.045118171335(3)
1.8	−0.63264446963(2)	−1.31165635723(4)	6876.64(8)	−0.025759676653(7)
1.9	−0.63443780313(2)	−1.28927957766(3)	6702.22(8)	−0.010738932319(2)
2.0	−0.63490371402(2)	−1.26794754871(2)	6529.92(8)	0.000929939656(5)
2.1	−0.63433874277(2)	−1.24770876810(2)	6360.83(9)	0.009985103532(6)
2.2	−0.63297502942(2)	−1.22858113806(2)	6195.75(9)	0.016985873064(8)
2.3	−0.63099566281(2)	−1.210561939709(8)	6035.30(9)	0.022360602552(9)
2.4	−0.62854598908(2)	−1.19363472384(4)	5879.89(10)	0.026440522632(2)
2.5	−0.62574204649(2)	−1.177774171737(5)	5730.17(9)	0.029483968477(10)
2.6	−0.62267693381(2)	−1.162949886186(7)	5585.75(9)	0.031693838997(9)
2.7	−0.61942570996(2)	−1.14913183653(2)	5443.78(9)	0.033229475329(4)
2.8	−0.61604970837(2)	−1.1363448521(4)	5240.3(2)	0.03419805881(10)
2.9	−0.6126373276449(9)	−1.1273877072(6)	1025.496(8)	0.0337541200(3)
3.0	−0.6092565809066(3)	−1.1169704761(2)	686.8614(6)	0.03384756185(6)
3.1	−0.6058760067337(2)	−1.107215086305(6)	728.1328(2)	0.033721589406(3)
3.2	−0.6025200367719(2)	−1.098279992182(2)	804.50572(7)	0.033362525425(2)
3.3	−0.5992098882292(2)	−1.090141364550(6)	899.20881(2)	0.0328116399726(8)
3.4	−0.59596291148758(9)	−1.08277065421(2)	1010.58055(3)	0.032104461401(3)
3.5	−0.59279322541713(7)	−1.076140686200(10)	1139.96220(3)	0.031270218466(3)
3.6	−0.58971230473326(7)	−1.070226837631(5)	1289.98488(2)	0.0303327143988(10)
3.7	−0.58672948045000(7)	−1.065007739046(6)	1464.27461(6)	0.029311141042(2)
3.8	−0.58385236783512(7)	−1.0604660320200(4)	1667.510(2)	0.028220711486(2)
3.9	−0.58108724022858(7)	−1.056589342884(5)	1905.53(4)	0.027073112197(2)
4.0	−0.57843936615047(9)	−1.05337158460(2)	2186.20482(9)	0.025876786926(4)
4.1	−0.575913326058(2)	−1.05081470268(3)	2518.7772(8)	0.024637060838(6)
4.2	−0.573513324467(2)	−1.04893098751(3)	2915.543(2)	0.023356109864(6)
4.3	−0.571243512561(7)	−1.0477460526(2)	3391.7(2)	0.02203278429(6)
4.4	−0.569108334546(3)	−1.04730246712(6)	3967.671(3)	0.02066231863(2)

4.5	−0.5671129053971(4)	−1.04766372527(6)	4666.929(3)	0.01923601901(2)
4.6	−0.565263411923(5)	−1.0489174690(2)	5519.01(6)	0.01774116408(3)
4.7	−0.563567493774(7)	−1.0511753560(2)	6557.4919(2)	0.01616162374(4)
4.8	−0.56203448904(2)	−1.0545642493(5)	7815.4358(6)	0.01448015183(9)
4.9	−0.56067530774(2)	−1.0591999694(3)	9317.460(2)	0.01268380532(6)
5.0	−0.559501546185(2)	−1.0651338718(3)	11063.43(2)	0.01077384411(4)
5.1	−0.55852340305(3)	−1.0722723195(2)	13007.53(7)	0.00877931109(5)
5.2	−0.55774628400(3)	−1.08029864685(10)	15042.66(6)	0.00676806175(3)
5.3	−0.55716691445(3)	−1.088663240174(10)	17006.75(5)	0.004843507293(10)
5.4	−0.55677086362(3)	−1.09669587688(9)	18722.96(4)	0.003119601917(9)
5.5	−0.556533310016(2)	−1.10380226580(3)	20054.675(10)	0.001684428042(3)
5.6	−0.55642303456(3)	−1.1096214112(3)	20940.17(3)	0.00057583178(4)
5.7	−0.55640761437(3)	−1.1140575306(4)	21390.23(2)	−0.00021794769(5)
5.8	−0.55645756958(4)	−1.1172097784(5)	21460.84(2)	−0.00074045504(6)
5.9	−0.55654851161(4)	−1.1192746870(5)	21224.60(2)	−0.00104706166(7)
6.0	−0.5566615832277(4)	−1.120471693419(5)	20751.9800(10)	−0.0011914211605(5)
6.5	−0.5571976881284(5)	−1.119337563057(6)	16549.4090(4)	−0.0007603364306(6)
7.0	−0.5573678766096(5)	−1.114291796186(5)	11685.406468(10)	0.0000634224333(3)
7.5	−0.5571787286781(3)	−1.1096549596025(5)	8572.7378(2)	0.0006269997002(2)
8.0	−0.5568167473350(2)	−1.1076182605094(10)	8607.9430(6)	0.0007519042699(3)
8.5	−0.5564710224949(2)	−1.107746149547(5)	9977.6354(5)	0.0006112818163(9)
9.0	−0.55621022322396(10)	−1.1084979781440(10)	11194.4591(7)	0.0004358298114(2)
9.5	−0.5560284445625(4)	−1.109217355762(3)	12019.8866(7)	0.0002988982484(5)
10.0	−0.55590423140963(5)	−1.1097665061842(6)	12531.0757(7)	0.00020419566346(9)
11.0	−0.55575951572416(3)	−1.1104239175269(3)	12959.4769(2)	0.00009955581098(6)
12.0	−0.55568609559565(2)	−1.1107324734532(3)	12948.9260(4)	0.00005330981150(3)
13.0	−0.55564496618165(2)	−1.1108806943325(5)	12715.79383(3)	0.00003147984851(5)
14.0	−0.555619726267830(10)	−1.1109576365463(2)	12355.235372(3)	0.00002012971352(2)
15.0	−0.555603120814325(8)	−1.11100171972292(5)	11902.07027(8)	0.000013634793710(7)
16.0	−0.555591642141235(10)	−1.11102932956862(3)	11356.2501(3)	0.000009622169611(4)
17.0	−0.555583416701015(2)	−1.11104774440(3)	10693.864(6)	0.000007005231(3)
18.0	−0.55557735193609(2)	−1.1110604726(2)	9872.84(2)	0.000005235066(2)
19.0	−0.55557276709809(2)	−1.1110693993(4)	8840.42(6)	0.000004007098(4)
20.0	−0.55556921894044(2)	−1.1110756876(9)	7553.4(2)	0.00000313751(2)

Table A61: Same as for Table A1, but for $4\,^3\Pi_u$ (ka state).

$4\,^3\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.031255144381749(1)	–	9.6696396	–
0.01	97.96900618942(5)	95.9385298243(3)	9.671(3)	−9999.94825545(2)
0.05	17.974768101(3)	15.96096723(2)	9.797(5)	−399.7713795(2)
0.1	7.990502264(5)	6.02010620(3)	10.160(6)	−99.6089833(2)
0.15	4.679688825(7)	2.76808275(5)	10.722(4)	−43.9419660(3)
0.2	3.040122589(3)	1.19548329(2)	11.463(4)	−24.42380941(5)
0.3	1.4353698795(4)	−0.267933132(2)	11.3(5)	−10.462242970(2)
0.4	0.667983504(2)	−0.898695376(10)	15.8(3)	−5.58665596(2)
0.5	0.23374572287(9)	−1.2082112364(8)	19.16(7)	−3.351405364(2)
0.6	−0.03608894287(4)	−1.3669192657(3)	23.04(8)	−2.1579022999(4)
0.7	−0.213901128076(6)	−1.44670967544(5)	27.69(4)	−1.45558202755(5)
0.8	−0.335762565642(3)	−1.48239404759(3)	33.02(2)	−1.01358614538(3)
0.9	−0.4215599335484(10)	−1.49242259240(3)	39.133(9)	−0.72144747256(2)
1.0	−0.4830835402668(2)	−1.48721116854(2)	46.099(7)	−0.52104408800(2)
1.1	−0.5277176991384(6)	−1.47291598011(2)	53.994(6)	−0.37952780167(2)
1.2	−0.5602898055072(3)	−1.45330108893(2)	62.904(5)	−0.277267898262(9)
1.3	−0.5840662193884(8)	−1.43072591192(2)	72.922(5)	−0.201994979341(8)
1.4	−0.6013203377653(5)	−1.40669542353(2)	84.154(5)	−0.145753391430(7)
1.5	−0.61367215601928(8)	−1.382179911621(8)	96.719(5)	−0.103223733054(4)
1.6	−0.62229928302782(7)	−1.357807353976(5)	110.751(5)	−0.070755492449(2)
1.7	−0.62807244783221(4)	−1.333982543620(4)	126.399(5)	−0.045786851738(2)
1.8	−0.63164499585127(5)	−1.310962662578(5)	143.839676(3)	−0.026484817153(3)
1.9	−0.63351345185437(10)	−1.288906215923(5)	163.25155(9)	−0.011515427481(3)
2.0	−0.63405938392257(5)	−1.267905267247(4)	184.848(6)	0.000106750299(2)
2.1	−0.63357888915233(7)	−1.248006982407(6)	208.887(8)	0.009119426618(2)
2.2	−0.63230370955222(4)	−1.229228198672(5)	235.640(5)	0.016081463833(2)
2.3	−0.6304165804424(5)	−1.211565366088(5)	265.41421(2)	0.021420780347(2)
2.4	−0.6280625362610(7)	−1.195001360578(2)	298.553(5)	0.025468213309(4)
2.5	−0.62535733780281(10)	−1.179510101449(10)	335.5333(7)	0.028481829663(4)
2.6	−0.6223938153247(3)	−1.16505933598(2)	377.18558(2)	0.030664728719(7)
2.7	−0.6192466480779(8)	−1.15160975853(6)	427.27644(4)	0.03217908801(2)
2.8	−0.6159754877121(7)	−1.1390636818(5)	550.437(2)	0.0331740335(2)
2.9	−0.61258993159(2)	−1.1245481385(3)	4697.85(10)	0.0347005946(2)
3.0	−0.60910147533(2)	−1.113279029676(5)	4982.86(8)	0.034974640313(10)
3.1	−0.60560614404(2)	−1.10306161859(3)	4902.78(10)	0.034887312724(6)
3.2	−0.60213193105(2)	−1.093666570131(6)	4804.30(9)	0.034561653684(8)
3.3	−0.59870014421(2)	−1.085049290070(8)	4705.82(7)	0.034045757009(8)
3.4	−0.59532785642(2)	−1.07717277441(4)	4610.73(3)	0.033377334831(4)
3.5	−0.59202872508(2)	−1.07000189273(2)	4521.28(10)	0.032587302068(5)
3.6	−0.58881359131(2)	−1.06350261764(2)	4437.34(10)	0.031701268030(8)
3.7	−0.585690956612(10)	−1.05764182627(3)	4359.77(4)	0.030740564043(2)
3.8	−0.58266736954(2)	−1.05238720974(5)	4288.42(3)	0.029723034037(7)
3.9	−0.57974774201(2)	−1.04770721178(6)	4223.78(3)	0.02866365952(2)
4.0	−0.57693560962(2)	−1.04357097927(4)	4166.00(9)	0.027575059986(4)
4.1	−0.57423334705(2)	−1.039948325815(9)	4115.90(6)	0.026467894695(8)
4.2	−0.57164234718(3)	−1.03680970154(3)	4073.41(7)	0.025351188818(7)
4.3	−0.56916317088(2)	−1.034126175118(10)	4039.15(6)	0.02423259692(2)
4.4	−0.56679567295(2)	−1.031869427504(2)	4013.54(6)	0.023118617849(8)

4.5	−0.56453910868(2)	−1.03001175342(3)	3997.13(3)	0.022014769813(6)
4.6	−0.562392224448(10)	−1.02852607261(3)	3990.28(6)	0.020925733966(9)
4.7	−0.56035333538(3)	−1.02738594937(5)	3993.855(9)	0.01985547268(3)
4.8	−0.55842039212(3)	−1.02656561414(6)	4008.18(2)	0.01880732715(3)
4.9	−0.556591038834(10)	−1.02603999172(4)	4033.86(6)	0.01778409916(2)
5.0	−0.55486266354(2)	−1.02578472765(4)	4071.56(8)	0.01678811985(2)
5.1	−0.553232443(2)	−1.02577623(2)	4121.5(2)	0.015821306(4)
5.2	−0.551697379(2)	−1.02599161(3)	4184.7(2)	0.014885221(4)
5.3	−0.550254333(2)	−1.02640881(3)	4261.2(2)	0.013981106(5)
5.4	−0.548900059(3)	−1.02700650(4)	4350.9(2)	0.013109929(6)
5.5	−0.547631222148(4)	−1.02776409927(6)	4454.34(5)	0.01227242636(2)
5.6	−0.546444435(4)	−1.02866185(5)	4569.4(2)	0.011469110(8)
5.8	−0.544303204(5)	−1.03080147(8)	4834.2(3)	0.00996637(2)
5.9	−0.543341814(6)	−1.03200686(9)	4980.2(3)	0.00926725(2)
6.0	−0.542448585689(4)	−1.03327914821(6)	5132.72(5)	0.00860300386(2)
6.5	−0.538883842724(2)	−1.04008265029(3)	5870.88(2)	0.005797697717(4)
7.0	−0.536515978508(2)	−1.04644266100(8)	6302.00(2)	0.003798470860(9)
7.5	−0.534974925145(4)	−1.051494656893(10)	6284.01(7)	0.002460692450(3)
8.0	−0.533975596442(6)	−1.05513476482(5)	5891.01(9)	0.00160205350(2)
8.5	−0.533319775267(6)	−1.05760097659(6)	5267.96(10)	0.00106336163(2)
9.0	−0.532879029864(5)	−1.05923111522(4)	4571.03(9)	0.000725216051(8)
9.5	−0.532574738980(6)	−1.06033221777(6)	3916.99(10)	0.000507080014(9)
10.0	−0.532360127292(5)	−1.06111408116(5)	3363.90(9)	0.000360617338(8)
11.0	−0.532095168365(4)	−1.06209449800(5)	2584.14(8)	0.000190530790(6)
12.0	−0.531947810466(4)	−1.06251299724(4)	2116.25(7)	0.000115218638(5)
13.0	−0.531849836075(3)	−1.06259045015(3)	1806.79(6)	0.000085324767(4)
14.0	−0.531771562618(3)	−1.06252417142(3)	1573.12(5)	0.000072782414(3)
15.0	−0.531702494600(3)	−1.06241794050(3)	1382.06(4)	0.000065803245(3)
16.0	−0.531639507384(3)	−1.06231496805(3)	1221.38(4)	0.000060252918(3)
17.0	−0.531581960211(2)	−1.06223201796(4)	1086.69(4)	0.000054817791(3)
18.0	−0.531529939877(2)	−1.06217447078(4)	976.26(3)	0.000049189387(3)
19.0	−0.531483627425(2)	−1.06214214987(4)	889.02(3)	0.000043426577(3)
20.0	−0.531443071566(2)	−1.06213195421(4)	823.67(3)	0.000037709445(3)

Table A62: Same as for Table A1, but for $5\,^3\Pi_u$ (kb state).

$5\,^3\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.01	97.97971004295(10)	95.9599372798(4)	7622.54(3)	−9999.94828061(2)
0.05	17.985469208(6)	15.982364081(5)	7640.32(2)	−399.7714870(2)
0.1	8.001196160(10)	6.0414764059(6)	7687.12(3)	−99.6091595(2)
0.15	4.690372809(8)	2.78941814(2)	7750.847(8)	−43.9421834(3)
0.2	3.050795082(6)	1.21678037(2)	7822.84(2)	−24.4240491(2)
0.3	1.446017738(3)	−0.246711290(2)	7968.00(2)	−10.46248925(5)
0.4	0.6786077743(9)	−0.877535530(5)	8090.39(2)	−5.58687770(2)
0.5	0.2443498092(4)	−1.187092949(3)	8174.79(2)	−3.351585138(6)
0.6	−0.0255003078(2)	−1.345818861(2)	8215.858(8)	−2.158030411(3)
0.7	−0.20332250258(10)	−1.4256025208(6)	8213.907(8)	−1.455653594(2)
0.8	−0.32518818511(2)	−1.4612558711(2)	8172.39(2)	−−
0.9	−0.410983962626(5)	−1.47123026544(4)	8096.30(4)	−0.72140260021(4)
1.0	−0.472500237400(6)	−1.46594313554(5)	3995.58(2)	−0.52094266074(3)
1.1	−0.517121522235(6)	−1.45155245623(4)	3931.24(3)	−0.37937219251(3)
1.2	−0.549675476136(6)	−1.43182410325(4)	3857.69(3)	−0.27706095914(2)
1.3	−0.573428757691(7)	−1.40911924970(4)	3777.23(3)	−0.20173979563(2)
1.4	−0.590655076624(7)	−1.38494450514(3)	3691.83(4)	−0.14545310849(2)
1.5	−0.602974740624(8)	−1.36027163373(3)	3603.17(4)	−0.102881434988(8)
1.6	−0.611565660309(9)	−1.33572991039(3)	3512.67(4)	−0.070374118607(7)
1.7	−0.617298848978(10)	−1.31172523652(3)	3421.45(4)	−0.045369140331(7)
1.8	−0.62082791420(2)	−1.28851571081(4)	3330.46(5)	−0.026033268007(8)
1.9	−0.62264961776(2)	−1.26626056380(5)	3240.43(5)	−0.01103227804(2)
2.0	−0.62314573773(2)	−1.24505239565(7)	3151.95(5)	0.00061953990(2)
2.1	−0.62261255296(3)	−1.22493872390(10)	3065.49(6)	0.00966018191(3)
2.2	−0.62128195851(3)	−1.2059365610(2)	2981.40(6)	0.01664879821(4)
2.3	−0.61933681423(4)	−1.1880423784(2)	2899.97(6)	0.02201358700(6)
2.4	−0.61692225251(4)	−1.1712389929(3)	2821.41(5)	0.02608563005(7)
2.5	−0.61415411267(5)	−1.1555004499(3)	2745.84(5)	0.02912311016(9)
2.6	−0.61112531252(5)	−1.1407960284(3)	5345.84(5)	0.03132869103(4)
2.62	−0.61049513548(3)	−1.1379765260(2)	5316.87(5)	0.03168463547(4)
2.64	−0.60985809867(3)	−1.1351970170(2)	5287.68(5)	0.03201484102(4)
2.66	−0.60921470678(3)	−1.1324574114(2)	5257.93(5)	0.03232030156(4)
2.68	−0.60856544557(3)	−1.1297577633(2)	2613.48(4)	0.03260191335(4)
2.6862	−0.608363056560(5)	−1.12892902702(4)	5217.106(6)	0.032684493374(9)
2.7	−0.60791078418(3)	−1.1270984133(2)	2596.85(4)	0.03286042782(4)
2.72	−0.60725117903(3)	−1.1244803157(2)	2577.81(4)	0.03309633911(4)
2.74	−0.60658708140(3)	−1.1219058855(2)	2553.51(4)	0.03330959028(3)
2.7581	−0.605982587124(5)	−1.11961881526(3)	5042.053(5)	0.033481874837(8)
2.76	−0.60591895554(3)	−1.11938149656(10)	2516.48(3)	0.03349870091(2)
2.78	−0.60524733087(3)	−1.116926112163(9)	2443.85(3)	0.033657751634(9)
2.7833	−0.60513622312(2)	−1.11653076545(2)	4849.109(6)	0.033680049144(4)
2.797	−0.604674260128(5)	−1.114938396636(5)	4593.986(8)	0.033754066361(2)
2.8	−0.60457298103(3)	−1.1146041404(4)	4507.28(4)	0.0337649363(2)
2.8061	−0.604366966334(5)	−1.11394694767(2)	4279.15(2)	0.033778904878(8)
2.8131	−0.604130502921(5)	−1.11323709850(3)	3910.12(2)	0.03377907196(2)
2.819	−0.603931240232(4)	−1.11267686202(4)	3503.60(2)	0.03376573907(2)
2.82	−0.60389747611(3)	−1.112584779(2)	3427.33(4)	0.0337624727(5)
2.8245	−0.603745581914(4)	−1.11217671448(4)	3068.48(3)	0.03374560076(2)

2.8299	−0.603563413494(4)	−1.11168987695(3)	2632.82(3)	0.03372449557(2)
2.8358	−0.603364495609(4)	−1.11114371374(2)	2200.78(4)	0.033706635681(9)
2.84	−0.60322294454(2)	−1.110739416(2)	970.21(4)	0.0336994623(6)
2.8428	−0.603128589406(4)	−1.1104621569700(5)	1791.06(4)	0.033697418682(3)
2.852	−0.602818557227(4)	−1.10951363429(2)	1421.36(5)	0.033703885052(3)
2.86	−0.60254886285(2)	−1.1086556476(7)	1215.05(5)	0.0337210063(3)
2.8656	−0.602359982491(4)	−1.10804429990(3)	1113.39(5)	0.033736622377(7)
2.88	−0.60187384982(2)	−1.1064538458(3)	948.59(6)	0.0337825881(2)
2.8908	−0.601508805770(4)	−1.10525644239(4)	878.47(6)	0.033818032777(9)
2.9	−0.601197545109(10)	−1.1042385555(2)	838.66(6)	0.03384708091(6)
2.92	−0.600520020230(7)	−1.10204113576(5)	394.25(5)	0.033903734488(10)
2.94	−0.599841468892(7)	−1.09987147915(5)	382.69(5)	0.03394947570(2)
2.96	−0.599162119658(7)	−1.09773316683(4)	378.16(5)	0.03398347040(2)
2.9627	−0.599070359270(5)	−1.09744698602(4)	755.88(7)	0.033987151085(9)
2.98	−0.598482208954(7)	−1.09562760514(3)	377.69(4)	0.03400564183(2)
3.0	−0.597801971421(10)	−1.09355533531(3)	759.71(7)	0.0340162025102(6)
3.1	−0.594403635832(10)	−1.08369380392(5)	409.61(10)	0.033907570239(10)
3.2	−0.591028241425(9)	−1.07464782021(6)	455.67(7)	0.03356520707(2)
3.3	−0.58769693047(2)	−1.06638657731(5)	512.17(9)	0.033032510193(8)
3.4	−0.584426874526(9)	−1.05887890215(2)	579.76(8)	0.0323455432054(7)
3.5	−0.581231972414(9)	−1.05209537283(2)	658.74(8)	0.0315338777135(7)
3.6	−0.578123446937(10)	−1.04600906259(2)	752.13(7)	0.0306216198000(5)
3.7	−0.575110348199(10)	−1.04059622409(3)	862.61(7)	0.0296282357585(3)
3.8	−0.57219998568(2)	−1.03583718712(3)	994.11(6)	0.028569153749(2)
3.9	−0.56939831109(2)	−1.03171765042(7)	1151.81(6)	0.027456146606(8)
4.0	−0.56671027407(2)	−1.02823059004(5)	1342.63(6)	0.026297489524(4)
4.1	−0.56414017436(3)	−1.02537910423(4)	1575.78(6)	0.02509786449(3)
4.2	−0.56169203862(3)	−1.023180652213(2)	1863.72(6)	0.02385795830(2)
4.3	−0.55937005516(3)	−1.021673286932(6)	2223.27(6)	0.022573679839(10)
4.4	−0.55717910961(3)	−1.02092448649(7)	2676.95(6)	0.021234939256(5)
4.5	−0.55512546075(3)	−1.0210424912(2)	3254.14(6)	0.01982409562(3)
4.6	−0.55321756360(3)	−1.0221870847(4)	3990.39(7)	0.01831479184(6)
4.7	−0.55146689839(4)	−1.0245676070(6)	4920.98(8)	0.01667365739(10)
4.8	−0.54988824296(5)	−1.0283944952(7)	6060.2(2)	0.0148712481(2)
4.9	−0.54849793818(6)	−1.0337213872(9)	7353.7(2)	0.0129131610(2)
5.0	−0.54730779182(8)	−1.0401443322(10)	8616.6(2)	0.0108942503(2)

Table A63: Same as for Table A1, but for $6\,^3\Pi_u$.

$6\,^3\Pi_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.01	97.9802584030(2)	95.9610342565(9)	10.6(2)	−9999.94825495(6)
0.05	17.986020367(7)	15.98347184(5)	8.3(7)	−399.7713779(6)
0.1	8.001754700(10)	6.04261145(7)	7.7(7)	−99.6089795(5)
0.15	4.690941554(8)	2.79058919(5)	8.2(7)	−43.9419594(3)
0.2	3.051375704(6)	1.21799126(4)	8.6(7)	−24.4238007(2)
0.5	0.2450031499(7)	−1.185686414(5)	11.7(9)	−−
0.6	−0.0248293383(5)	−1.344385888(4)	14.7(10)	−−
0.7	−0.20263897749(4)	−1.4241662588(3)	18.9(9)	−3.351385427(7)
0.8	−0.3244974985(4)	−1.459839088(2)	23.6(8)	−2.157878685(4)
0.9	−0.41029157506(3)	−1.4698545538(2)	29.8(2)	−1.4555547198(3)
1.0	−0.47181151067(5)	−1.46462847737(4)	35.5(3)	−0.7214126707(2)
1.1	−0.51644161177(3)	−1.4503170150(2)	42.1(2)	−0.52100545617(7)
1.2	−0.54900926552(2)	−1.43068417055(7)	49.918413(2)	−0.379485264899(2)
1.3	−0.57278082204(6)	−1.4080892919(2)	58.35(2)	−0.2772213662448(7)
1.4	−0.59002966655(7)	−1.3840372697(2)	67.90(2)	−0.2019443442850(5)
1.5	−0.60237578063(3)	−1.35949829364(5)	78.64(3)	−0.1456985261031(3)
1.6	−0.61099675704(2)	−1.33510022458(5)	90.70(3)	−0.1031644882651(2)
1.7	−0.616763306008(10)	−1.31124771736(2)	104.20(3)	−0.07069169407645(5)
1.8	−0.620328751135(9)	−1.28819779131(2)	119.29(3)	−0.0457182972716(2)
1.9	−0.622189591884(7)	−1.26610876020(2)	136.15(3)	−0.0264112717069(3)
2.0	−0.622727367083(6)	−1.245072463050(9)	154.97(3)	−0.0114366191960(4)
2.1	−0.622238140051(4)	−1.225135802419(4)	175.97(3)	0.0001911355345(5)
2.2	−0.620953613862(6)	−1.206315306949(5)	199.39(4)	0.0092097512590(5)
2.3	−0.619056478902(6)	−1.188607064035(3)	225.54(3)	0.0161781457813(3)
2.4	−0.616691717720(3)	−1.17199351825(4)	254.71(2)	0.0215243016120(2)
2.5	−0.613975030575(7)	−1.15644804640(5)	287.239041(2)	0.0255791321656(7)
2.5452	−0.6126571940941(2)	−1.149763326264(5)	323.555(6)	0.028600805924(2)
2.6	−0.610999173148(6)	−1.1419375082(8)	364.252(3)	0.029683742702(2)
2.62	−0.610379740479(6)	−1.13915617045(8)	384.409(2)	0.0307926303833(2)
2.64	−0.609753490645(7)	−1.13641420247(10)	410.91(2)	0.03114630172(3)
2.66	−0.609120920978(7)	−1.1337111017(2)	210.63(5)	0.03147453743(4)
2.68	−0.608482506095(8)	−1.13104621837(10)	216.26(5)	0.03177847377(5)
2.6862	−0.608283481821(3)	−1.13022772973(3)	222.41(6)	0.03205925143(3)
2.7	−0.607838697365(8)	−1.1284186136(4)	229.35(6)	0.032141774220(6)
2.72	−0.607189920764(7)	−1.1258267299(3)	463.43(6)	0.0323180673338(10)
2.7338	−0.606739576363(3)	−1.12405769129(4)	475.75(6)	0.0325562906(4)
2.74	−0.606536570970(7)	−1.12326754923(10)	247.5(7)	0.032709584257(10)
2.7581	−0.605941638246(4)	−1.12097402820(4)	518.74(5)	0.0327757632(4)
2.76	−0.605878994763(7)	−1.1207340926(3)	264.2(7)	0.032960823866(4)
2.773	−0.605449429025(4)	−1.11909304391(5)	582.54(6)	0.0329796722(5)
2.78	−0.605217440325(8)	−1.118206791(2)	293.9(6)	0.03310703720(2)
2.7833	−0.605107907055(4)	−1.11778717415(5)	661.24(5)	0.0331755715(7)
2.7909	−0.604855231643(4)	−1.11681282886(5)	359.6(6)	0.0332082923139(2)
2.797	−0.604651987810(4)	−1.11601786067(7)	757.54(6)	0.03328590578(2)
2.8	−0.604551879654(10)	−1.115620628(3)	870(9)	0.033352204147(5)
2.8019	−0.604488423111(4)	−1.11536635678(8)	1003.28(6)	0.033386833473(7)
2.8061	−0.604347992124(4)	−1.11479558052(8)	1088.06(8)	0.03340964683(3)
2.8098	−0.604224086472(4)	−1.11428137744(9)	1149.58(5)	0.033462957059(10)

2.8131	−0.604113412063(4)	−1.11381295494(10)	1312.03(5)	0.03351370044(3)
2.8161	−0.604012655937(4)	−1.11337921019(2)	1489.01(4)	0.03356221580(2)
2.819	−0.603915122054(5)	−1.1129536750(2)	1676.46(5)	0.03360892784(4)
2.82	−0.60388145765(2)	−1.112805797(4)	1871.06(4)	0.03365610825(2)
2.8217	−0.603824189758(5)	−1.1125534300(2)	2079.15(4)	0.033672737(2)
2.8245	−0.603729759785(5)	−1.1121362951(2)	1077.20(9)	0.03370129694(4)
2.8272	−0.603638576785(3)	−1.11173434820(9)	2286.72(4)	0.03374870759(2)
2.8299	−0.603547272373(5)	−1.11133494592(10)	2510.75(4)	0.03379414451(3)
2.8328	−0.603449073880(3)	−1.11091099699(10)	2729.03(4)	0.03383850981(2)
2.8358	−0.603347353788(5)	−1.11047973216(9)	2943.00(3)	0.03388419612(4)
2.8392	−0.603233(2)	−1.110002(2)	3162.10(3)	0.03392868873(2)
2.84	−0.60320473151(3)	−1.109890306(3)	3371.35(3)	0.03397526887(3)
2.8428	−0.603109522927(5)	−1.10950686084(8)	3583.24(2)	0.0339856185(8)
2.847	−0.602966538691(5)	−1.10894505682(7)	1814.41(5)	0.034020045404(6)
2.852	−0.602796080084(5)	−1.10829452209(6)	3776.77(2)	0.03406674414(2)
2.858	−0.602591230474(5)	−1.10753497607(6)	3964.30(2)	0.0341155813916(3)
2.86	−0.60252288225(7)	−1.1072859493(10)	4140.930(10)	0.03416636979(2)
2.8656	−0.602331350999(5)	−1.10659757175(5)	4299.73(2)	0.0341817536(3)
2.8759	−0.601978534882(5)	−1.10535790795(5)	2171.15(5)	0.034221499954(4)
2.88	−0.60183792164(3)	−1.1048717510(7)	4440.951(7)	0.03428462805(2)
2.8908	−0.601467112878(6)	−1.10360629092(5)	4563.401(9)	0.0343069765(2)
2.9	−0.60115081479(7)	−1.1025425621(6)	2298.70(5)	0.034360016203(6)
2.9151	−0.600630943128(5)	−1.10081989572(5)	4661.879(5)	0.034399678488(2)
2.92	−0.60046207016(7)	−1.1002664201(6)	4696.734(8)	0.03445576156(2)
2.94	−0.59977205030(7)	−1.0980328313(6)	4730(2)	0.0344718220(2)
2.96	−0.59908106012(7)	−1.0958376153(6)	2368.34(4)	0.0345276426(2)
2.9627	−0.598987717351(6)	−1.09554407833(5)	2375.17(4)	0.0345690895(2)
2.98	−0.59838937483(7)	−1.0936787688(6)	2375.28(4)	0.034573651186(7)
3.0	−0.59769725048(3)	−1.0915551565(6)	4750.050(4)	0.0345973090(2)
3.1	−0.59423809870(8)	−1.0814445571(6)	2371.63(4)	0.0346131148574(2)
3.1037	−0.594110366005(7)	−1.08108626977(6)	4731.595(2)	0.0345263355998(3)
3.2	−0.59079979260(8)	−1.0721441383(6)	4645.063(2)	0.03451830468(2)
3.3	−0.58740341011(8)	−1.0636142038(6)	4641.477(4)	0.03420482717974(6)
3.4	−0.58406587906(8)	−1.0558180867(7)	4545.956(2)	0.0336947322650(2)
3.5	−0.58080073121(9)	−1.0487204086(7)	4447.149(3)	0.0330334328064(6)
3.6	−0.57761869032(9)	−1.0422867702(7)	4351.988(4)	0.0322517296754(10)
3.7	−0.57452814578(9)	−1.0364836456(7)	4261.745(6)	0.0313751695840(4)
3.8	−0.57153553803(9)	−1.0312783194(8)	4177.057(5)	0.0304250395(2)
3.9	−0.56864567435(9)	−1.0266388371(8)	4098.326784(2)	0.0294191465271(7)
4.0	−0.56586198901(10)	−1.0225339639(8)	4025.881(4)	0.028372438896(2)
4.1	−0.56318675854(9)	−1.0189331520(7)	3960.030(3)	0.027297503566(2)
4.2	−0.56062128109(9)	−1.0158065197(7)	3901.098(3)	0.026204967126(3)
4.3	−0.5581660265(2)	−1.0131248409(10)	3849.442(4)	0.025103819669(3)
4.4	−0.5558207625(2)	−1.0108595464(9)	3805.459(8)	0.024001677258(2)
4.5	−0.5535846622(2)	−1.0089827371(8)	3769.60(2)	0.022904995179(2)
4.6	−0.5514563950(2)	−1.0074672069(8)	3742.34(2)	0.0218192416648(10)
4.7	−0.5494342054(2)	−1.0062864758(8)	3724.23(2)	0.020749039832(2)
4.8	−0.54751598067(10)	−1.0054148301(7)	3715.81(2)	0.019698284050(2)
4.9	−0.54569931051(10)	−1.0048273693(7)	3717.69(2)	0.018670235714(3)
5.0	−0.54398153856(10)	−1.0045000594(6)	3730.445(10)	0.017667602419(4)

Table A64: Same as for Table A1, but for $7\,^3\Pi_u$.

$7\,^3\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.466086340413(9)	95.9726239638(9)	4368.9(2)	−9999.94826931(6)
1.1	−0.510709214153(6)	15.99505552(5)	4378.76(3)	−399.7714385(5)
1.2	−0.543266645076(6)	6.0541798(2)	4404.15(2)	−99.6090802(7)
1.3	−0.567025156652(6)	2.80213749(8)	4438.592(7)	−43.9420840(3)
1.4	−0.584258314712(2)	1.22951750(5)	4477.2(2)	−24.42393839(9)
1.5	−0.596586280425(5)	−0.23393810(4)	4554.31(4)	−10.46237211(8)
1.6	−0.605186819026(8)	−0.86473041(2)	4617.521(5)	−5.58676732(3)
1.7	−0.61093080374(5)	−1.17426316(2)	4658.59(2)	−3.35148900(2)
1.8	−0.614471706838(2)	−1.332973078(5)	4674.81(2)	−2.157952690(6)
1.9	−0.616306162332(2)	−1.4127498373(6)	4666.720(2)	−−
2.0	−0.616815827555(6)	−1.4484052426(3)	4636.389(4)	−1.0135635513(2)
2.1	−0.616296868131(6)	−1.4583901508(3)	4586.82(2)	−−
2.2	−0.614981071804(6)	−1.4531213000(4)	2260.6301(5)	−0.5209486677(3)
2.3	−0.613051198053(5)	−1.4387558721(6)	4442.984848(2)	−0.3793977241(4)
2.4	−0.610652279638(4)	−1.4190589148(5)	4354.676189(2)	−0.2771047318(4)
2.5	−0.607900059151(3)	−1.3963907815(5)	4259.041(3)	−0.2018004000(3)
2.6	−0.604887329548(4)	−1.37225729712(9)	4158.307(2)	−0.14552908244(5)
2.62	−0.604260369364(4)	−1.3476294908(5)	4054.350(2)	−0.1029713143(3)
2.64	−0.603626543953(4)	−1.32313595898(8)	3948.718(2)	−0.07047647108(4)
2.66	−0.602986356427(4)	−1.2991819837(5)	3842.672(2)	−0.0454825875(2)
2.68	−0.6023402808(4)	−1.2760251009(7)	3737.227(2)	−0.0261564980(3)
2.7	−0.601688774355(3)	−1.2538240314(2)	3633.184(2)	−0.01116405233(8)
2.72	−0.601032298927(4)	−1.2326709143(6)	3531.176(2)	0.00048038471(10)
2.74	−0.600371282819(4)	−1.2126128476(5)	3431.6985(4)	0.0095147353(2)
2.76	−0.599706081968(4)	−1.1936664603(5)	3335.135479(2)	0.0164980798(2)
2.78	−0.59903708812(3)	−1.1758278675(5)	3241.792(2)	0.0218585524(2)
2.8	−0.598364742068(10)	−1.1590795455(4)	3151.904(3)	0.0259271801(2)
2.82	−0.597689338351(5)	−1.1433951931(3)	3065.552(3)	0.02896210580(10)
2.84	−0.597011233012(3)	−1.143092147(2)	3063.81(2)	0.0290137324(6)
2.86	−0.596330790575(2)	−1.12874370776(3)	2981.881(2)	0.03116597517(2)
2.88	−0.595648256266(3)	−1.12593461499(3)	1482.42(5)	0.03152167472(2)
2.9	−0.594963983436(5)	−1.12316546503(3)	1473.81(5)	0.03185166174(2)
2.92	−0.594278252955(5)	−1.12043619474(3)	1464.89(3)	0.03215691908(2)
2.94	−0.593591336041(6)	−1.11982761190(4)	2925.675(3)	0.03222228572(2)
2.96	−0.59290349615(2)	−1.11774692938(3)	1455.17(4)	0.03243831611(2)
2.98	−0.592214995144(2)	−1.116921444(3)	−−	0.0325208188(7)
3.0	−0.591526069565(6)	−1.11509819649(4)	2888.024036(2)	0.03269653578(2)
3.1	−0.588083003004(6)	−1.114272431(2)	−−	0.0327731408(6)
3.2	−0.58466046763(10)	−1.11249146896(4)	1429.38(4)	0.03293188577(2)
3.3	−0.58127997743(9)	−1.11018450759(4)	2819.740(5)	0.03312367849(2)
3.4	−0.57795808(2)	−1.10993072820(5)	1406.94(5)	0.03314375042(3)
3.5	−0.57470822413(7)	−1.10883358(4)	2783.97(9)	0.03322792(2)
3.6	−0.57154111047(7)	−1.1076622531(2)	2737.96(3)	0.0333125763(3)
3.7	−0.56846506922(8)	−1.10742760734(7)	1362.99(5)	0.03332878451(3)
3.8	−0.5654864931(9)	−1.10696077737(4)	2699.184(8)	0.03336017667(2)
3.9	−0.56261014104(7)	−1.10642484068(2)	2661.11(2)	0.033394649999(7)
4.0	−0.55983940264(8)	−1.10527696673(5)	2541.53(2)	0.03346141026(2)
4.1	−0.5571765089(3)	−1.10501899152(8)	1252.16(8)	0.03347475568(3)

4.2	−0.5546227137(2)	−1.10420247446(5)	2352.82(2)	0.03351179430(2)
4.3	−0.5521784434(2)	−1.10404464130(4)	2316.19(3)	0.03351791764(2)
4.4	−0.54984343(2)	−1.10341339516(5)	2142.15(3)	0.03353866246(2)
4.5	−0.5476167853(5)	−1.1032827617(4)	2100.50(3)	0.0335422004(2)
4.6	−0.5454971583(5)	−1.102788284(6)	1927.098359(2)	0.033553465(3)
4.7	−0.54348277(4)	−1.10275631932(4)	1915.02(3)	0.03355409580(2)
4.8	−0.54157143(4)	−1.102628796(3)	−−	0.0335564966(9)
4.9	−0.53976073(6)	−1.10216390277(4)	1683.84(4)	0.03356430589(2)
5.0	−0.5380479038(7)	−1.102005847(2)	1621.173284(2)	0.0335668036(6)

Table A65: Same as for Table A1, but for $8\,^3\Pi_u$.

$8\,^3\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.465690182387(9)	95.9732587811(3)	6.49(2)	−9999.948254568(7)
1.1	−0.510318419897(6)	15.99569650(5)	6.57(2)	−399.7713763(7)
1.2	−0.542884025181(6)	6.0548364(2)	5.4(4)	−99.6089771(10)
1.3	−0.566653343625(6)	2.8028149(2)	7.13(3)	−43.941956(2)
1.4	−0.58389975385(2)	1.23021757(10)	7.61(3)	−24.4237968(10)
1.5	−0.596243231089(5)	−0.23319284(2)	8.85(5)	−10.4622246(3)
1.6	−0.60486135926(8)	−0.86394696(7)	10.53(4)	−5.5866323(3)
1.7	−0.610624839555(5)	−1.17345247(4)	12.58(5)	−3.3513763(2)
1.8	−0.614186983932(2)	−1.332147988(6)	15.05(5)	−2.15786781(3)
1.9	−0.61604427876(2)	−1.4119237432(8)	18.01(2)	−1.4555421386(8)
2.0	−0.616578248131(6)	−1.447591253(2)	21.34(4)	−1.013540820(6)
2.1	−0.616084938581(6)	−1.457600691(2)	23.4(9)	−0.7213966331(6)
2.2	−0.614796033561(6)	−1.4523678547(6)	13.1(5)	−0.5209876463(4)
2.3	−0.612894203361(5)	−1.4380488725(4)	15.5(6)	−0.3794656405(2)
2.4	−0.610524407021(4)	−1.4184077191(3)	19.0(5)	−0.2771998784(2)
2.5	−0.607802329314(3)	−1.395803702(4)	21.2(8)	−0.201920934(2)
2.6	−0.604820722113(4)	−1.3717416775(2)	26.5(3)	−0.14567312761(6)
2.62	−0.604200101599(4)	−1.34719177353(5)	29.5(9)	−0.10313702114(2)
2.64	−0.603572653961(4)	−1.32278179236(3)	34.5(5)	−0.07066206598(2)
2.66	−0.602938882248(4)	−1.29891631599(3)	39.1(6)	−0.045686401039(8)
2.68	−0.602299260444(4)	−1.275852278(2)	44.2(8)	−0.0263769834(2)
2.7	−0.601654245835(3)	−1.25374789094(4)	50.6(8)	−0.01139979471(2)
2.72	−0.601004300293(4)	−1.23269487550(4)	58.2(5)	0.00023066189(2)
2.74	−0.600349852192(4)	−1.2127399957(7)	66.5(3)	0.0092521707(3)
2.76	−0.59969125758(4)	−1.1938996179(8)	75.0(4)	0.0162236784(3)
2.78	−0.599028908346(3)	−1.17616964317(3)	83.5(8)	0.021573199432(10)
2.8	−0.598363245468(10)	−1.15953230694(4)	95.9(3)	0.02563168042(2)
2.82	−0.597694563706(5)	−1.14396076267(2)	108.1(3)	0.028657320850(4)
2.84	−0.597023219355(3)	−1.129421649079(5)	122.5(2)	0.030853451207(4)
2.86	−0.596349577247(2)	−1.126634268249(4)	125.8(2)	0.031208029663(3)
2.88	−0.595673882954(3)	−1.123886125442(3)	129.2(4)	0.031537194411(3)
2.9	−0.594996490213(5)	−1.121176686625(2)	133.78(10)	0.031842092986(3)
2.92	−0.594317680344(5)	−1.120572328390(4)	270.05(6)	0.0319074692085(9)
2.94	−0.593637725029(6)	−1.118505225235(8)	138.5(4)	0.032123893297(2)
2.96	−0.592956888264(2)	−1.117684624294(4)	281.86(6)	0.0322067540900(10)
2.98	−0.592275432486(2)	−1.11587060897(2)	145.6(2)	0.032383861023(3)
3.0	−0.591593594876(6)	−1.1150484(2)	−−	0.03246134(7)
3.1	−0.588186634587(6)	−1.11327075735(2)	155.8(2)	0.032623552832(5)
3.2	−0.584801666638(8)	−1.1109569318749(8)	343.75(6)	0.032823884415(3)
3.3	−0.581459816569(9)	−1.11070107917(3)	174.1(2)	0.032845368492(8)
3.4	−0.578178104198(10)	−1.10839166499(2)	417.47(6)	0.033034795818(4)
3.5	−0.574970289256(2)	−1.10814932974(5)	214.11(8)	0.03305436093(2)
3.6	−0.571847412283(2)	−1.107664224522(10)	454.03(5)	0.033093487083(6)
3.7	−0.568818302604(2)	−1.10586417942(3)	606.34(5)	0.03324039425(2)
3.8	−0.565890005294(2)	−1.105578011264(5)	321.14(2)	0.033474755672(2)
3.9	−0.56306816043(2)	−1.10514620205(5)	705.06(5)	0.03330117783(2)
4.0	−0.560357355244(3)	−1.10464455854(4)	791.59(5)	0.03334489530(2)
4.1	−0.557761480584(3)	−1.10369300728(5)	999.66(4)	0.03343103815(2)

4.2	−0.555284125821(4)	−1.10331281566(8)	1098(5)	0.03346653042(3)
4.3	−0.552929070435(4)	−1.102903118(5)	606.1(2)	0.033505239(2)
4.4	−0.550700944411(5)	−1.10286204951(5)	1224.60(4)	0.03350913558(2)
4.5	−0.548606162023(5)	−1.10209443878(5)	1453.79(3)	0.03358192833(2)
4.6	−0.546654197088(6)	−1.10206704943(10)	1462.09(3)	0.03358450831(4)
4.7	−0.544858945398(3)	−1.10133109750(4)	1681.72(3)	0.03365262567(2)
4.8	−0.543238661872(3)	−1.10111494919(10)	1743.45(3)	0.03367202937(3)
4.9	−0.541809990451(3)	−1.10052666817(3)	1900.66(2)	0.03372299061(2)
5.0	−0.540570747925(3)	−1.10032836610(9)	1949.45(2)	0.03373949424(3)

Table A66: Same as for Table A1, but for $9\,^3\Pi_u$.

$9\,^3\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.01	97.9863723285(2)	95.973262114(2)	0.423(4)	−9999.94825428(7)
0.05	17.99213435(2)	15.99569994(8)	0.433(5)	−399.771375(2)
0.1	8.00786889(8)	6.0548406(4)	0.4612(9)	−99.608972(2)
0.15	4.69705599(4)	2.8028190(2)	0.507(8)	−43.9419530(9)
0.3	1.45273993(2)	−0.2331856(2)	0.750(7)	−10.4622183(4)
0.4	0.685356405(10)	−0.86393674(5)	0.99(2)	−5.58662388(8)
0.5	0.251122197(6)	−1.17343864(3)	1.30(2)	−3.35136606(3)
0.6	−0.018708178(6)	−1.33212984(4)	1.69(3)	−2.15785581(4)
0.7	−0.196515348(3)	−1.41190049(2)	2.15(3)	−1.45552827(2)
0.8	−0.31837105(2)	−1.44756217(8)	2.673(9)	−1.01352509(7)
0.9	−0.404161930(2)	−1.45756491(2)	3.30(3)	−0.72137894(2)
1.0	−0.465678304(2)	−1.452324568(9)	2.04(2)	−0.520967960(7)
1.1	−0.5103044622(6)	−1.437997206(5)	2.45(2)	−0.379443893(3)
1.2	−0.5428677796(5)	−1.418346750(4)	2.91(2)	−0.277175992(2)
1.3	−0.5666345922(4)	−1.395732448(2)	3.4(7)	−0.2018948179(6)
1.4	−0.5838782692(3)	−1.3716590812(10)	3.999(9)	−0.1456446734(4)
1.5	−0.5962187734(2)	−1.3470967061(9)	4.652(10)	−0.1031061063(4)
1.6	−0.6048336754(2)	−1.3226730269(6)	5.38(2)	−0.0706285476(3)
1.7	−0.61059366029(10)	−1.2987925147(5)	6.18(2)	−0.0456501142(2)
1.8	−0.61415202231(3)	−1.2757119726(3)	7.04(2)	−0.02633773775(9)
1.9	−0.61600522721(3)	−1.2535894604(2)	8.04(5)	−0.01135737155(8)
2.0	−0.6165347749(2)	−1.232516520(2)	9.13(3)	0.0002765148(5)
2.1	−0.6160366835(2)	−1.2125397050(10)	10.31(3)	0.0093017438(4)
2.2	−0.6147426047(2)	−1.1936751431(7)	11.60(4)	0.0162773029(3)
2.3	−0.61283517003(7)	−1.1759184697(6)	13.02(4)	0.0216312480(2)
2.4	−0.61045929621(6)	−1.1592516561(5)	14.57(4)	0.0256945568(2)
2.5	−0.60773061340(5)	−1.1436477235(4)	16.26(4)	0.0287254013(2)
2.6	−0.604741822(3)	−1.1290740031(3)	18.08(2)	0.030926779(2)
2.62	−0.60411968400(5)	−1.1262797486(5)	18.467(2)	0.0312822975(2)
2.64	−0.60349069654(5)	−1.1235249635(6)	18.82(3)	0.0316122839(2)
2.66	−0.60285535573(6)	−1.1208093453(6)	19.27(2)	0.0319178068(2)
2.68	−0.60221414056(6)	−1.1181325890(6)	19.681(7)	0.0321998851(2)
2.7	−0.60156751011(6)	−1.1154943877(7)	20.10(3)	0.0324594935(2)
2.72	−0.60091590439(6)	−1.1128944332(7)	20.53(5)	0.0326975646(3)
2.74	−0.60025974515(7)	−1.1103324157(8)	21.09(7)	0.0329149907(3)
2.76	−0.59959943669(7)	−1.1078080246(8)	21.55(8)	0.0331126264(3)
2.78	−0.59893536657(7)	−1.1053209486(9)	21.80(3)	0.0332912894(3)
2.8	−0.59826790637(7)	−1.1028708756(9)	22.49(8)	0.0334517633(3)
2.82	−0.59759741229(7)	−1.1004574935(10)	22.749(8)	0.0335947983(3)
2.84	−0.59692422590(8)	−1.098080490(2)	23.25(6)	0.0337211134(4)
2.86	−0.59624867462(8)	−1.0957395519(10)	23.709(9)	0.0338313977(4)
2.88	−0.59557107245(8)	−1.093434368(2)	24.21(5)	0.0339263115(4)
2.9	−0.59489172040(8)	−1.091164625(2)	25.03(10)	0.0340064881(4)
2.92	−0.59421090696(3)	−1.0889300116(3)	25.219(10)	0.03407253505(6)
2.94	−0.593528911(2)	−1.08673026(5)	25.738(4)	0.03412502(2)
2.96	−0.59284599217(3)	−1.0845649341(3)	26.26(5)	0.03416454400(8)
2.98	−0.59216241041(3)	−1.0824338493(4)	26.76(7)	0.03419160118(10)
3.0	−0.59147840772(4)	−1.0803366549(4)	27.36(4)	0.03420672017(8)

3.1	−0.5880599328(6)	−1.070348311(6)	30.26(4)	0.034119856(2)
3.2	−0.58466046763(10)	−1.0603781270(9)	1259.66(2)	0.0340446276(3)
3.3	−0.58127997743(9)	−1.0518876620(8)	1232.23(2)	0.0335370585(2)
3.4	−0.57795808(2)	−1.04412852(2)	1204.6(4)	0.032878704(10)
3.5	−0.57470822413(7)	−1.0370646924(6)	1179.23(2)	0.0321005017(2)
3.6	−0.57154111047(7)	−1.0306616527(6)	1154.97(2)	0.0312279356(2)
3.7	−0.56846506922(8)	−1.0248856731(7)	1132.39(2)	0.0302822879(2)
3.8	−0.5654864931(9)	−1.019703846(3)	1111.32(9)	0.02928135270(10)
3.9	−0.56261014104(7)	−1.0150840175(6)	1092.62(2)	0.0282400678(2)
4.0	−0.55983940264(8)	−1.0109947624(7)	1075.61(2)	0.0271710107(2)
4.1	−0.5571765089(3)	−1.007405341(3)	1060.64(3)	0.0260847993(5)
4.2	−0.5546227137(2)	−1.0042856823(9)	1047.86(2)	0.0249904155(2)
4.3	−0.5521784434(2)	−1.001606383(2)	1037.37(2)	0.0238954660(2)
4.4	−0.54984343(2)	−0.99933872(2)	1029.1(2)	0.022806391(4)
4.5	−0.5476167853(5)	−0.997454584(4)	1018(6)	0.0217286637(6)
4.6	−0.5454971583(5)	−0.995926681(3)	1020.97(2)	0.0206668772(5)
4.7	−0.54348277(4)	−0.99472847(8)	1021.1(2)	0.019624909(2)
4.8	−0.54157143(4)	−0.99383402(9)	1024.4(2)	0.018606008(4)
4.9	−0.53976073(6)	−0.9932185(2)	1030.8(3)	0.017612843(9)
5.0	−0.5380479038(7)	−0.992857735(3)	1040.49(5)	0.0166476145(4)

Table A67: Same as for Table A1, but for $10\,^3\Pi_u$.

$10\,^3\Pi_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.462248426393(4)	95.980230075(2)	2733.234(10)	−9999.94826364(10)
1.1	−0.506872219001(3)	16.0026640(2)	2739.06(4)	−399.771414(2)
1.2	−0.539431521022(3)	6.061794616(6)	2754.40(6)	−99.6090391(10)
1.3	−0.56319278626(2)	2.80976021(6)	2775.0(2)	−43.9420342(2)
1.4	−0.580429507616(4)	1.23714895(8)	2797.9(6)	−24.4238828(2)
1.5	−0.592761771998(9)	−0.22628863(7)	2844.0(2)	−10.4623135(2)
1.6	−0.601367271715(6)	−0.85706507(6)	2880.97(10)	−5.58671226(5)
1.7	−0.607116808834(4)	−1.16658569(3)	2903.88(3)	−3.35144136(7)
1.8	−0.610663788581(4)	−1.32528788(2)	2911.2(2)	−2.15791445(2)
1.9	−0.61250478104(5)	−1.405061520(3)	2903.61(2)	−1.455568649(8)
2.0	−0.613021383774(2)	−1.440718346(6)	2882.18(9)	−1.013546610(6)
2.1	−0.612509706282(3)	−1.4507089268(4)	2849.08(2)	−0.721381842(2)
2.2	−0.611201483977(2)	−1.445449662(3)	1403.1098(10)	−0.520952875(2)
2.3	−0.609279427903(7)	−1.431097320(3)	1377.768(4)	−0.3794117745(8)
2.4	−0.606888525467(7)	−1.4114165277(10)	1349.452(5)	−0.2771279656(4)
2.5	−0.604144472982(2)	−1.3887672269(5)	1318.963(6)	−0.2018320983(2)
2.6	−0.601140030158(8)	−1.3646548485(3)	1286.986(7)	−0.14556850346(7)
2.62	−0.600514738747(4)	−1.3400500537(2)	1254.096(8)	−0.10301771851(3)
2.64	−0.599882581905(10)	−1.31558110063(6)	1220.767(10)	−0.07052913741(2)
2.66	−0.599244068363(9)	−1.29165296248(3)	1187.38(2)	−0.045540823791(7)
2.68	−0.598599667484(4)	−1.26852289531(2)	1154.24(2)	−0.026219647040(4)
2.7	−0.597949847796(4)	−1.246349366722(9)	1121.60(2)	−0.011231494412(2)
2.72	−0.597295067429(2)	−1.225224285764(5)	1089.64(2)	0.0004092310818(6)
2.74	−0.596635712122(5)	−1.205194541447(3)	1058.51(3)	0.00944041470788(2)
2.76	−0.595972179345(5)	−1.1862765694946(6)	1028.343(8)	0.0164211022403(4)
2.78	−0.595304899532(4)	−1.1684663026668(8)	999.15(2)	0.0217793977983(9)
2.8	−0.594634224613(2)	−1.151746033948(2)	971.14(2)	0.025846305701(2)
2.82	−0.593960496626(2)	−1.139459417(4)	1900.227(5)	0.0282873766(10)
2.84	−0.593284093157(5)	−1.136089248588(3)	944.23(3)	0.028879963310(2)
2.86	−0.592605323969(2)	−1.121464491146(4)	918.06(2)	0.031083063887(2)
2.88	−0.591924463859(7)	−1.118660581506(3)	912.73(2)	0.031438684518(2)
2.9	−0.591241877511(7)	−1.11632235742(5)	1816.225(4)	0.03171912464(2)
2.92	−0.590557830734(10)	−1.115896536400(3)	907.21(2)	0.031768624418(2)
2.94	−0.589872585472(2)	−1.113172279051(4)	901.33(2)	0.032073870355(2)
2.96	−0.589186434115(2)	−1.110487926813(4)	894.72(2)	0.032355293276(2)
2.98	−0.588499605987(2)	−1.10908155799(5)	1781.378(5)	0.03249503083(2)
3.0	−0.587812355672(2)	−1.10784403237(3)	886.55(2)	0.032613565508(6)
3.1	−0.584377636817(8)	−1.10550042583(5)	−−	0.03282643764(2)
3.2	−0.580963625948(5)	−1.105242232831(3)	874.86(2)	0.0328489337063(6)
3.3	−0.577591254345(4)	−1.10334651619(5)	1722.156(7)	0.03300793537(2)
3.4	−0.574277344276(2)	−1.10268722897(2)	854.24(2)	0.033060522386(4)
3.5	−0.571035341941(2)	−1.10188132942(4)	1687.314(8)	0.03312268978(2)
3.6	−0.567875890428(8)	−1.10079714455(4)	1646.886(10)	0.033202172266(8)
3.7	−0.564807303558(8)	−1.10019335610(4)	807.74(3)	0.03324402356(2)
3.8	−0.561835948809(5)	−1.09997299408(3)	1601.97(2)	0.033258802907(6)
3.9	−0.558966561516(3)	−1.09929303151(2)	1550.99(2)	0.033302514175(3)
4.0	−0.556202505994(8)	−1.098729730003(7)	1495.74(2)	0.033336270236(2)
4.1	−0.55354599013(2)	−1.098232764728(4)	1434.77(2)	0.033363936680(6)

4.2	−0.550998244324(2)	−1.09780027186(2)	1371.04(2)	0.033386263793(9)
4.3	−0.548559672112(3)	−1.09740719054(3)	1304.12(3)	0.03340511716(2)
4.4	−0.546229975866(10)	−1.09702931580(4)	1232.20(3)	0.03342202159(2)
4.5	−0.544008264826(3)	−1.09667705983(4)	1159.66(3)	0.03343685589(2)
4.6	−0.541893146209(3)	−1.09632669753(5)	1084.11(3)	0.03345094718(2)
4.7	−0.539882804232(9)	−1.09598864046(5)	1010.15(3)	0.03346416609(3)
4.8	−0.537975068324(10)	−1.09563951801(5)	935.02(4)	0.03347769370(3)
4.9	−0.536167472618(10)	−1.0955268151(2)	455.57(8)	0.03348207421(6)
5.0	−0.534457308827(10)	−1.09526727254(5)	858.72(4)	0.03349224191(2)

Table A68: Same as for Table A1, but for $11\,^3\Pi_u$.

$11\,^3\Pi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.01	97.9900561042(3)	95.980629664(2)	4.18(2)	−9999.9482544(2)
0.05	17.99581814(4)	16.0030677(2)	4.20(6)	−399.771372(3)
0.1	8.0115526(2)	6.0622081(5)	4.35(8)	−99.608970(2)
0.15	4.7007396(2)	2.8101865(6)	4.4(2)	−43.941951(2)
0.2	3.0611740(2)	1.2375898(4)	4.8(2)	−24.4237911(2)
0.3	1.4564231(3)	−0.225821(2)	5.65(10)	−10.462223(5)
0.4	0.68903918(9)	−0.8565729(5)	6.75(6)	−5.5866282(8)
0.5	0.25480450(5)	−1.16607651(3)	7.96(10)	−3.3513714(3)
0.6	−0.01502645(3)	−1.32477014(8)	9.6(2)	−2.15786208(5)
0.7	−0.192835(2)	−1.40454350(2)	11.45(8)	−1.4555120(8)
0.8	−0.314690772(10)	−1.44020826(6)	13.1(4)	−1.01353340(5)
0.9	−0.400482545(10)	−1.45021459(9)	16.09(5)	−0.72138834(7)
1.0	−0.4619999009(3)	−1.44497817859(8)	8.5(6)	−0.5209783777(6)
1.1	−0.50662715654(3)	−1.43065527923(3)	10.0(3)	−0.37945542380(2)
1.2	−0.53919168454(6)	−1.411009792(2)	11.5(5)	−0.277188686(2)
1.3	−0.5629598273694(9)	−1.388401010(2)	14.2(3)	−0.2019087351(10)
1.4	−0.5802049607(4)	−1.3643337560(7)	16.7(3)	−0.14565988168(3)
1.5	−0.59254705314(9)	−1.339778133(2)	18.3(6)	−0.1031226849(9)
1.6	−0.6011636857(6)	−1.315361913(3)	21.3(4)	−0.0706465886(6)
1.7	−0.60692555222(4)	−1.2914896326(3)	24.5(6)	−0.04566972244(9)
1.8	−0.61048595847(4)	−1.2684181786(3)	28.0(5)	−0.0263590342(2)
1.9	−0.61234138315(5)	−1.2463057077(3)	32.7(4)	−0.0113804955(2)
2.0	−0.61287334104(2)	−1.22524387430(9)	37.1(3)	0.00025140389(3)
2.1	−0.61237786774(3)	−1.2052793654(2)	41.7(7)	0.00927446192(6)
2.2	−0.61108663429(2)	−1.1864284582(2)	47(3)	0.01624764110(4)
2.3	−0.60918229449(3)	−1.1686869522(2)	53.05(4)	0.02159897253(5)
2.4	−0.60680978929(3)	−1.1520369736(2)	60(2)	0.02565941876(5)
2.4779	−0.604667741703(9)	−1.13961094634(3)	−−	0.028138559692(2)
2.5	−0.6040847730(2)	−1.1364515835(2)	68.7(4)	0.0286871848(2)
2.6	−0.60109995342(3)	−1.1218974454(3)	78.0(5)	0.03088556210(8)
2.62	−0.60047864858(4)	−1.1191069489(3)	80.3(5)	0.03124059091(10)
2.6369	−0.599948290332(3)	−1.116779570014(6)	166.43(5)	0.03152072913212(9)
2.64	−0.59985049923(2)	−1.1163556708(4)	82.8(4)	0.0315701999(2)
2.66	−0.59921600242(5)	−1.1136430874(5)	85.8(4)	0.0318755329(2)
2.68	−0.59857563201(4)	−1.1109684769(7)	89.6(5)	0.0321577564(3)
2.6906	−0.598234009089(4)	−1.109565963251(8)	186.05(5)	0.0322983925245(6)
2.7	−0.59792983777(4)	−1.1083306785(9)	95.1(10)	0.0324181575(2)
2.718	−0.597344334596(4)	−1.10598632251(2)	207.58(5)	0.032635153304(2)
2.72	−0.597279041100(10)	−1.10572744428(5)	104.2(4)	0.032658322774(2)
2.7348	−0.596794457109(4)	−1.10382042858(2)	233.84(4)	0.032824515737(3)
2.74	−0.596623622530(5)	−1.1031534602(2)	122.4(4)	0.03288094338(4)
2.7464	−0.596412965241(4)	−1.10233404411(2)	265.85(4)	0.032949274094(5)
2.7551	−0.596125907680(4)	−1.10122116589(3)	304.21(4)	0.033040778728(7)
2.76	−0.595963882309(5)	−1.10059377577(6)	166.7(3)	0.03309202495(2)
2.7618	−0.595904299706(4)	−1.10036299656(4)	347.55(4)	0.033110870755(10)
2.7674	−0.595718714072(4)	−1.09964327880(5)	397.24(4)	0.03316981620(2)
2.7721	−0.595562698420(4)	−1.09903636255(6)	451.41(4)	0.03321995393(2)
2.7763	−0.595423079198(4)	−1.09849107982(7)	511.43(4)	0.03326552555(3)

2.78	−0.595299921387(4)	−1.09800811718(8)	574.34(3)	0.03330637611(3)
2.7834	−0.595186615074(4)	−1.09756220810(9)	640.50(3)	0.03334447871(3)
2.7867	−0.595076516704(5)	−1.09712781636(10)	711.70(3)	0.03338185562(4)
2.7898	−0.594972978295(5)	−1.09671886914(10)	783.57(3)	0.03341712218(4)
2.7929	−0.594869330663(5)	−1.0963098036(2)	858.45(3)	0.03345227461(4)
2.7959	−0.594768923268(5)	−1.0959146186(2)	931.77(2)	0.03348590005(4)
2.799	−0.594665063987(5)	−1.0955077998(2)	1006.23(2)	0.03351994577(4)
2.8	−0.5946315386020(10)	−1.095377028(3)	514.6(4)	0.033530732(2)
2.8023	−0.594554389796(5)	−1.0950772768(2)	1081.83(2)	0.03355511643(4)
2.8057	−0.594440242735(5)	−1.0946371228(2)	1153.88(2)	0.03358996425(4)
2.8094	−0.594315892377(5)	−1.09416251997(10)	1224.17(2)	0.03362613540(4)
2.8136	−0.594174580271(5)	−1.09362945405(10)	1293.13(2)	0.03366495113(3)
2.8183	−0.594016258178(5)	−1.09303974554(9)	1357.217(9)	0.03370569876(3)
2.82	−0.593958946465(3)	−1.0928280902(2)	688.6(2)	0.03371978821(4)
2.8239	−0.593827378065(5)	−1.09234553139(8)	1417.841(8)	0.03375092062(3)
2.8306	−0.593601077010(6)	−1.09152516835(8)	1472.420(7)	0.03380095586(3)
2.8393	−0.593306745721(6)	−1.09047342724(7)	1522.169(6)	0.03386048118(2)
2.84	−0.59328304180(2)	−1.09038937544(9)	762.61(4)	0.03386503809(2)
2.8509	−0.592913540866(6)	−1.08908996550(7)	1564.473(5)	0.03393213239(2)
2.86	−0.59260452297(2)	−1.0880171120(2)	792.80(3)	0.03398319369(6)
2.8677	−0.592342696271(6)	−1.08711681558(6)	1598.360(4)	0.03402328590(2)
2.88	−0.59192384272(7)	−1.0856917588(2)	805.89(3)	0.03408191896(3)
2.8951	−0.591408714585(6)	−1.08396286582(6)	1621.273(4)	0.03414547454(2)
2.9	−0.59124135550(2)	−1.08340650522(10)	811.4(2)	0.03416420884(8)
2.92	−0.590557373848(10)	−1.0811586108(2)	813.3(2)	0.03423155375(4)
2.94	−0.58987218654(2)	−1.0789467297(2)	813.2(2)	0.03428491270(4)
2.96	−0.58918606564(2)	−1.07798469385(6)	1625.873(4)	0.03430415481(2)
2.98	−0.58849926967(2)	−1.076770059346(6)	811.9(2)	0.03432502429(2)
3.0	−0.58781204522(2)	−1.074628033947(6)	809.8(2)	0.03435251857(3)
3.1	−0.58436492493(3)	−1.07252022(8)	807.3(2)	0.03436796(3)
3.1078	−0.58411006759(2)	−1.06293645935(7)	791.2(2)	0.034126900167(9)
3.2	−0.58096343046(5)	−1.061733(2)	1580.053658(2)	0.034264(2)
3.3	−0.57759108301(4)	−1.05324602(7)	773.3(2)	0.03396276(2)
3.4	−0.574277189289(8)	−1.0447766170(3)	1511.96(6)	0.03345622697(6)
3.5	−0.571035198119(2)	−1.03703665861(5)	1478.02(4)	0.03279932939(2)
3.6	−0.567875755256(3)	−1.02999049468(2)	1415.0(3)	0.032022829018(4)
3.7	−0.564807175100(2)	−1.02360346602(2)	64.9(2)	0.031152234582(5)
3.8	−0.56183582528(2)	−1.01784176039(2)	−551(7)	0.030208808057(3)
3.9	−0.558966441870(7)	−1.01267236573(6)	−523(7)	0.02921033810(3)
4.0	−0.556202389305(7)	−1.00806302659(3)	86.6(2)	0.028171758236(10)
4.1	−0.553545875476(7)	−1.00398220690(3)	95.5(2)	0.02710564292(2)
4.2	−0.550998130963(7)	−1.00039906000(4)	105.1(2)	0.02602260754(2)
4.3	−0.548559559079(10)	−0.99728340973(4)	−−	0.02493163147(2)
4.4	−0.546229862302(10)	−0.994605742821(6)	−378(6)	0.023840319837(6)
4.5	−0.544008149494(10)	−0.99233721367(2)	140.9(2)	0.022755116112(7)
4.6	−0.541893027489(9)	−0.99044966122(2)	155.5(2)	0.021681475052(8)
4.7	−0.539882679927(9)	−0.98891563816(2)	171.7(2)	0.020624003648(8)
4.8	−0.537974935723(10)	−0.98770845256(3)	189.8(2)	0.019586576012(9)
4.9	−0.536167329192(10)	−0.98680222429(5)	210.0(2)	0.01857242648(2)
5.0	−0.534457153946(10)	−0.98617196544(5)	−164(5)	0.01758422304(2)

Table A69: Same as for Table A1, but for $1\,^1\Delta_g$ (J state).

		$1\,^1\Delta_g$		
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.055620732852246(6)	–	249.3999921(1)	–
0.01	97.94464063225(8)	95.8897987253(4)	249.495(5)	−9999.94825392(3)
0.05	17.950402758(2)	15.91223701(2)	251.715(2)	−399.7713702(3)
0.1	7.966137799(2)	5.971379772(8)	257.7675(3)	−99.60895827(6)
0.15	4.655326122(10)	2.71936403(9)	266.582(4)	−43.9419215(5)
0.2	3.0157626470(4)	1.146776579(3)	277.4901(10)	−24.42374358(2)
0.3	1.4110187858(2)	−0.316601808(2)	303.983(2)	−10.462131266(4)
0.4	0.64364598011(10)	−0.9473064696(9)	334.9933(8)	−5.586496075(2)
0.5	0.20942662468(5)	−1.2567450891(5)	369.2268(7)	−3.3511966770(9)
0.6	−0.06038473758(7)	−1.4153564736(8)	405.8327(4)	−2.157644997(2)
0.7	−0.238168788667(6)	−1.4950313299(3)	444.1652(7)	−1.4552767894(4)
0.8	−0.359997345352(5)	−1.5305818482(3)	483.6862(6)	−1.0132339469(3)
0.9	−0.445757193490(3)	−1.5404589218(3)	523.9099(3)	−0.7210494831(2)
1.0	−0.507238765568(2)	−1.5350791419(2)	564.38021(3)	−0.5206016107(2)
1.1	−0.551826510264(2)	−1.5205994788(2)	604.65916(9)	−0.3790422348(2)
1.2	−0.584347966331(2)	−1.5007847822(2)	644.3213(2)	−0.2767407079(2)
1.3	−0.608069642915(2)	−1.4779952685(2)	682.9511(2)	−0.20142767898(10)
1.4	−0.625265089996(2)	−1.4537367149(2)	720.1432(3)	−0.14514752492(9)
1.5	−0.637554458244(2)	−1.4289802064(2)	755.50399(9)	−0.10258085994(8)
1.6	−0.646115512699(2)	−1.4043545041(2)	788.6509(10)	−0.07007717418(7)
1.7	−0.651819138081(2)	−1.3802651611(2)	819.2249(3)	−0.04507463820(6)
1.8	−0.655318833653(2)	−1.3569700867(2)	846.8729(2)	−0.02574023302(6)
1.9	−0.6571112747985(9)	−1.3346284697(2)	871.2699(2)	−0.01073995792(5)
2.0	−0.657578175515(2)	−1.3133330016(2)	892.1116(2)	0.00091167472(5)
2.1	−0.6570157725599(9)	−1.2931314085(2)	909.118451(5)	0.00995244599(5)
2.2	−0.655655939719(2)	−1.2740410080(2)	922.0376(2)	0.01694130518(4)
2.3	−0.6536815346421(8)	−1.2560586436(2)	930.6464(2)	0.02230627202(4)
2.4	−0.651237703586(2)	−1.2391675119(2)	934.75261(10)	0.02637828968(4)
2.5	−0.648440309661(2)	−1.22334187472(10)	934.1976(2)	0.02941549784(4)
2.6	−0.645382285520(2)	−1.20855031659(10)	928.8582(2)	0.03162086710(4)
2.7	−0.642138469418(2)	−1.19475799353(2)	918.6476(2)	0.03315516493(4)
2.8	−0.6387693202308(8)	−1.1819281760(2)	903.5176(2)	0.03414659445(4)
2.9	−0.635323795042(2)	−1.1700232967(2)	883.4601(2)	0.03469803220(3)
3.0	−0.6318415950686(8)	−1.1590056488(2)	858.5083(2)	0.03489251378(3)
3.1	−0.628354930861(2)	−1.1488378379(2)	828.7376(2)	0.03479742705(3)
3.2	−0.624889918637(2)	−1.1394830604(2)	794.2667(2)	0.03446774277(3)
3.3	−0.621467691419(2)	−1.1309052612(2)	755.2582(2)	0.03394852171(3)
3.4	−0.6181052881259(8)	−1.1230692072(2)	711.91896(9)	0.03327687324(3)
3.5	−0.614816368695(2)	−1.1159405055(2)	664.4998(2)	0.03248349484(3)
3.6	−0.611611792070(2)	−1.1094855841(2)	613.2956(2)	0.03159388889(3)
3.7	−0.608500085550(2)	−1.1036716527(2)	558.6440(2)	0.03062932930(3)
3.8	−0.605487827630(2)	−1.0984666501(2)	500.9243(2)	0.02960763294(3)
3.9	−0.602579961668(2)	−1.0938391903(2)	440.5554(2)	0.02854377771(3)
4.0	−0.599780054032(2)	−1.0897585092(2)	377.9932(2)	0.02745039972(4)
4.1	−0.59709050752(2)	−1.0861944183(2)	313.7279(2)	0.02633819432(4)
4.2	−0.59451273861(2)	−1.0831172663(2)	248.2795(2)	0.02521624070(4)
4.3	−0.59204732551(2)	−1.0804979108(2)	182.1937(2)	0.02409226517(4)
4.4	−0.58969413232(2)	−1.0783077013(2)	116.0364(2)	0.02297285531(4)

4.5	−0.587452413905(2)	−1.0765184726(2)	50.3879(2)	0.02186363450(4)
4.6	−0.58532090495(2)	−1.0751025488(2)	−14.1644(2)	0.02076940458(4)
4.7	−0.58329789605(2)	−1.0740327578(2)	−77.0331(2)	0.01969426262(4)
4.8	−0.58138129929(2)	−1.0732824534(2)	−137.6389(2)	0.01864169692(3)
4.9	−0.57956870499(2)	−1.0728255467(2)	−195.4192(2)	0.01761466598(3)
5.0	−0.5778574313451(9)	−1.07263654358(4)	−249.8371(2)	0.016615663821(6)
5.1	−0.57624456807(2)	−1.0726905879(2)	−300.39034(6)	0.01564677417(3)
5.2	−0.57472701512(2)	−1.0729635094(2)	−346.62071(6)	0.01470971554(3)
5.3	−0.57330151724(2)	−1.0734318762(2)	−388.12233(6)	0.01380587891(3)
5.4	−0.57196469513(2)	−1.0740730496(2)	−424.55003(6)	0.01293635939(2)
5.5	−0.5707130736461(10)	−1.0748652412(2)	−455.62660(7)	0.01210198292(3)
5.6	−0.56954310754(2)	−1.0757875721(2)	−481.14855(5)	0.01130332911(2)
5.7	−0.56845120509(2)	−1.0768201322(2)	−500.99099(5)	0.01054075052(2)
5.8	−0.56743374995(2)	−1.07794403860(10)	−515.10989(5)	0.00981438988(2)
5.9	−0.56648712138(2)	−1.07914149229(10)	−523.54296(4)	0.00912419500(2)
6.0	−0.5656077130156(8)	−1.0803958311(2)	−526.40821(6)	0.00846993250(2)
6.5	−0.5620958545227(7)	−1.08702241688(2)	−466.342356(8)	0.005718352641(3)
7.0	−0.5597588069529(6)	−1.09327995541(2)	−319.624503(7)	0.003748236927(2)
7.5	−0.5582430041811(6)	−1.09844500090(2)	−143.919569(6)	0.002405467662(2)
8.0	−0.5572765084694(5)	−1.10235713531(7)	16.25444(4)	0.001524485205(7)
8.5	−0.5566657784146(4)	−1.10516157937(5)	139.17337(3)	0.000961173819(5)
9.0	−0.5562807673480(4)	−1.10710387325(5)	221.20754(3)	0.000606406828(4)
9.5	−0.5560373516877(3)	−1.10842077012(4)	268.18138(2)	0.000384624554(3)
10.0	−0.5558823395249(3)	−1.10930212830(3)	288.86959(2)	0.000246255076(2)
11.0	−0.5557172626635(2)	−1.11027501915(2)	283.074177(10)	0.0001054096526(8)
12.0	−0.5556442468329(2)	−1.11070175639(2)	249.94157(2)	0.0000488947732(7)
13.0	−0.55560891584507(8)	−1.11089271310(2)	211.74911(2)	0.0000250091226(6)
14.0	−0.55559002375800(7)	−1.110982666208(10)	176.94278(2)	0.0000140986650(3)
15.0	−0.55557895352912(6)	−1.111028620149(9)	147.72163(2)	0.0000086191274(2)
16.0	−0.55557198533841(5)	−1.111054497715(4)	123.921656(7)	0.00000559206019(3)
17.0	−0.55556737127515(3)	−1.111070483806(2)	104.691749(8)	0.00000377992608(6)
18.0	−0.55556420810772(2)	−1.1110811031163(5)	89.121911(6)	0.00000262850542(7)
19.0	−0.55556198592162(2)	−1.1110885180730(4)	76.434402(4)	0.0000018659878(2)
20.0	−0.555560395819745(10)	−1.1110938651653(7)	66.013132(3)	0.00000134632363(9)

Table A70: Same as for Table A1, but for $2\,^1\Delta_g$ (S state).

$2\,^1\Delta_g$				
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.031279846178687(7)	–	129.1751887(8)	–
0.01	97.9689815171(6)	95.938480492(7)	129.1(2)	−9999.9482542(6)
0.05	17.974743568(4)	15.96091845(3)	130.27(9)	−399.7713737(5)
0.1	7.990478260(5)	6.02005964(4)	133.49(10)	−99.6089688(3)
0.15	4.679665835(4)	2.76804054(3)	138.20(10)	−43.9419408(2)
0.2	3.040101130(3)	1.19544761(3)	144.05(10)	−24.42377326(9)
0.3	1.435353191(2)	−0.26794865(2)	158.34(9)	−10.46218345(4)
0.4	0.667973981(2)	−0.89868087(2)	175.20(9)	−5.58657208(3)
0.5	0.233745815(3)	−1.20815680(3)	194.058(5)	−3.35129687(5)
0.6	−0.036076769(3)	−1.36681506(3)	214.249(5)	−2.15776921(4)
0.7	−0.2138744247(7)	−1.446546050(7)	235.6(5)	−1.455424573(9)
0.8	−0.3357189126(6)	−1.482161560(7)	257.7(2)	−1.013404669(7)
0.9	−0.4214969484(5)	−1.492112037(6)	280.31(7)	−0.721242378(6)
1.0	−0.4829988831(5)	−1.486813583(6)	303.37(7)	−0.520815817(5)
1.1	−0.5276090751(4)	−1.472422645(5)	326.53(6)	−0.379276813(4)
1.2	−0.5601549662(4)	−1.452703523(5)	349.58(6)	−0.276994659(4)
1.3	−0.5839029627(4)	−1.430015856(5)	372.29(5)	−0.201699947(3)
1.4	−0.6011265066(3)	−1.405864824(4)	394.44(5)	−0.145437007(3)
1.5	−0.6134456363(3)	−1.381220891(4)	415.83(4)	−0.102886412(3)
1.6	−0.6220380003(3)	−1.356712180(4)	436.23(4)	−0.070397612(2)
1.7	−0.6277743631(2)	−1.332743588(4)	455.47(3)	−0.045408742(2)
1.8	−0.6313081002(2)	−1.309572348(4)	473.35(3)	−0.026086749(2)
1.9	−0.6331357600(2)	−1.287356959(4)	489.68(3)	−0.011097600(2)
2.0	−0.6336389265(2)	−1.266189406(4)	504.31(2)	0.000544224(2)
2.1	−0.6331137032(2)	−1.246116692(4)	516.63(10)	0.009576531(2)
2.2	−0.6317918279(2)	−1.227155397(4)	527.4(2)	0.016558299(2)
2.3	−0.6298560197(2)	−1.209301614(4)	535.9(2)	0.021917576(2)
2.4	−0.6274512833(2)	−1.192537773(4)	542.2(2)	0.025985331(2)
2.5	−0.62469333803(10)	−1.176837358(4)	546.1(2)	0.029019727(2)
2.6	−0.62167497012(10)	−1.162168163(4)	547.6(2)	0.031223761(2)
2.7	−0.61847086911(9)	−1.148494542(4)	546.5(2)	0.032758221(2)
2.8	−0.61514134299(8)	−1.135778956(4)	542.9(2)	0.0337513320(10)
2.9	−0.61173519588(8)	−1.123983019(4)	536.6(2)	0.0343059907(10)
3.0	−0.60829197421(7)	−1.113068200(4)	527.7(2)	0.0345052495(10)
3.1	−0.60484373213(7)	−1.102996279(4)	516.1(2)	0.0344165114(10)
3.2	−0.60141642811(7)	−1.093729629(4)	502.0(2)	0.0340947587(10)
3.3	−0.59803103643(6)	−1.085231374(4)	485.2(2)	0.0335850603(9)
3.4	−0.59470443667(6)	−1.077465474(4)	466.1(2)	0.0329245293(9)
3.5	−0.59145012934(6)	−1.070396743(4)	444.6(2)	0.0321438617(9)
3.6	−0.58827881435(5)	−1.063990841(4)	420.7(2)	0.0312685523(9)
3.7	−0.58519886109(5)	−1.058214239(4)	394.6(2)	0.0303198605(9)
3.8	−0.58221669200(5)	−1.053034178(4)	366.5(3)	0.0293155805(8)
3.9	−0.57933709708(5)	−1.048418626(5)	336.9(2)	0.0282706585(9)
4.0	−0.57656349303(5)	−1.044336233(5)	305.3(2)	0.0271976883(10)
4.1	−0.5738981379(4)	−1.040756299(5)	272.4(2)	0.0261073114(9)
4.2	−0.5713423091(4)	−1.037648749(5)	238.2(2)	0.0250085404(9)
4.3	−0.5688964534(4)	−1.034984119(4)	203.1(2)	0.0239090205(8)
4.4	−0.5665603124(4)	−1.032733554(4)	167.3(2)	0.0228152434(8)

4.5	$-0.56433302860(4)$	$-1.030868818(4)$	$131.1(2)$	$0.0217327198(7)$
4.6	$-0.5622132368(4)$	$-1.029362313(4)$	$94.7(2)$	$0.0206661219(7)$
4.7	$-0.5601991410(4)$	$-1.028187105(4)$	$58.4(2)$	$0.0196193993(6)$
4.8	$-0.5582885830(3)$	$-1.027316968(4)$	$22.5(2)$	$0.0185958747(6)$
4.9	$-0.5564790998(3)$	$-1.026726416(4)$	$-12.6(2)$	$0.0175983232(6)$
5.0	$-0.55476797555(3)$	$-1.026390758(4)$	$-46.485(2)$	$0.0166290386(6)$
5.1	$-0.5531522871(2)$	$-1.026286143(2)$	$-79.4315(7)$	$0.0156898885(3)$
5.2	$-0.5516289434(2)$	$-1.026389605(2)$	$-110.8608(7)$	$0.0147823619(3)$
5.3	$-0.5501947219(2)$	$-1.026679113(2)$	$-140.5207(6)$	$0.0139076095(3)$
5.4	$-0.5488463004(2)$	$-1.027133611(2)$	$-168.1766(6)$	$0.0130664796(3)$
5.5	$-0.54758028570(3)$	$-1.027733055(2)$	$-193.6151(6)$	$0.0122595485(2)$
5.6	$-0.5463932394(2)$	$-1.028458445(2)$	$-216.6473(6)$	$0.0114871488(2)$
5.7	$-0.5452817009(2)$	$-1.029291853(2)$	$-237.1121(5)$	$0.0107493945(2)$
5.8	$-0.5442422082(2)$	$-1.030216435(2)$	$-254.8786(5)$	$0.0100462036(2)$
5.9	$-0.5432713164(2)$	$-1.031216447(2)$	$-269.8489(5)$	$0.0093773196(2)$
6.0	$-0.54236561426(2)$	$-1.032277247(2)$	$-281.9597(5)$	$0.0087423303(2)$
6.5	$-0.53869960442(2)$	$-1.0380567891(7)$	$-299.9114(4)$	$0.00605267996(9)$
7.0	$-0.53619200485(2)$	$-1.0437716053(6)$	$-256.6901(3)$	$0.00408748635(6)$
7.5	$-0.53451438596(3)$	$-1.0487145211(4)$	$-176.8895(3)$	$0.00270856678(4)$
8.0	$-0.533409627363(7)$	$-1.0526346196(3)$	$-87.8654(3)$	$0.00177307939(3)$
8.5	$-0.532688724014(5)$	$-1.0555684285(2)$	$-8.9711(2)$	$0.00115400230(2)$
9.0	$-0.532219837300(4)$	$-1.05768436195(10)$	$51.4683(2)$	$0.000750590296(7)$
9.5	$-0.531914529402(2)$	$-1.05917808133(5)$	$93.2808(2)$	$0.000489576577(3)$
10.0	$-0.531714996043(2)$	$-1.06022288149(3)$	$120.2700(2)$	$0.0003207110602(6)$
11.0	$-0.5314981603599(7)$	$-1.06147956779(7)$	$147.16930(8)$	$0.000137886631(5)$
12.0	$-0.531405525917(3)$	$-1.0620946507(4)$	$138.12363(8)$	$0.00005970010(3)$
13.0	$-0.531361214888(5)$	$-1.0622847559(4)$	$98.81519(9)$	$0.00003366722(3)$
14.0	$-0.531333519958(5)$	$-1.0623473884(3)$	$70.29746(9)$	$0.00002283225(2)$
15.0	$-0.531314154695(5)$	$-1.0623827543(3)$	$53.13734(9)$	$0.00001637034(2)$
16.0	$-0.531300061427(5)$	$-1.0624066413(3)$	$42.10912(9)$	$0.00001209260(2)$
17.0	$-0.531289529900(4)$	$-1.0624236023(3)$	$34.38081(9)$	$0.000009144559(9)$
18.0	$-0.531281491309(4)$	$-1.0624361620(2)$	$28.59996(9)$	$0.000007045589(8)$
19.0	$-0.531275253649(3)$	$-1.0624459037(2)$	$24.09626(6)$	$0.000005505454(4)$
20.0	$-0.531270354143(3)$	$-1.06245378378(9)$	$20.50273(5)$	$0.000004346226(3)$

Table A71: Same as for Table A1, but for $3\,^1\Delta_g$.

$3\,^1\Delta_g$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.020015836159984(4)	–	71.883131(6)	–
0.01	97.980245529(5)	95.96100853(5)	71.86(4)	−9999.948252(4)
0.05	17.98600758(2)	15.98344649(9)	72.51(4)	−399.771373(2)
0.1	8.00174219(3)	6.0425873(2)	74.28(6)	−99.608970(4)
0.15	4.69092953(2)	2.7905671(2)	76.90(7)	−43.9419463(6)
0.2	3.05136446(2)	1.21797248(10)	80.19(7)	−24.4237822(4)
0.3	1.446615227(10)	−0.24542957(8)	88.25(6)	−10.4622001(3)
0.4	0.679233933(8)	−0.87617091(7)	97.78(6)	−5.5865969(2)
0.5	0.245002857(8)	−1.18565933(7)	108.37(6)	−3.35133009(10)
0.6	−0.02482075981(3)	−1.3443566609(3)	3.258(2)	−2.1578585688(4)
0.7	−0.20262823114(3)	−1.42412848659(2)	3.8803(6)	−1.45553146343(9)
0.8	−0.324484267791(10)	−1.45979147600(5)	4.58869(5)	−1.01352867552(4)
0.9	−0.410275539110(6)	−1.46979576992(4)	5.40304(3)	−0.72138299077(3)
1.0	−0.471792341600(3)	−1.46455714368(2)	6.326945(5)	−0.520972460483(9)
1.1	−0.516418973735(4)	−1.45023169847(3)	7.368367(9)	−0.37944886454(2)
1.2	−0.548982812872(3)	−1.43058337193(3)	8.536557(8)	−0.27718145515(2)
1.3	−0.572750197621(2)	−1.40797143246(2)	9.841779(7)	−0.20190079786(2)
1.4	−0.589994499745(3)	−1.38390067775(3)	11.295451(8)	−0.14565119875(2)
1.5	−0.602335685102(2)	−1.35934118596(3)	12.910269(8)	−0.10311321051(2)
1.6	−0.610951328144(2)	−1.33492068687(3)	14.700317(7)	−0.07063626912(2)
1.7	−0.616712117902(2)	−1.31104368066(2)	16.681248(6)	−0.045658496972(10)
1.8	−0.620271353389(2)	−1.28796700419(2)	18.870468(5)	−0.026346831894(8)
1.9	−0.622125505637(2)	−1.26584875641(2)	21.287345(4)	−0.011367234282(7)
2.0	−0.6226560805980(7)	−1.244780524050(7)	23.95346839(2)	0.000265818573(3)
2.1	−0.622159103652(2)	−1.22480891484(2)	26.892898(3)	0.009290139270(7)
2.2	−0.620866234232(2)	−1.20595011697(2)	30.132527(3)	0.016264705222(7)
2.3	−0.618960112991(2)	−1.18819983612(3)	33.702399(3)	0.021617560808(8)
2.4	−0.616585666905(3)	−1.17154012524(3)	37.636135(4)	0.025679670239(9)
2.5	−0.613858537891(3)	−1.15594410005(3)	41.971406(4)	0.028709190293(10)
2.6	−0.610871435917(3)	−1.14137920080(4)	46.750460(5)	0.03090910424(2)
2.7	−0.607698975532(4)	−1.12780944559(4)	52.020736(5)	0.03244018721(2)
2.8	−0.604401391425(2)	−1.115196979360(4)	57.835574(2)	0.03343064410335(5)
2.9	−0.601027416646(4)	−1.10350312872(6)	64.254979(7)	0.03398334640(2)
3.0	−0.597616529274(10)	−1.0926891085(2)	71.34661(2)	0.03418131668(4)
3.1	−0.59420071848(2)	−1.0827164840(2)	79.1862(4)	0.03409192033(5)
3.2	−0.59080588190(2)	−1.0735474610(2)	87.8620(9)	0.03377009463(5)
3.3	−0.58745293793(2)	−1.0651450579(2)	97.46971(6)	0.03326085393(5)
3.4	−0.58415871625(2)	−1.0574731960(2)	108.1208(4)	0.03260124604(5)
3.5	−0.58093667459(2)	−1.0504967369(3)	119.94097(4)	0.03182188922(6)
3.6	−0.57779747858(2)	−1.0441814875(3)	133.07352(3)	0.03094818602(6)
3.7	−0.57474947340(2)	−1.0384941867(3)	147.68172(5)	0.03000128651(6)
3.8	−0.57179906915(2)	−1.0334024864(3)	163.95228(5)	0.02899885575(6)
3.9	−0.56895105754(2)	−1.0288749346(3)	182.09917(5)	0.02795568731(5)
4.0	−0.56620887362(2)	−1.0248809676(3)	202.36831(5)	0.02688419490(5)
4.1	−0.563574813217(5)	−1.02139091720(8)	225.0414(10)	0.02579480713(2)
4.2	−0.561050215121(5)	−1.01837603642(8)	250.4518(2)	0.02469628424(2)
4.3	−0.558635614663(5)	−1.01580854864(8)	278.9745(8)	0.02359597225(2)
4.4	−0.556330874661(6)	−1.01366172450(8)	311.0542(2)	0.02250000564(2)

4.5	−0.55413529822(2)	−1.0119099911(3)	347.21066(6)	0.02141346786(5)
4.6	−0.552047727289(5)	−1.01052907920(8)	388.05181(6)	0.02034051639(2)
4.7	−0.550066630351(5)	−1.00949621840(9)	434.29629(2)	0.01928447709(2)
4.8	−0.548190181945(5)	−1.00879038834(9)	486.79518(3)	0.01824791157(2)
4.9	−0.546416336826(6)	−1.00839264490(9)	546.56083(3)	0.01723265893(2)
5.0	−0.54474290121(6)	−1.0082865417(10)	614.8017(3)	0.0162398521(2)
5.1	−0.54316760344(2)	−1.0084586730(3)	692.96548(5)	0.01526990861(4)
5.2	−0.54168816772(2)	−1.0088993914(3)	782.78671(5)	0.01432248924(4)
5.3	−0.54030239268(2)	−1.0096037279(3)	886.34353(5)	0.01339642594(4)
5.4	−0.53900823979(2)	−1.0105725927(3)	1006.11187(4)	0.01248960867(5)
5.5	−0.53780393483(2)	−1.0118142927(3)	1145.00707(4)	0.01159883217(5)
5.6	−0.53668808661(2)	−1.0133463660(3)	1306.38205(3)	0.01071960844(5)
5.7	−0.53565982494(2)	−1.0151975807(4)	1493.92352(2)	0.00984597705(5)
5.8	−0.53471895438(3)	−1.0174095824(4)	1711.336777(8)	0.00897040111(6)
5.9	−0.53386610648(3)	−1.0200369111(6)	1961.636077(6)	0.00808394947(8)
6.0	−0.53310284405(3)	−1.0231427458(6)	2245.78077(3)	0.00717715704(10)
6.5	−0.53071320415(6)	−1.045964723(2)	3768.18470(9)	0.0023787208(3)
7.0	−0.53036271505(8)	−1.063480641(2)	3646.6948(2)	−0.0003936016(2)
7.5	−0.53069709275(8)	−1.066977502(2)	2672.5991(2)	−0.0007444422(2)
8.0	−0.53102272770(7)	−1.0663320411(8)	1869.1923(2)	−0.00053582321(9)
8.5	−0.53123243163(6)	−1.0651220685(7)	1297.1556(2)	−0.00031261239(7)
9.0	−0.53134699728(6)	−1.0641086033(7)	897.6494(2)	−0.00015717874(6)
9.5	−0.53139969576(6)	−1.0633887598(6)	619.7807(2)	−0.00006203877(6)
10.0	−0.53141584831(6)	−1.0629109010(6)	426.3823(2)	−0.00000792044(5)
11.0	−0.53139704439(5)	−1.0623979304(5)	195.2441(2)	0.00003601440(3)
12.0	−0.53135574744(4)	−1.06220947639(9)	95.2160(2)	0.000041834873(2)
13.0	−0.53132000903(2)	−1.06226615858(4)	72.0434(2)	0.00002875842243(2)
14.0	−0.53129727480(2)	−1.06234791395(4)	61.5091(2)	0.0000176168325(10)
15.0	−0.531283198196(8)	−1.06239921337(3)	52.0714(2)	0.0000111455346(10)
16.0	−0.531274082048(7)	−1.06242958327(3)	43.7143(2)	0.0000074113018(8)
17.0	−0.531267896346(5)	−1.06244848971(2)	36.6592(3)	0.0000051354697(6)
18.0	−0.531263544934(4)	−1.06246106290(2)	30.8478(3)	0.0000036681647(4)
19.0	−0.531260402126(3)	−1.062469898203(10)	26.1040(2)	0.0000026792658(3)
20.0	−0.531258087002(3)	−1.062476355620(8)	22.2333(2)	0.0000019909192(2)

Table A72: Same as for Table A1, but for $1\,^3\Delta_g$ (j state).

$1\,^3\Delta_g$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.055620732852246(6)	–	−25.322839(1)	–
0.01	97.94462504930(8)	95.8897675464(9)	−25.35573(6)	−9999.94825522(7)
0.05	17.950387042(5)	15.91220533(4)	−26.09617(10)	−399.7713751(5)
0.1	7.966121699(10)	5.97134665(7)	−28.2619(3)	−99.6089675(5)
0.15	4.6553094399(8)	2.719328728(6)	−31.674(5)	−43.94193434(3)
0.2	3.0157452463(4)	1.146738665(3)	−36.223(6)	−24.42375914(2)
0.3	1.4109996263(2)	−0.316645940(2)	−48.556(2)	−10.462150644(3)
0.4	0.64362474137(7)	−0.9473577703(7)	−65.07352(2)	−5.586518132(2)
0.5	0.20940307854(4)	−1.2568041734(4)	−85.694007(5)	−3.3512206610(7)
0.6	−0.06041075435(4)	−1.4154237141(5)	−110.38069(8)	−2.1576703423(7)
0.7	−0.23819738850(2)	−1.4951069019(2)	−139.1039(4)	−1.4553030355(3)
0.8	−0.360028598215(2)	−1.5306657564(7)	−171.8273(5)	−1.013260701(2)
0.9	−0.445791132413(2)	−1.5405510218(10)	−208.490(3)	−0.7210763965(7)
1.0	−0.507275390884(2)	−1.5351791582(9)	−249.014(4)	−0.5206283763(6)
1.1	−0.551865793188(2)	−1.5207070223(4)	−293.314(2)	−0.3790685784(6)
1.2	−0.584389852239(6)	−1.5008993679(4)	−341.2821(7)	−0.2767663864(5)
1.3	−0.6081140544401(10)	−1.4781163328(3)	−392.790(3)	−0.2014524802(4)
1.4	−0.625311930040(2)	−1.4538636329(10)	−447.7023(3)	−0.1451712662(6)
1.5	−0.637603612891(2)	−1.4291123072(10)	−505.8724(3)	−0.1026033875(5)
1.6	−0.646166854039(2)	−1.4044910871(10)	−567.1388(8)	−0.0700983618(5)
1.7	−0.651872526918(2)	−1.3804055102(2)	−631.3291(2)	−0.04509438610(6)
1.8	−0.655374122083(2)	−1.3571134842(10)	−698.274(2)	−0.0257584667(5)
1.9	−0.6571683086315(8)	−1.3347742060(2)	−767.784(4)	−0.0107566258(2)
2.0	−0.657636796522(2)	−1.3134803887(10)	−839.663(2)	0.0008966022(5)
2.1	−0.6570758205306(7)	−1.29327978465(10)	−913.7167(2)	0.00993897925(4)
2.2	−0.6557172543224(7)	−1.27418974794(10)	−989.7472(2)	0.01692943668(4)
2.3	−0.653743957076(2)	−1.25620716262(10)	−1067.5422(2)	0.02229597893(4)
2.4	−0.6513010780162(7)	−1.23931526982(9)	−1146.892(5)	0.02636953583(10)
2.5	−0.6485044844504(7)	−1.22348837915(8)	−1227.565(5)	0.02940823581(9)
2.6	−0.6454471142490(7)	−1.20869512355(6)	−1309.340(5)	0.03161504027(9)
2.7	−0.6422038117048(7)	−1.19490070783(10)	−1391.97425(7)	0.03315070947(3)
2.8	−0.6388350423590(8)	−1.1820684492(3)	−1475.2380(5)	0.0341434412(2)
2.9	−0.6353897704070(7)	−1.17016082620(3)	−1558.879(6)	0.03469610840(7)
3.0	−0.631907704457(2)	−1.159140176(2)	−1642.623(4)	0.0348917445(3)
3.1	−0.628421062577(2)	−1.148969140(2)	−1726.208(5)	0.0347977370(3)
3.2	−0.624955968495(3)	−1.139610953(2)	−1809.350(5)	0.0344690574(3)
3.3	−0.6215335626069(8)	−1.13102958908(2)	−1891.755(6)	0.03395076845(6)
3.4	−0.618170890977(2)	−1.123189844(2)	−1973.113(5)	0.0332799818(3)
3.5	−0.6148816203646(8)	−1.11605734361(5)	−2053.110(7)	0.03248739912(5)
3.6	−0.611676616151(2)	−1.109598538(2)	−2131.407(6)	0.0315985263(3)
3.7	−0.608564411632(2)	−1.103780647(2)	−2207.662(6)	0.0306346424(4)
3.8	−0.605551590831(2)	−1.098571620(2)	−2281.517(6)	0.0296135689(4)
3.9	−0.602643102140(2)	−1.093940079(2)	−2352.600(6)	0.0285502886(4)
4.0	−0.599842516471(2)	−1.089855263(2)	−2420.532(6)	0.0274574425(4)
4.1	−0.597152240675(7)	−1.08628698426(9)	−2484.91710(7)	0.02634573100(2)
4.2	−0.594573694841(7)	−1.08320559281(9)	−2545.37141(7)	0.02522423735(2)
4.3	−0.592107460330(7)	−1.08058194455(8)	−2601.49028(7)	0.02410069212(2)
4.4	−0.589743404029(7)	−1.078387387333(1)	−2652.87520(7)	0.022977141068(4)

4.5	−0.5875107832469(10)	−1.076593756(2)	−2699.140(7)	0.0218728469(4)
4.6	−0.585368334828(4)	−1.07517346(6)	−2739.883(4)	0.02077461(2)
4.7	−0.583354351324(4)	−1.07409906378(5)	−2774.743295(6)	0.019704178482(8)
4.8	−0.581436746574(4)	−1.07334419028(5)	−2803.381918(7)	0.018651938097(7)
4.9	−0.579623112577(4)	−1.07288266639(4)	−2825.475753(8)	0.017625216075(7)
5.0	−0.5779107691510(7)	−1.0726890053(2)	−2840.742633(4)	0.01662650660(4)
5.1	−0.576296807654(6)	−1.07273836078(6)	−2848.9437(2)	0.015657893045(10)
5.2	−0.574778129728(6)	−1.07300657564(6)	−2849.8905(2)	0.014721093041(9)
5.3	−0.573351481941(6)	−1.07347023344(6)	−2843.4525(2)	0.013817496310(9)
5.4	−0.572013486940(5)	−1.07410671348(6)	−2829.5632(2)	0.012948196370(8)
5.5	−0.5707606716936(8)	−1.0748942480(2)	−2808.22564(3)	0.01211401735(2)
5.6	−0.569589493266(5)	−1.07581198016(5)	−2779.5176(2)	0.011315536853(7)
5.7	−0.568496362453(5)	−1.07684002364(5)	−2743.5929(2)	0.010553105485(6)
5.8	−0.567477665622(5)	−1.07795951993(5)	−2700.6835(2)	0.009826864019(6)
5.9	−0.566529784916(4)	−1.07915269460(4)	−2651.0982(2)	0.009136758514(6)
6.0	−0.5656491170275(6)	−1.0804029094(2)	−2595.21896(6)	0.00848255411(3)
6.5	−0.5621309641209(6)	−1.087011918600(7)	−2239.09406(2)	0.0057307707138(8)
7.0	−0.5597879212474(5)	−1.09325801162(3)	−1811.0158(6)	0.003759690125(3)
7.5	−0.5582667435321(5)	−1.098417534964(6)	−1385.58400(3)	0.0024154602799(6)
8.0	−0.5572956569909(4)	−1.102328492734(6)	−1013.92884(5)	0.0015328526558(5)
8.5	−0.5566811365466(3)	−1.105134321154(3)	−716.962011(5)	0.0009679943456(3)
9.0	−0.5562930619288(3)	−1.107079221805(4)	−493.75996(4)	0.0006118780057(4)
9.5	−0.5560472002632(3)	−1.10839913564(3)	−332.87618(5)	0.000388975251(3)
10.0	−0.5558902474374(3)	−1.10928348864(3)	−220.21685(3)	0.000249700624(2)
11.0	−0.5557224198360(2)	−1.110261603490(8)	−90.6807789(4)	0.0001075669258(5)
12.0	−0.55564767706476(2)	−1.110692286359(5)	−32.667748551(3)	0.0000502556477(3)
13.0	−0.55561124984318(9)	−1.110886058163(9)	−7.645756(7)	0.0000258801173(5)
14.0	−0.55559165020191(7)	−1.110977966709(6)	2.71341(6)	0.0000146666925(2)
15.0	−0.55558011398760(5)	−1.111025264127(4)	6.68030(4)	0.00000899758997(10)
16.0	−0.55557283203673(4)	−1.111052064170(3)	7.89325(2)	0.00000584999403(7)
17.0	−0.55556800184259(3)	−1.111068688028(2)	7.938663(3)	0.00000395974459(2)
18.0	−0.55556468643292(2)	−1.1110797536846(5)	7.50969(4)	0.00000275662117(2)
19.0	−0.55556235472174(2)	−1.1110874859744(4)	6.91140(2)	0.00000195912994(2)
20.0	−0.555560684284435(9)	−1.1110930626904(3)	6.2781(2)	0.00000141529389(4)

Table A73: Same as for Table A1, but for $2\,^3\Delta_g$ (s state).

$2\,^3\Delta_g$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.031279846178687(7)	–	−29.442651(2)	–
0.01	97.9689725121(7)	95.938462474(8)	−29.469(3)	−9999.9482550(6)
0.05	17.974734485(4)	15.96090013(4)	−30.01(5)	−399.7713769(5)
0.1	7.990468955(6)	6.02004048(4)	−31.46(2)	−99.6089743(3)
0.15	4.679656209(10)	2.76802020(7)	−33.7075(9)	−43.9419481(3)
0.2	3.040091094(3)	1.19542577(3)	−36.68(2)	−24.42378207(10)
0.3	1.435342162(2)	−0.26797399(2)	−44.50(2)	−10.46219438(5)
0.4	0.667961781(2)	−0.89871023(2)	−54.65(2)	−5.58658448(3)
0.5	0.2337323229(10)	−1.208190492(10)	−66.996(10)	−3.35131028(2)
0.6	−0.0360916399(7)	−1.366853264(8)	−81.468(10)	−2.157783306(10)
0.7	−0.2138907282(6)	−1.446588820(7)	−97.996(10)	−1.455439091(8)
0.8	−0.3357366789(5)	−1.482208857(6)	−116.517(7)	−1.013419374(6)
0.9	−0.4215161861(4)	−1.492163735(5)	−136.969(4)	−0.721257070(5)
1.0	−0.4830195816(3)	−1.486869480(5)	−159.282(3)	−0.520830317(4)
1.1	−0.5276312074(3)	−1.472482477(5)	−183.379(2)	−0.379290966(4)
1.2	−0.5601784906(2)	−1.452766973(4)	−209.1785(9)	−0.277008326(3)
1.3	−0.5839278245(2)	−1.430082564(4)	−236.5913(7)	−0.201713011(3)
1.4	−0.6011526405(2)	−1.405934398(4)	−265.5248(7)	−0.145449369(3)
1.5	−0.6134729678(2)	−1.381292919(4)	−295.8820(8)	−0.102897989(2)
1.6	−0.6220664474(2)	−1.356786237(4)	−327.58(2)	−0.070408339(2)
1.7	−0.62780383818(2)	−1.332819244(3)	−360.4655(9)	−0.045418569(2)
1.8	−0.63133851155(10)	−1.309649179(3)	−394.4858(9)	−0.026095642(2)
1.9	−0.63316701315(9)	−1.287434551(3)	−429.5186(10)	−0.011105539(2)
2.0	−0.63367092550(8)	−1.266267361(3)	−465.4583(10)	0.000537245(2)
2.1	−0.63314635209(7)	−1.246194635(3)	−502.1985(10)	0.009570509(2)
2.2	−0.63182503171(7)	−1.227232979(3)	−539.6328(10)	0.016553220(2)
2.3	−0.62988968521(6)	−1.209378513(4)	−577.6546(10)	0.021913416(2)
2.4	−0.62748532021(6)	−1.192613701(4)	−616.1572(9)	0.025982058(2)
2.5	−0.62472765933(6)	−1.176912056(4)	−655.0335(9)	0.029017305(2)
2.6	−0.62170949287(5)	−1.162241406(4)	−694.1763(9)	0.031222146(2)
2.7	−0.61850551483(5)	−1.148566136(4)	−733.4775(10)	0.032757368(2)
2.8	−0.61517603792(5)	−1.135848738(4)	−772.8280(8)	0.0337511920(10)
2.9	−0.61176987127(4)	−1.124050855(4)	−812.1178(8)	0.0343065130(10)
3.0	−0.60832656637(4)	−1.11313399(2)	−851.25(2)	0.034506381(4)
3.1	−0.60487818243(4)	−1.103059926(4)	−890.0658(8)	0.0344182061(10)
3.2	−0.60145068294(4)	−1.093791078(4)	−928.4939(8)	0.0340969651(10)
3.3	−0.59806504702(4)	−1.085290582(4)	−966.4002(6)	0.0335877309(9)
3.4	−0.59473815889(4)	−1.077522413(4)	−1003.666(5)	0.0329276190(10)
3.5	−0.59148352338(3)	−1.070451397(4)	−1040.158(2)	0.0321473285(10)
3.6	−0.58831184448(3)	−1.064043203(5)	−1075.756(5)	0.0312723574(10)
3.7	−0.58523149528(3)	−1.058264307(5)	−1110.318(2)	0.0303239686(10)
3.8	−0.58224890156(3)	−1.053081955(5)	−1143.717(2)	0.0293199600(10)
3.9	−0.57936885630(3)	−1.048464116(5)	−1175.812(3)	0.0282752813(10)
4.0	−0.57659477884(3)	−1.044379438(5)	−1206.450(3)	0.0272025301(10)
4.1	−0.5739289295(5)	−1.040797219(6)	−1235.497(6)	0.026112351(2)
4.2	−0.5713725875(5)	−1.037687381(6)	−1262.795(6)	0.025013760(2)
4.3	−0.5689262015(5)	−1.035020456(6)	−1288.197(5)	0.023914406(2)
4.4	−0.5665895141(5)	−1.032767585(6)	−1311.552(5)	0.022820783(2)

4.5	$-0.56436166909(3)$	$-1.030900528(6)$	$-1332.708(5)$	$0.0217384024(10)$
4.6	$-0.5622413022(4)$	$-1.029391681(5)$	$-1351.516(5)$	$0.0206719399(10)$
4.7	$-0.5602266182(4)$	$-1.028214111(5)$	$-1367.831(5)$	$0.0196253458(9)$
4.8	$-0.5583154593(4)$	$-1.027341588(5)$	$-1381.513(5)$	$0.0186019439(9)$
4.9	$-0.5565053632(4)$	$-1.026748628(5)$	$-1392.426(5)$	$0.0176045099(8)$
5.0	$-0.55479361463(2)$	$-1.026410541(4)$	$-1400.44484(10)$	$0.0166353376(6)$
5.1	$-0.5531772909(2)$	$-1.026303479(2)$	$-1405.4641(2)$	$0.0156962946(2)$
5.2	$-0.5516533014(2)$	$-1.026404484(2)$	$-1407.3816(2)$	$0.0147888689(2)$
5.3	$-0.5502184245(2)$	$-1.026691531(2)$	$-1406.1164(2)$	$0.0139142109(2)$
5.4	$-0.54886933846(10)$	$-1.027143573(2)$	$-1401.6063(2)$	$0.0130731674(2)$
5.5	$-0.54760265103(2)$	$-1.0277405768(10)$	$-1393.8112(2)$	$0.0122663137(2)$
5.6	$-0.54641492477(9)$	$-1.0284635559(10)$	$-1382.7146(2)$	$0.0114939810(2)$
5.7	$-0.54530270018(9)$	$-1.0292945940(10)$	$-1368.3266(2)$	$0.0107562818(2)$
5.8	$-0.54426251653(9)$	$-1.0302168624(9)$	$-1350.6849(2)$	$0.0100531329(2)$
5.9	$-0.54329093035(8)$	$-1.0312146314(9)$	$-1329.8563(2)$	$0.0093842762(2)$
6.0	$-0.54238453182(2)$	$-1.0322732727(8)$	$-1305.9379(2)$	$0.0087492985(2)$
6.5	$-0.53871507082(2)$	$-1.0380437812(6)$	$-1145.4508(2)$	$0.00605944007(8)$
7.0	$-0.536204237204(9)$	$-1.0437533092(5)$	$-937.8097(2)$	$0.00409359503(6)$
7.5	$-0.534523796106(7)$	$-1.0486947488(4)$	$-717.6113(2)$	$0.00271371246(4)$
8.0	$-0.533416729668(5)$	$-1.0526161254(3)$	$-515.4714(2)$	$0.00177716675(3)$
8.5	$-0.532694032132(4)$	$-1.0555525791(2)$	$-348.8171(2)$	$0.00115711590(2)$
9.0	$-0.532223797072(3)$	$-1.0576714852(2)$	$-221.4210(2)$	$0.000752900992(9)$
9.5	$-0.531917496946(2)$	$-1.05916800312(7)$	$-128.38712(10)$	$0.000491262187(5)$
10.0	$-0.5317172469052(10)$	$-1.06021538919(4)$	$-61.39762(9)$	$0.000321910462(2)$
11.0	$-0.5314996327340(6)$	$-1.06147873220(5)$	$25.43585(7)$	$0.000138230297(4)$
12.0	$-0.531407019747(2)$	$-1.0620995850(3)$	$55.14599(6)$	$0.00005953787(2)$
13.0	$-0.531362675665(4)$	$-1.0622850013(3)$	$35.41638(5)$	$0.00003387308(2)$
14.0	$-0.531334713043(4)$	$-1.0623456789(3)$	$21.79898(5)$	$0.00002312480(2)$
15.0	$-0.531315067671(4)$	$-1.0623806803(2)$	$16.47654(3)$	$0.000016630336(9)$
16.0	$-0.531300740548(3)$	$-1.0624046820(2)$	$14.51684(2)$	$0.000012299941(7)$
17.0	$-0.531290026783(3)$	$-1.0624219029(2)$	$13.59824(2)$	$0.000009302982(6)$
18.0	$-0.531281850639(3)$	$-1.06243475293(10)$	$12.87428(2)$	$0.000007163798(4)$
19.0	$-0.531275511183(2)$	$-1.06244477030(9)$	$12.09832(2)$	$0.000005592215(3)$
20.0	$-0.531270537434(2)$	$-1.06245289313(7)$	$11.23870(2)$	$0.000004409087(3)$

Table A74: Same as for Table A1, but for $3\,^3\Delta_g$.

		$3\,^3\Delta_g$		
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.020015836159984(4)	–	−19.56885(1)	–
0.01	97.980240336(6)	95.96099815(6)	−19.66(4)	−9999.948252(5)
0.05	17.98600234(2)	15.9834359(2)	−19.97(4)	−399.771375(2)
0.1	8.00173682(3)	6.0425762(2)	−20.90(6)	−99.608974(2)
0.15	4.69092398(3)	2.7905554(2)	−22.38(4)	−43.9419503(8)
0.2	3.05135868(2)	1.2179599(2)	−24.03(7)	−24.4237871(6)
0.3	1.44660888(2)	−0.2454441(2)	−28.63(6)	−10.4622063(4)
0.4	0.67922692(2)	−0.87618769(6)	−34.56(6)	−5.5866038(2)
0.5	0.2450098726(6)	−1.185664469(2)	2.72786(4)	−3.351368428(2)
0.6	−0.02482075993(2)	−1.3443566621(2)	3.25513(2)	−2.1578585705(2)
0.7	−0.20262823103(2)	−1.4241284873(2)	3.87182(2)	−1.4555314646(2)
0.8	−0.32448426727(7)	−1.459791455(6)	4.541(8)	−1.013528650(7)
0.9	−0.41027553947(2)	−1.46979576872(4)	5.3951(2)	−0.721382988716(8)
1.0	−0.471792341884(4)	−1.46455714418(2)	6.321800(10)	−0.520972460410(9)
1.1	−0.516418974033(5)	−1.45023169936(4)	7.363100(6)	−0.37944886481(2)
1.2	−0.548982813206(3)	−1.43058337311(3)	8.530611(4)	−0.27718145558(2)
1.3	−0.572750198003(3)	−1.40797143393(3)	9.834862(3)	−0.20190079841(2)
1.4	−0.589994500187(3)	−1.38390067954(3)	11.287318(3)	−0.14565119940(2)
1.5	−0.602335685614(3)	−1.35934118812(3)	12.900662(3)	−0.10311321126(2)
1.6	−0.610951328737(3)	−1.33492068945(3)	14.688959(3)	−0.07063626998(2)
1.7	−0.616712118588(3)	−1.31104368370(3)	16.667831(4)	−0.04565849796(2)
1.8	−0.620271354180(2)	−1.28796700777(3)	18.854643(5)	−0.026346833004(10)
1.9	−0.622125506546(2)	−1.26584876060(2)	21.268721(5)	−0.011367235528(9)
2.0	−0.6226560816383(9)	−1.244780528913(9)	23.931594(3)	0.000265817182(4)
2.1	−0.622159104839(2)	−1.22480892046(3)	26.867283(6)	0.009290137724(8)
2.2	−0.620866235582(3)	−1.20595012344(3)	30.102592(6)	0.016264703510(9)
2.3	−0.618960114521(3)	−1.18819984353(3)	33.667497(5)	0.021617558919(9)
2.4	−0.616585668633(3)	−1.17154013368(3)	37.595537(6)	0.025679668162(10)
2.5	−0.613858539837(3)	−1.15594410963(4)	41.924287(6)	0.02870918802(2)
2.6	−0.610871438101(4)	−1.14137921164(4)	46.695893(6)	0.03090910175(2)
2.7	−0.607698977976(4)	−1.12780945780(5)	51.957680(5)	0.03244018450(2)
2.8	−0.604401394151(2)	−1.115196993063(6)	57.762856(3)	0.0334306411570(6)
2.9	−0.601027419679(5)	−1.10350314404(6)	64.171318(5)	0.03398334321(2)
3.0	−0.59761653264(2)	−1.0926891256(2)	71.250577(8)	0.03418131323(4)
3.1	−0.59420072221(2)	−1.0827165029(2)	79.069(5)	0.03409191662(5)
3.2	−0.59080588601(2)	−1.0735474819(2)	87.74(2)	0.03377009065(5)
3.3	−0.58745294245(2)	−1.0651450810(2)	97.3262(4)	0.03326084967(5)
3.4	−0.58415872121(2)	−1.0574732213(3)	107.958(6)	0.03260124151(5)
3.5	−0.58093668001(2)	−1.0504967646(3)	119.755627(3)	0.03182188442(6)
3.6	−0.57779748450(2)	−1.0441815176(3)	132.8631(3)	0.03094818095(6)
3.7	−0.57474947984(2)	−1.0384942193(3)	147.444688(6)	0.03000128119(6)
3.8	−0.57179907613(2)	−1.0334025214(3)	163.68533(6)	0.02899885021(6)
3.9	−0.56895106509(2)	−1.0288749720(3)	181.79943(2)	0.02795568158(6)
4.0	−0.56620888174(2)	−1.0248810073(3)	202.03283(2)	0.02688418904(6)
4.1	−0.563574821934(5)	−1.02139095893(9)	224.63(3)	0.02579480120(2)
4.2	−0.561050224431(5)	−1.01837607986(8)	250.036(6)	0.02469627833(2)
4.3	−0.558635624559(5)	−1.01580859333(9)	278.51(2)	0.02359596646(2)
4.4	−0.556330885125(5)	−1.01366176988(9)	310.542(3)	0.02250000008(2)

4.5	−0.55413530922(2)	−1.0119100365(3)	346.65317(3)	0.02141346266(5)
4.6	−0.552047738789(5)	−1.01052912393(9)	387.4423(4)	0.02034051166(2)
4.7	−0.550066642295(6)	−1.00949626186(9)	433.63260(5)	0.01928447292(2)
4.8	−0.548190194278(6)	−1.00879043036(10)	486.07540(5)	0.01824790796(2)
4.9	−0.546416349499(6)	−1.00839268615(10)	545.78230(4)	0.01723265568(2)
5.0	−0.54474291421(7)	−1.0082865847(10)	613.9605(2)	0.0162398488(2)
5.1	−0.54316761682(2)	−1.0084587230(3)	692.05452(4)	0.01526990404(5)
5.2	−0.54168818170(2)	−1.0088994598(3)	781.79311(4)	0.01432248147(5)
5.3	−0.54030240773(2)	−1.0096038350(3)	885.24361(4)	0.01339641141(5)
5.4	−0.53900825687(2)	−1.0105727748(3)	1004.86318(4)	0.01248958129(5)
5.5	−0.53780395569(2)	−1.0118146116(3)	1143.53539(4)	0.01159878178(5)
5.6	−0.53668811432(2)	−1.0133469251(4)	1304.56053(3)	0.01071951849(5)
5.7	−0.53565986467(3)	−1.0151985489(4)	1491.53991(3)	0.00984582113(6)
5.8	−0.53471901464(3)	−1.0174112285(5)	1708.043105(9)	0.00897013806(7)
5.9	−0.53386620088(3)	−1.0200396499(6)	1956.874302(8)	0.00808351726(8)
6.0	−0.53310299371(3)	−1.0231471870(6)	2238.68008(3)	0.00717646674(9)
6.5	−0.53071433556(6)	−1.045989737(2)	3719.45614(7)	0.0023752206(3)
7.0	−0.53036577326(7)	−1.063510617(2)	3516.44777(6)	−0.0003970101(2)
7.5	−0.53070140753(6)	−1.0669989292(9)	2492.69263(5)	−0.00074614856(10)
8.0	−0.53102760234(5)	−1.0663467826(7)	1669.88804(4)	−0.00053644723(7)
8.5	−0.53123744011(5)	−1.0651317884(6)	1095.46340(4)	−0.00031257744(6)
9.0	−0.53135188012(5)	−1.0641144711(6)	702.96166(4)	−0.00015674566(5)
9.5	−0.53140429877(5)	−1.0633916497(5)	436.81907(4)	−0.00006137391(5)
10.0	−0.53142008190(5)	−1.0629113374(5)	256.79895(5)	−0.00000711736(4)
11.0	−0.53140034308(4)	−1.0623922987(4)	49.83448(9)	0.00003712613(3)
12.0	−0.53135777423(3)	−1.0621987740(2)	−27.0889(2)	0.000043064539(5)
13.0	−0.53132114819(2)	−1.06226085837(6)	−23.6165(2)	0.000029341385(2)
14.0	−0.531297999916(10)	−1.06234527030(5)	−14.1428(2)	0.000017909252(2)
15.0	−0.531283697742(8)	−1.06239760563(4)	−8.8833(2)	0.000011319324(2)
16.0	−0.531274440851(6)	−1.06242848435(3)	−6.0545(2)	0.0000075248344(10)
17.0	−0.531268160774(5)	−1.06244769217(3)	−4.4091(2)	0.0000052134928(7)
18.0	−0.531263743501(4)	−1.06246046509(2)	−3.3601(2)	0.0000037234398(5)
19.0	−0.531260553538(3)	−1.06246944097(2)	−2.6373(2)	0.0000027192686(3)
20.0	−0.531258204003(2)	−1.062476000706(8)	−2.1102(2)	0.0000020203650(2)

Table A75: Same as for Table A1, but for $1\,^1\Delta_u$.

$1\,^1\Delta_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.031255144381749(1)	–	10.0242694(2)	–
0.01	97.9690062215(9)	95.93850(2)	10.03(3)	−9999.951(2)
0.05	17.974768201(3)	15.9609672(4)	10.083(9)	−399.771385(8)
0.1	7.990502596(4)	6.02010742(3)	10.404697(2)	−99.6089776(2)
0.15	4.679689561(4)	2.76808562(2)	10.819212(8)	−43.94195659(4)
0.2	3.04012386(2)	1.1954878(5)	11.31(3)	−24.423800(3)
0.3	1.4353727318(6)	−0.2679224(6)	12.66(3)	−10.462226(2)
0.4	0.6679885497(2)	−0.8986760(7)	14.34(3)	−5.586633(2)
0.5	0.23375357935(8)	−1.208179919(2)	16.370(3)	−3.351374156(4)
0.6	−0.03607765666(3)	−1.3668742649(2)	18.654(2)	−2.1578649194(2)
0.7	−0.213885795914(4)	−1.4466485349(2)	21.2968(10)	−1.4555384901(2)
0.8	−0.335742572079(5)	−1.4823143080(2)	24.2450(4)	−1.0135364547(2)
0.9	−0.42153466310(2)	−1.4923217876(4)	27.542(2)	−0.7213916238(4)
1.0	−0.483052376483(2)	−1.4870868193(3)	31.215(2)	−0.5209820664(2)
1.1	−0.527680023498(3)	−1.4727655857(3)	35.26(2)	−0.3794595807(2)
1.2	−0.560244996210(2)	−1.4531221184(3)	39.8032(9)	−0.2771934383(2)
1.3	−0.5840136499432(10)	−1.4305157935(3)	44.7910(5)	−0.2019142258(2)
1.4	−0.601259375370(4)	−1.4064515320(2)	50.29691(5)	−0.1456662723(2)
1.5	−0.613602159689(2)	−1.3818995538(3)	56.36880(6)	−0.1031301563(2)
1.6	−0.622219601438(2)	−1.3574877512(2)	63.06233(4)	−0.07065534268(9)
1.7	−0.627982416814(2)	−1.3336208112(3)	70.43936(6)	−0.0456799868(2)
1.8	−0.631543935499(2)	−1.3105557856(2)	78.5696(3)	−0.02637106367(8)
1.9	−0.633400663171(2)	−1.2884510211(2)	87.5325(3)	−0.01139457618(7)
2.0	−0.6339341449639(10)	−1.2673983899(2)	97.417179(9)	0.00023495004(6)
2.1	−0.6334404506109(10)	−1.2474448293(2)	108.3239(2)	0.00925527233(6)
2.2	−0.6321512898081(5)	−1.2286069088(2)	120.36757(2)	0.01622530492(5)
2.3	−0.6302493602476(7)	−1.2108807752(2)	133.67740(5)	0.02157301970(5)
2.4	−0.6278796537133(5)	−1.1942489931(2)	148.4007(2)	0.02562929763(5)
2.5	−0.6251578858732(5)	−1.1786852727(2)	164.7049(2)	0.02865219961(4)
2.6	−0.6221768507539(10)	−1.1641577462(2)	182.7808(2)	0.03084459820(4)
2.7	−0.6190112588871(10)	−1.1506312391(2)	202.84595(6)	0.03236714025(4)
2.8	−0.6157214547842(6)	−1.13806884120(2)	225.149057(7)	0.03334788156(4)
2.9	−0.6123562974337(10)	−1.12643298788(10)	249.9749(2)	0.03388951965(3)
3.0	−0.608955409700(2)	−1.1156862000(2)	277.65094(5)	0.03407487315(3)
3.1	−0.6055509476900(7)	−1.1057915868(2)	308.5530(2)	0.03397106730(3)
3.2	−0.6021690021118(7)	−1.0967131881(2)	343.1154(2)	0.03363275503(3)
3.3	−0.598830715508(2)	−1.0884162111(2)	381.8397(2)	0.03310461208(3)
3.4	−0.5955531787935(5)	−1.0808672039(3)	425.30830(3)	0.03242328049(8)
3.5	−0.592350155523(2)	−1.0740341990(2)	474.1980(2)	0.03161888915(4)
3.6	−0.589232671193(2)	−1.0678868580(3)	529.29969(3)	0.03071624567(6)
3.7	−0.586209496693(2)	−1.0623966370(2)	591.53929(7)	0.02973577200(4)
3.8	−0.583287548851(2)	−1.0575370076(3)	662.00586(2)	0.02869423425(7)
3.9	−0.580472226530(2)	−1.0532837537(3)	741.98433(4)	0.02760530753(5)
4.0	−0.577767697396(3)	−1.0496153895(3)	832.99621(8)	0.02648000131(6)
4.1	−0.57517714819(3)	−1.0465137343(5)	936.8489(3)	0.0253269664(2)
4.2	−0.57270300980(4)	−1.0439647094(6)	1055.6943(3)	0.0241526929(2)
4.3	−0.57034716783(4)	−1.0419594391(7)	1192.0964(3)	0.0229616039(2)
4.4	−0.56811116901(5)	−1.0404957531(9)	1349.1058(4)	0.0217560420(2)

4.5	−0.5659964346176(7)	−1.039580229(2)	1530.3327(5)	0.0205361424(3)
4.6	−0.56400449281(6)	−1.039230917(2)	1739.9972(6)	0.0192995801(3)
4.7	−0.56213724247(7)	−1.039480884(2)	1982.9156(7)	0.0180411916(3)
4.8	−0.56039726043(8)	−1.040382531(2)	2264.3379(9)	0.0167524978(4)
4.9	−0.55878815724(9)	−1.042012243(2)	2589.4757(8)	0.0154212391(4)
5.0	−0.557314967322(2)	−1.044473803(3)	2962.4477(10)	0.0140312264(5)
5.1	−0.55598451220(2)	−1.0478967533(4)	3384.221(9)	0.01256319040(7)
5.2	−0.55480557796(2)	−1.0524220088(5)	3849.173(8)	0.01099791291(8)
5.3	−0.55378858966(3)	−1.0581627304(6)	4340.116(6)	0.00932348094(10)
5.4	−0.55294429515(3)	−1.0651302729(7)	4823.567(5)	0.0075478366(2)
5.5	−0.552281020395(6)	−1.0731365176(8)	5249.445(4)	0.0057137315(2)
5.6	−0.55180072019(4)	−1.0817308097(9)	5560.935(3)	0.0039054698(2)
5.7	−0.55149536294(5)	−1.0902582112(10)	5714.5482(9)	0.0022337745(2)
5.8	−0.55134599995(5)	−1.0980552082(10)	5698.61866(2)	0.0007994468(2)
5.9	−0.55132561055(6)	−1.1046623373(10)	5535.5912(7)	−0.0003408672(2)
6.0	−0.551404212282(3)	−1.1099102658(3)	5267.7377(2)	−0.00118364021(4)
6.5	−0.552457242666(2)	−1.1207431144(2)	3570.4699(5)	−0.00243517370(2)
7.0	−0.553570837250(2)	−1.12068767251(9)	2319.5660(3)	−0.001935142572(10)
7.5	−0.5543760645948(6)	−1.11852171002(4)	1527.9872(2)	−0.001302610777(4)
8.0	−0.5548993990952(5)	−1.11635144667(3)	1017.97888(9)	−0.000819081059(3)
8.5	−0.5552214294901(4)	−1.11462656199(2)	681.77655(7)	−0.000492200354(2)
9.0	−0.5554112429334(4)	−1.11337238662(2)	457.44891(7)	−0.000283322305(2)
9.5	−0.5555180750562(3)	−1.11250600870(2)	307.25722(5)	−0.0001547219569(10)
10.0	−0.5555745677120(3)	−1.111929535416(10)	206.88872(3)	−0.0000780399992(7)
11.0	−0.5556116632044(2)	−1.111326455803(7)	95.928484(10)	−0.0000093753994(5)
12.0	−0.5556094183824(2)	−1.111106750184(5)	47.706156(4)	0.0000093405484(3)
13.0	−0.55559818668317(10)	−1.111043171085(3)	26.881845(10)	0.0000117847909(2)
14.0	−0.55558722244837(6)	−1.111036302095(2)	17.665346(3)	0.00000986734301(7)
15.0	−0.55557861625837(4)	−1.1110465948261(10)	13.266111(2)	0.00000737584605(3)
16.0	−0.55557232288398(4)	−1.1110597914484(7)	10.862844(3)	0.00000530339498(2)
17.0	−0.55556782624247(3)	−1.1110714817502(4)	9.313753(2)	0.000003774749106(3)
18.0	−0.55556462424462(3)	−1.1110807713516(2)	8.1634812(4)	0.00000269317430(2)
19.0	−0.55556233179299(2)	−1.11108786405500(2)	7.2296381(8)	0.00000193681740(2)
20.0	−0.55556067537094(2)	−1.11109320801738(3)	6.436203(3)	0.000001407136212(10)

Table A76: Same as for Table A1, but for $2\,^1\Delta_u$.

R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.0200029371587427(5)	–	5.7042946(4)	–
0.01	97.9802584250(2)	95.9610343042(7)	5.71(2)	−9999.94825457(5)
0.05	17.986020428(3)	15.98347205(2)	5.728(10)	−399.7713762(3)
0.1	8.001754885(6)	6.04261216(4)	5.88(3)	−99.6089761(3)
0.15	4.690941940(4)	2.79059070(2)	6.03(5)	−43.94195451(9)
0.2	3.051376373(3)	1.21799389(2)	6.415(4)	−24.42379425(5)
0.3	1.446625532(2)	−0.245415170(7)	7.173(8)	−10.46222078(2)
0.4	0.6792417239(6)	−0.876167283(3)	8.12(2)	−5.586626827(5)
0.5	0.2450071975(3)	−1.185670290(2)	9.308(2)	−3.351369370(3)
0.6	−0.0248235261(2)	−1.3443627192(9)	10.6164(3)	−2.1578594450(10)
0.7	−0.2026310824(2)	−1.4241347733(10)	12.098(6)	−1.4555322979(10)
0.8	−0.32448720197(10)	−1.4597980084(10)	13.768(6)	−1.0135295057(9)
0.9	−0.41027855831(6)	−1.469802597(2)	15.634(7)	−0.7213838676(9)
1.0	−0.47179545330(10)	−1.464564349(2)	17.711(8)	−0.5209734423(10)
1.1	−0.51642219173(7)	−1.450239404(2)	20.013(9)	−0.3794500184(10)
1.2	−0.5489861580(2)	−1.430591744(2)	22.561(9)	−0.2771828570(2)
1.3	−0.5727536989(2)	−1.407980691(2)	25.374(4)	−0.201902533(2)
1.4	−0.5899981953(2)	−1.383911100(3)	28.4756(7)	−0.145653364(2)
1.5	−0.6023396232(2)	−1.359353116(3)	31.81(6)	−0.103115913(2)
1.6	−0.61095556851(6)	−1.334934547(3)	35.646(5)	−0.070639631(2)
1.7	−0.6167167331(2)	−1.311059981(3)	39.74(3)	−0.045662656(2)
1.8	−0.62027643075(4)	−1.287986357(4)	44.328(9)	−0.026351942(2)
1.9	−0.62213114877(2)	−1.265871891(4)	49.335(5)	−0.011373470(2)
2.0	−0.62266241179(3)	−1.244808306(4)	54.846(10)	0.000258259(2)
2.1	−0.62216626631(3)	−1.224842369(4)	60.918(10)	0.009281030(2)
2.2	−0.62087439576(5)	−1.205990450(5)	67.611(10)	0.016253792(2)
2.3	−0.61896946815(6)	−1.188248471(5)	74.998(3)	0.021604550(2)
2.4	−0.61659644175(10)	−1.171598736(5)	83.153(4)	0.025664228(2)
2.5	−0.6138709943(2)	−1.156014657(6)	92.170(3)	0.028690933(2)
2.6	−0.6108858770(2)	−1.141464022(6)	102.137(10)	0.030887589(2)
2.7	−0.60771575189(5)	−1.127911266(7)	113.21(2)	0.032414903(3)
2.8	−0.60442090900(5)	−1.115319028(7)	125.502(6)	0.033400997(3)
2.9	−0.60105014550(5)	−1.103649227(8)	139.168(6)	0.033948643(3)
3.0	−0.59764301454(3)	−1.092863796(8)	154.381(10)	0.034140744(3)
3.1	−0.59423159359(4)	−1.082925172(9)	171.384(9)	0.034044521(3)
3.2	−0.59084188475(4)	−1.073796630(9)	190.35(5)	0.033714731(3)
3.3	−0.58749493087(6)	−1.065442509(10)	211.7347(5)	0.033196168(3)
3.4	−0.58420771064(4)	−1.057828379(9)	235.701(7)	0.032525601(3)
3.5	−0.5809938625(2)	−1.05092118(2)	262.7296(10)	0.031733298(3)
3.6	−0.5778642720(2)	−1.04468937(2)	293.267(3)	0.030844215(3)
3.7	−0.57482755547(4)	−1.03910310(2)	327.876(4)	0.029878922(3)
3.8	−0.57189046072(4)	−1.03413449(2)	367.0(2)	0.028854324(4)
3.9	−0.56905820467(4)	−1.02975800(2)	412.11(8)	0.027784208(4)
4.0	−0.56633476490(5)	−1.02595101(2)	463.707(3)	0.026679629(3)
4.1	−0.5637231394(8)	−1.02269474(2)	522.975(4)	0.025549155(3)
4.2	−0.5612255888(9)	−1.01997557(2)	591.4735(6)	0.024398954(4)
4.3	−0.558843881(2)	−1.01778716(3)	670.957(2)	0.023232698(6)
4.4	−0.556579553(2)	−1.01613380(3)	763.611(6)	0.022051205(6)

4.5	−0.5544342336(4)	−1.01503575(4)	871.919(4)	0.020851714(8)
4.6	−0.552410057(2)	−1.01453785(4)	998.66(3)	0.019626580(8)
4.7	−0.550510252(3)	−1.01472351(6)	1146.44(2)	0.01836106(2)
4.8	−0.548740018(3)	−1.01573692(6)	1316.34(2)	0.01702982(2)
4.9	−0.547107820(4)	−1.01781520(9)	1504.60(5)	0.01559193(2)
5.0	−0.5456271965(2)	−1.0213220(2)	1694.79(3)	0.01398648(3)
5.1	−0.5443186361(10)	−1.02673184(3)	1841.454(5)	0.012138319(5)
5.2	−0.543209274(2)	−1.03440445(4)	1846.834(5)	0.010002712(7)
5.3	−0.542324503(2)	−1.04391901(5)	1561.970(5)	0.007684905(8)
5.4	−0.541666251(3)	−1.05334652(5)	879.629(5)	0.005552960(8)
5.5	−0.54119190728(7)	−1.06000091(2)	−119.2819(8)	0.004069618(3)
5.6	−0.540824448(3)	−1.06255765(3)	−1190.551(4)	0.003409150(5)
5.7	−0.540488775(3)	−1.06168831(2)	−2111.479(4)	0.003384077(3)
5.8	−0.540136970(2)	−1.05892056(2)	−2780.598(3)	0.003681618(2)
5.9	−0.539750144(2)	−1.055591451(9)	−3197.414(3)	0.0040523452(10)
6.0	−0.53932875809(2)	−1.0525079096(6)	−3410.568(4)	0.00435826778(6)
6.5	−0.53706500341(2)	−1.0459524996(7)	−3120.9978(3)	0.00433500112(7)
7.0	−0.53516264823(2)	−1.0476809760(6)	−2413.6087(2)	0.00323490293(7)
7.5	−0.53381654251(2)	−1.0512110784(6)	−1789.4912(2)	0.00218960088(6)
8.0	−0.53292651986(2)	−1.0545151815(6)	−1275.7014(2)	0.00141723228(6)
8.5	−0.532356879819(10)	−1.0570783293(6)	−871.4457(2)	0.00089828592(5)
9.0	−0.531997121138(10)	−1.0588975861(5)	−569.2333(2)	0.00056629513(5)
9.5	−0.531769855665(10)	−1.0601266972(5)	−353.9179(2)	0.00035926464(4)
10.0	−0.531624732783(10)	−1.0609345138(5)	−206.6814(2)	0.00023149518(4)
11.0	−0.531467232329(8)	−1.0617971680(4)	−46.4463(2)	0.00010339061(3)
12.0	−0.531393202225(7)	−1.0621616214(4)	18.39651(10)	0.00005206526(3)
13.0	−0.531353596798(7)	−1.0623155779(3)	41.64360(9)	0.00003012428(2)
14.0	−0.531329076802(6)	−1.0623767103(3)	45.56992(8)	0.00002010309(2)
15.0	−0.531311891879(5)	−1.0624029108(3)	41.70288(8)	0.000014724867(10)
16.0	−0.531299010885(6)	−1.0624180411(3)	35.76210(8)	0.00001124879(2)
17.0	−0.531289073605(4)	−1.0624293881(2)	29.93463(6)	0.000008750536(7)
18.0	−0.531281304700(4)	−1.0624389031(2)	24.88175(6)	0.000006872572(5)
19.0	−0.531275183021(3)	−1.0624471402(2)	20.70012(5)	0.000005432939(4)
20.0	−0.531270331255(3)	−1.06245432054(9)	17.30076(5)	0.000004317099(3)

Table A77: Same as for Table A1, but for $3\,^1\Delta_u$.

$3\,^1\Delta_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.0138906838155497(3)	–	3.482257(7)	–
0.01	97.9863706789(2)	95.973258814(2)	3.4845(9)	−9999.94825443(8)
0.05	17.992132698(6)	15.99569663(4)	3.520(2)	−399.7713753(6)
0.1	8.00786719(2)	6.05483686(7)	3.616(2)	−99.6089751(5)
0.15	4.697054287(9)	2.80281557(6)	3.760(2)	−43.9419534(3)
0.2	3.057488778(6)	1.23021897(4)	3.944(2)	−24.4237929(2)
0.3	1.452738091(3)	−0.23318953(2)	4.410(2)	−10.46221904(4)
0.4	0.685354474(8)	−0.86394094(5)	4.994(2)	−5.58662473(8)
0.5	0.251120177(5)	−1.17344310(4)	5.684(3)	−3.35136692(5)
0.6	−0.018710282(2)	−1.33213454(2)	6.480(2)	−2.15785663(2)
0.7	−0.196517540(3)	−1.41190546(2)	7.386(3)	−1.45552912(3)
0.8	−0.3183733219(10)	−1.447567399(9)	8.403(3)	−1.013525944(8)
0.9	−0.404164302(3)	−1.45757051(2)	9.542(4)	−0.72137990(2)
1.0	−0.4656807788(3)	−1.452330595(2)	10.805(3)	−0.520969038(2)
1.1	−0.5103070537(3)	−1.438003765(3)	12.207(3)	−0.379445143(2)
1.2	−0.5428705074(3)	−1.418353981(3)	13.757(3)	−0.277177472(2)
1.3	−0.5666374826(4)	−1.395740536(3)	15.466(3)	−0.201896593(2)
1.4	−0.5838813553(4)	−1.371668256(4)	17.350(4)	−0.145646818(2)
1.5	−0.5962220960(5)	−1.347107249(4)	19.423(4)	−0.103108704(2)
1.6	−0.6048372847(5)	−1.322685279(5)	21.68(2)	−0.070631694(3)
1.7	−0.6105976163(6)	−1.298806888(5)	24.17(3)	−0.045653915(3)
1.8	−0.6141563963(6)	−1.275728957(6)	26.95(2)	−0.026342314(3)
1.9	−0.6160101034(7)	−1.253609638(7)	29.94(5)	−0.011362859(3)
2.0	−0.6165402518(7)	−1.232540580(8)	33.30(3)	0.000269962(3)
2.1	−0.6160428765(8)	−1.212568460(8)	36.96(3)	0.009293949(4)
2.2	−0.6147496477(9)	−1.193709550(9)	41.030(10)	0.016268066(4)
2.3	−0.6128432184(9)	−1.175959654(10)	45.47(5)	0.021620340(4)
2.4	−0.6104685299(10)	−1.15930094(2)	50.37(4)	0.025681716(4)
2.5	−0.6077412403(10)	−1.14370666(2)	55.80(3)	0.028710327(4)
2.6	−0.604754079(2)	−1.12914443(2)	61.83(2)	0.030909126(5)
2.7	−0.601581682(2)	−1.11557846(2)	68.494(9)	0.032438854(5)
2.8	−0.598284310(2)	−1.10297114(2)	75.890(2)	0.033427673(5)
2.9	−0.594910728(2)	−1.09128409(2)	84.08(3)	0.033978401(5)
3.0	−0.591500451(2)	−1.08047892(2)	93.23(3)	0.034173994(5)
3.1	−0.588085511(2)	−1.07051765(2)	103.45(2)	0.034081734(5)
3.2	−0.584691860(2)	−1.06136308(2)	114.900(8)	0.033756452(5)
3.3	−0.581340483(2)	−1.05297898(2)	127.732(2)	0.033243025(5)
3.4	−0.578048291(2)	−1.04533028(2)	142.164(10)	0.032578325(5)
3.5	−0.574828842(2)	−1.03838311(3)	158.463(10)	0.031792736(5)
3.6	−0.571692932(2)	−1.03210500(3)	176.92(2)	0.030911351(6)
3.7	−0.568649070(2)	−1.02646500(3)	197.90(2)	0.029954902(6)
3.8	−0.565703880(2)	−1.02143393(3)	221.845(10)	0.028940481(6)
3.9	−0.562862436(2)	−1.01698475(3)	249.289(9)	0.027882083(6)
4.0	−0.560128550(2)	−1.01309315(3)	280.898(8)	0.026790987(6)
4.1	−0.557505033(2)	−1.00973856(3)	317.488(7)	0.025675978(7)
4.2	−0.554993938(2)	−1.00690571(4)	360.077(5)	0.024543373(8)
4.3	−0.552596820(2)	−1.00458743(4)	409.89(3)	0.023396792(9)
4.4	−0.550315030(2)	−1.00278941(4)	468.48(2)	0.022236511(9)

4.5	−0.548150116(3)	−1.00153902(7)	537.46(4)	0.02105805(2)
4.6	−0.546104413(4)	−1.00090155(8)	618.48(4)	0.01984941(2)
4.7	−0.544182053(4)	−1.0010124(2)	711.72(5)	0.01858546(3)
4.8	−0.542390760(6)	−1.0021402(2)	812.62(7)	0.01721694(3)
4.9	−0.540745177(7)	−1.0048019(3)	900.96(6)	0.01565070(4)
5.0	−0.53927242(2)	−1.0098994(6)	910.5(4)	0.0137291(2)
5.1	−0.538016806(7)	−1.0184245(2)	673.69(4)	0.01129591(4)
5.2	−0.537022853(9)	−1.0292670(3)	−53.08(4)	0.00861128(4)
5.3	−0.536266717(10)	−1.0367730(2)	−1184.57(4)	0.00674725(3)
5.4	−0.535621928(9)	−1.03684041(3)	−2142.23(4)	0.006371009(3)
5.5	−0.534963991(7)	−1.03225380(3)	−2570.29(3)	0.006849846(7)
5.6	−0.534251065(5)	−1.02720191(4)	−2568.51(3)	0.007375035(8)
5.7	−0.533498616(4)	−1.02355641(3)	−2351.60(2)	0.007621194(6)
5.8	−0.532736666(3)	−1.02154336(3)	−2057.460(10)	0.007574132(5)
5.9	−0.531991304(2)	−1.02090673(2)	−1743.876(6)	0.007300995(4)
6.0	−0.5312820635(4)	−1.021410847(5)	−1425.0905(4)	0.0068588798(9)
6.5	−0.5288103544(2)	−1.04245138(2)	512.7440(4)	0.002333743(2)
7.0	−0.5288765327(2)	−1.068388550(2)	1194.3729(4)	−0.0015193550(3)
7.5	−0.5296762085(2)	−1.070450782(2)	788.0294(6)	−0.0014797819(2)
8.0	−0.53030077042(6)	−1.0687730069(5)	492.4044(3)	−0.00102143326(5)
8.5	−0.53071413808(4)	−1.0669769046(4)	307.7319(3)	−0.00065277982(3)
9.0	−0.53097318465(3)	−1.0655538013(3)	192.2463(3)	−0.00040082577(2)
9.5	−0.53112974957(2)	−1.0645175269(2)	120.1860(2)	−0.000237687133(9)
10.0	−0.53122092310(2)	−1.06379300113(8)	75.64031(10)	−0.000135115493(6)
11.0	−0.531297076365(7)	−1.06296751572(5)	30.98206(6)	−0.000033942090(3)
12.0	−0.53131019485(2)	−1.0626058774(2)	11.0989(2)	0.000001209356(10)
13.0	−0.531302926288(5)	−1.06246509850(5)	0.50351(4)	0.000010827237(3)
14.0	−0.531291562605(5)	−1.06242762606(4)	−3.79490(5)	0.000011107082(2)
15.0	−0.531281477286(4)	−1.06242881069(3)	−4.68382(5)	0.0000089429252(10)
16.0	−0.531273682281(3)	−1.06244004176(2)	−4.35421(4)	0.0000067076753(6)
17.0	−0.531267903022(3)	−1.062451914015(9)	−3.71557(4)	0.0000049348253(3)
18.0	−0.531263656125(2)	−1.062461991741(6)	−3.07409(4)	0.0000036289172(2)
19.0	−0.531260523877(2)	−1.062469989263(4)	−2.51771(3)	0.00000268728899(6)
20.0	−0.5312581938707(8)	−1.062476197047(2)	−2.05942(3)	0.00000200953471(2)

Table A78: Same as for Table A1, but for $4\,^1\Delta_u$.

$4\,^1\Delta_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.4656774229388(8)	−1.4523210696(2)	1.78898(6)	−0.52096622372(7)
1.1	−0.5103033999480(4)	−1.43799299519(6)	2.11779(4)	−0.37944199571(3)
1.2	−0.54286651978(2)	−1.41834176047(7)	2.48763(2)	−0.27717393409(4)
1.3	−0.5666331188303(2)	−1.39572661877(2)	2.90151(2)	−0.201892600853(5)
1.4	−0.5838765663248(9)	−1.371652350119(5)	3.36271(2)	−0.145642298192(3)
1.5	−0.5962168251322(2)	−1.34708901183(2)	3.87478(6)	−0.103103574376(8)
1.6	−0.604831466264(2)	−1.322664309176(9)	4.44176(5)	−0.070625860405(4)
1.7	−0.6105911747706(8)	−1.298782713687(6)	5.06789(5)	−0.045647273027(3)
1.8	−0.614149245075(7)	−1.27570102874(3)	5.75788(7)	−0.026334743662(4)
1.9	−0.616002142978(2)	−1.253577314149(4)	6.51699(6)	−0.01135422536508(8)
2.0	−0.616531368355(2)	−1.232503111071(4)	7.3508(2)	0.0002798128194(3)
2.1	−0.6160329396740(8)	−1.21252497418(2)	8.2657(2)	0.009305192939(5)
2.2	−0.6147385084296(7)	−1.19365902997(2)	9.2687(2)	0.016280903132(5)
2.3	−0.6128307061987(8)	−1.175900912456(10)	10.3673(2)	0.021634999975(4)
2.4	−0.610454449575(2)	−1.15923259142(2)	11.5699(3)	0.025698461555(6)
2.5	−0.607725368615(2)	−1.14362708614(3)	12.8860(4)	0.028729460435(8)
2.6	−0.604736159740(2)	−1.12905172509(3)	14.3259(4)	0.030930997843(9)
2.7	−0.601561422035(2)	−1.11547039684(4)	15.9012(5)	0.032463869344(10)
2.8	−0.598261372545(2)	−1.10284509638(4)	17.6245(6)	0.03345630311(2)
2.9	−0.594884724188(3)	−1.09113697655(6)	19.5108(3)	0.03401119718(2)
3.0	−0.591470932070(3)	−1.08030705097(7)	21.5746(3)	0.03421160439(2)
3.1	−0.588051959161(4)	−1.07031665163(7)	23.8341(2)	0.03412492474(3)
3.2	−0.584653673174(4)	−1.06112771405(8)	26.3084(5)	0.03380613509(3)
3.3	−0.581296958360(5)	−1.05270294259(10)	29.02178(3)	0.03330029519(3)
3.4	−0.577998605383(5)	−1.0450058937(2)	31.9955(4)	0.03264450503(3)
3.5	−0.574772027328(6)	−1.0380010041(2)	35.2600(3)	0.03186944301(4)
3.6	−0.571627838751(6)	−1.0316535852(2)	38.8442(9)	0.03100058119(4)
3.7	−0.568574326217(7)	−1.0259297962(2)	42.7833(2)	0.03005915033(5)
3.8	−0.565617832523(8)	−1.0207966091(2)	47.1167(3)	0.02906290947(5)
3.9	−0.562763071924(8)	−1.0162217715(3)	51.8878(3)	0.02802676214(5)
4.0	−0.560013390033(9)	−1.0121737743(3)	57.1467(4)	0.02696325144(6)
4.1	−0.557370979210(10)	−1.0086218268(3)	62.9491(2)	0.02588295894(6)
4.2	−0.55483705803(2)	−1.0055358429(3)	69.3586(3)	0.02479482694(7)
4.3	−0.5524120217002(10)	−1.0028864401(4)	76.4469(2)	0.02370641937(7)
4.4	−0.5500955689825(8)	−1.0006449509(4)	84.29696(2)	0.02262413343(8)
4.5	−0.5478868099187(6)	−0.9987834476(5)	93.0013(2)	0.02155337161(9)
4.6	−0.5457843581020(4)	−0.9972747810(5)	102.66700(3)	0.02049868156(10)
4.7	−0.543786410249(2)	−0.9960926303(6)	113.41701(10)	0.0194638703(2)
4.8	−0.5418908154674(2)	−0.9952115655(6)	125.3925(2)	0.0184520970(2)
4.9	−0.540095136090(6)	−0.994607124(5)	138.7568(9)	0.0174659486(9)
5.0	−0.538396701669(10)	−0.994255885(6)	153.70184(3)	0.0165075036(10)

Table A79: Same as for Table A1, but for $5\,^1\Delta_u$.

$5\,^1\Delta_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46199401603(2)	−1.4449546609(9)	7.0142(4)	−0.5209666291(7)
1.1	−0.50662003734(2)	−1.4306267964(7)	7.9233(4)	−0.3794424757(6)
1.2	−0.53918321103(2)	−1.410975859(2)	8.9280(4)	−0.2771745314(8)
1.3	−0.56294987733(2)	−1.388361113(2)	10.0362(5)	−0.2018933526(9)
1.4	−0.58019340974(2)	−1.364287369(2)	11.2566(5)	−0.1456432498(10)
1.5	−0.59253377598(2)	−1.3397247051(8)	12.5994(5)	−0.103104777(2)
1.6	−0.601148552510(10)	−1.315300900(3)	14.0757(6)	−0.070627372(2)
1.7	−0.606908430521(8)	−1.291420431(3)	15.6982(6)	−0.045649159(2)
1.8	−0.610466711384(6)	−1.268340162(4)	17.4812(6)	−0.026337078(2)
1.9	−0.612319868721(5)	−1.246218210(4)	19.4408(7)	−0.011357091(2)
2.0	−0.612849411348(3)	−1.225146180(4)	21.5951(7)	0.000276321(2)
2.1	−0.6123513678484(2)	−1.205170705(5)	23.9648(7)	0.009300967(2)
2.2	−0.611057401267(3)	−1.186307999(6)	26.5732(7)	0.016275819(2)
2.3	−0.609150156385(5)	−1.168553804(7)	29.4471(7)	0.021628916(3)
2.4	−0.606774564949(7)	−1.151890210(8)	32.6168(7)	0.025691216(3)
2.5	−0.604046274456(9)	−1.136290383(8)	36.1171(6)	0.028720866(3)
2.6	−0.60105800148(2)	−1.121721820(6)	39.9881(6)	0.030920839(2)
2.7	−0.59788436852(2)	−1.108148625(4)	44.2757(5)	0.032451893(2)
2.8	−0.59458561989(2)	−1.095533043(3)	49.0331(4)	0.0334422130(7)
2.9	−0.59121050052(2)	−1.083836525(7)	54.3220(2)	0.033994647(2)
3.0	−0.58779850327(2)	−1.073020454(9)	60.21429(5)	0.034192184(3)
3.1	−0.58438163593(2)	−1.063046620(8)	66.7938(3)	0.034102146(3)
3.2	−0.58098581986(2)	−1.05387753(2)	74.1596(6)	0.033779410(5)
3.3	−0.57763200408(2)	−1.045476605(9)	82.4288(10)	0.033268910(3)
3.4	−0.57433705813(2)	−1.037808315(9)	91.741(2)	0.032607589(3)
3.5	−0.57111449224(2)	−1.03083828(2)	102.261(3)	0.031825916(5)
3.6	−0.56797504205(2)	−1.024533368(9)	114.192(3)	0.030949088(2)
3.7	−0.56492714712(2)	−1.018861816(9)	127.778(4)	0.029997967(3)
3.8	−0.561977346483(7)	−1.013793423(9)	143.316(5)	0.028989808(2)
3.9	−0.5591306106095(2)	−1.00929988(2)	161.177(7)	0.027938807(7)
4.0	−0.556390626278(9)	−1.00535529(4)	181.818(8)	0.026856491(8)
4.1	−0.55376005065(3)	−1.001937117(10)	205.82(2)	0.025751948(3)
4.2	−0.55124075250(5)	−0.99902777(2)	233.88(2)	0.024631841(3)
4.3	−0.54883406510(8)	−0.99661754(6)	266.91(2)	0.02350014(2)
4.4	−0.5465410908(2)	−0.99471012(3)	305.94(3)	0.022357288(6)
4.5	−0.54436313256(7)	−0.99333355(4)	352.07(3)	0.021198381(8)
4.6	−0.5423024117(4)	−0.99256361(6)	405.91(4)	0.02000896(2)
4.7	−0.54036343326(3)	−0.99257615(9)	465.65(5)	0.01875547(2)
4.8	−0.5385558577(5)	−0.9937697(2)	520.20(6)	0.01736292(3)
4.9	−0.5369007741(6)	−0.9970309(3)	524.77(7)	0.01566748(6)
5.0	−0.5354420343(7)	−1.0039525(5)	327.99(9)	0.01338631(9)

Table A80: Same as for Table A1, but for $6\,^1\Delta_u$.

$6\,^1\Delta_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46199182388246(7)	−1.444948415984(7)	1.18596747(4)	−0.520964768217(3)
1.1	−0.506617648372(2)	−1.430619737573(4)	1.40124579(2)	−0.379440400754(2)
1.2	−0.53918060171715(3)	−1.410967842698(3)	1.6433545577(5)	−0.2771721993854(8)
1.3	−0.56294702029734(3)	−1.3883519842163(10)	1.91428604(2)	−0.2018907258716(6)
1.4	−0.58019027324450(3)	−1.364276941381(2)	2.21622341(4)	−0.1456402820657(5)
1.5	−0.59253032333397(3)	−1.339712770504(2)	2.55155924(6)	−0.1031014158904(6)
1.6	−0.6011447414333(3)	−1.315287175585(2)	2.927(4)	−0.0706235579489(6)
1.7	−0.6069042124114(2)	−1.291404626491(2)	3.3331774(2)	−0.0456448245106(7)
1.8	−0.6104620304649(2)	−1.268321924519(2)	3.7855041(2)	−0.0263321464383(8)
1.9	−0.6123146610690(2)	−1.246197126940(3)	4.11(7)	−0.0113514762114(9)
2.0	−0.6128436037722(3)	−1.225121771756(3)	4.8306362(3)	0.000282717894(2)
2.1	−0.6123448765913(3)	−1.205142409850(4)	5.23(8)	0.009308258730(2)
2.2	−0.6110501304970(4)	−1.186275163148(5)	6.0906599(4)	0.016284135385(2)
2.3	−0.6091419964379(4)	−1.168515660190(5)	6.8132628(4)	0.021638405516(2)
2.4	−0.6067653902652(5)	−1.151845864270(6)	7.6050346(4)	0.025702048442(3)
2.5	−0.6040359411616(5)	−1.136238787004(7)	8.4723166(4)	0.028733238128(3)
2.6	−0.60104634452415(5)	−1.121661747818(9)	9.4221486(3)	0.030934977396(3)
2.7	−0.59787119824370(5)	−1.108078624707(10)	10.4623549(2)	0.032468063623(3)
2.8	−0.59457071797775(5)	−1.09545140029(2)	11.60164393(7)	0.033460727023(4)
2.9	−0.59119361503996(5)	−1.08374121302(2)	12.84971925(10)	0.034015867953(4)
3.0	−0.58777934268899(6)	−1.07290905985(2)	14.2174083(3)	0.034216541843(4)
3.1	−0.58435986176614(6)	−1.06291625348(2)	15.7168079(6)	0.034130151630(5)
3.2	−0.58096103754783(6)	−1.05372470721(2)	17.3614516(9)	0.033811677465(5)
3.3	−0.57760375150183(7)	−1.04529709986(2)	19.166501(2)	0.033306182772(5)
3.4	−0.574304791117(4)	−1.03759695859(6)	42.297930(10)	0.03265077166(2)
3.5	−0.5710775658640(2)	−1.03058868675(2)	23.327968(2)	0.031876127138(5)
3.6	−0.567932686209(2)	−1.02423755752(2)	51.450035(5)	0.031007726362(5)
3.7	−0.564878434083(2)	−1.01850968686(3)	28.364378(3)	0.030066805759(5)
3.8	−0.561921147051(2)	−1.01337199765(3)	31.273459(4)	0.029071130646(5)
3.9	−0.559065533479(4)	−1.00879218217(6)	68.96653(4)	0.02803561148(2)
4.0	−0.556314932364(2)	−1.00473866879(3)	38.029088(5)	0.026972798984(6)
4.1	−0.553671528651(2)	−1.00118059684(3)	41.950907(6)	0.025893283039(6)
4.2	−0.551136532634(2)	−0.99808780225(3)	46.294451(7)	0.024806015004(6)
4.3	−0.548710330306(2)	−0.99543081568(3)	51.112024(8)	0.023718568589(6)
4.4	−0.546392610174(2)	−0.99318087399(3)	56.463704(9)	0.022637351446(6)
4.5	−0.544182470980(2)	−0.99130994536(4)	62.418779(10)	0.021567777021(7)
4.6	−0.542078513893(3)	−0.98979076810(4)	69.05753(2)	0.020514404279(7)
4.7	−0.540078922080(3)	−0.98859690290(4)	76.47346(2)	0.019481051332(8)
4.8	−0.538181530014(3)	−0.98770279899(5)	84.77623(2)	0.018470887715(8)
4.9	−0.536383884474(3)	−0.98708387550(5)	94.09536(2)	0.017486508867(9)
5.0	−0.534683298881(4)	−0.98671662183(6)	104.58541(2)	0.016529995187(10)

Table A81: Same as for Table A1, but for $1\,^3\Delta_u$.

$1\,^3\Delta_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.031255144381749(1)	–	9.6696396	–
0.01	97.9690061972(7)	95.938522(5)	9.67(2)	−9999.9490(5)
0.05	17.974768177(3)	15.9609670(4)	9.763(9)	−399.771387(9)
0.1	7.990502571(4)	6.0201070(4)	10.026(9)	−99.608983(5)
0.15	4.679689534(3)	2.76808560(7)	10.42540(2)	−43.9419565(3)
0.2	3.040123847(2)	1.1954878(5)	10.922(10)	−24.423800(3)
0.3	1.4353726991(6)	−0.2679225(5)	12.20(2)	−10.462226(2)
0.4	0.6679885115(2)	−0.8986760(6)	13.79(2)	−5.586633(2)
0.5	0.2337535344(2)	−1.2081808(7)	15.68(2)	−3.351376(2)
0.6	−0.03607770954(10)	−1.3668744214(6)	17.859(2)	−2.1578650039(7)
0.7	−0.213885857835(6)	−1.4466487259(5)	20.329(2)	−1.4555385861(5)
0.8	−0.335742644206(3)	−1.48231453851(9)	23.1102(7)	−1.01353656262(9)
0.9	−0.421534746601(4)	−1.4923220623(2)	26.215(2)	−0.7213917434(2)
1.0	−0.483052472506(3)	−1.4870871424(2)	29.674(2)	−0.5209821974(2)
1.1	−0.527680133189(3)	−1.4727659616(2)	33.511(2)	−0.3794597229(2)
1.2	−0.560245120680(3)	−1.4531225511(2)	37.7655(9)	−0.2771935915(2)
1.3	−0.584013790252(5)	−1.4305162866(2)	42.4725(2)	−0.2019143893(2)
1.4	−0.601259532509(2)	−1.4064520884(2)	47.6749(6)	−0.14566644528(9)
1.5	−0.613602334566(2)	−1.3819001758(2)	53.4251(6)	−0.10313033778(8)
1.6	−0.622219794846(2)	−1.3574884401(2)	59.7800(2)	−0.07065553152(8)
1.7	−0.627982629417(2)	−1.3336215674(2)	66.8034(6)	−0.04568018150(8)
1.8	−0.631544167799(2)	−1.3105566082(2)	74.5703(2)	−0.02637126257(7)
1.9	−0.633400915489(2)	−1.2884519077(2)	83.1631(4)	−0.01139477725(7)
2.0	−0.6339344174044(8)	−1.2673993366(2)	92.6771(6)	0.00023474908(7)
2.1	−0.633440743036(2)	−1.2474458305(2)	103.2210(2)	0.00925507409(6)
2.2	−0.632151601801(2)	−1.2286079564(2)	114.9162(2)	0.01622511234(6)
2.3	−0.63024969107(2)	−1.2108818591(2)	127.90297(8)	0.02157283612(6)
2.4	−0.627880002297(2)	−1.1942501003(2)	142.3400660(10)	0.02562912680(5)
2.5	−0.625158250729(2)	−1.1786863871(2)	158.40868(5)	0.02865204574(5)
2.6	−0.622177229955(2)	−1.1641588483(2)	176.315952(5)	0.03084446601(5)
2.7	−0.619011650005(2)	−1.1506323054(2)	196.29833(6)	0.03236703505(5)
2.8	−0.615721854827(2)	−1.1380698436(2)	218.62686(8)	0.03334780932(5)
2.9	−0.6123567027750(10)	−1.1264338930(3)	243.61238(2)	0.03388948710(7)
3.0	−0.608955815994(2)	−1.1156869681(2)	271.61185(10)	0.03407488797(5)
3.1	−0.605551349778(2)	−1.1057921712(2)	303.0369(2)	0.03397113816(5)
3.2	−0.602169393902(2)	−1.0967135337(2)	338.3626(3)	0.03363289189(5)
3.3	−0.598831089842(3)	−1.0884162526(3)	378.1391(3)	0.03310482637(6)
3.4	−0.595553527284(3)	−1.0808668639(3)	423.0052(2)	0.03242358550(6)
3.5	−0.592350468349(3)	−1.0740333859(3)	473.7049(3)	0.03161930023(6)
3.6	−0.589232936864(2)	−1.0678854621(3)	531.1085(3)	0.03071678100(7)
3.7	−0.5862097017438(7)	−1.0623945276(3)	596.2369(3)	0.02973645295(7)
3.8	−0.583287677482(3)	−1.0575340266(4)	670.2926(4)	0.02869508640(8)
3.9	−0.580472260143(2)	−1.0532797109(4)	754.6982(4)	0.02760636137(8)
4.0	−0.577767614025(2)	−1.0496100525(5)	851.1424(4)	0.02648129388(9)
4.1	−0.57517692178(4)	−1.0465068186(7)	961.6374(3)	0.0253285427(2)
4.2	−0.57270260933(5)	−1.0439558647(7)	1088.5875(6)	0.0241546081(2)
4.3	−0.57034655613(5)	−1.0419482315(9)	1234.870(2)	0.0229639258(2)
4.4	−0.56811030137(6)	−1.0404816429(10)	1403.9309(5)	0.0217588545(3)

4.5	−0.5659952569707(9)	−1.039562543(2)	1599.8717(6)	0.0205395491(3)
4.6	−0.56400293958(7)	−1.039208820(2)	1827.5351(6)	0.0193037085(3)
4.7	−0.56213523395(8)	−1.039453341(2)	2092.5193(8)	0.0180461972(4)
4.8	−0.56039469994(9)	−1.040348290(2)	2401.0474(9)	0.0167585646(4)
4.9	−0.55878492842(10)	−1.041969841(3)	2759.515(2)	0.0154285748(5)
5.0	−0.557310932621(2)	−1.044421656(3)	3173.415(2)	0.0140400418(5)
5.1	−0.5559795149(4)	−1.04783343(2)	3644.9(3)	0.012573648(3)
5.2	−0.5547994504(3)	−1.05234669(2)	4170.0(3)	0.011010040(3)
5.3	−0.5537811750(3)	−1.058076179(8)	4731.8(3)	0.009337013(2)
5.4	−0.5529354845(2)	−1.065035853(6)	5295.1(2)	0.007562058(2)
5.5	−0.552270801744(5)	−1.073040750(5)	5805.6(2)	0.0057274279(9)
5.6	−0.55178921992(10)	−1.081642333(3)	6199.4(2)	0.0039171619(6)
5.7	−0.55148284732(9)	−1.090184966(3)	6424.6(2)	0.0022422331(5)
5.8	−0.55133282504(8)	−1.098001533(2)	6463.2(2)	0.0008041581(4)
5.9	−0.55131214327(7)	−1.104628130(2)	6335.4(2)	−0.0003396345(3)
6.0	−0.551390765309(2)	−1.10989234515(6)	6085.1296(2)	−0.001185135754(7)
6.5	−0.552445964036(2)	−1.12075438028(9)	4335.37950(10)	−0.00244037726(2)
7.0	−0.5535618672438(8)	−1.12069717962(5)	2986.8741(2)	−0.001939063589(6)
7.5	−0.5543687420831(5)	−1.11852767170(3)	2114.45541(5)	−0.001305358338(4)
8.0	−0.5548932494056(5)	−1.11635517878(3)	1539.98381(5)	−0.000821084996(3)
8.5	−0.5552161581127(3)	−1.11462915363(2)	1150.57100(3)	−0.000493745577(2)
9.0	−0.5554066658714(3)	−1.11337450547(2)	880.667066(10)	−0.000284574858(2)
9.5	−0.5555140718032(3)	−1.11250801819(2)	690.37336(2)	−0.0001557762721(9)
10.0	−0.5555710538164(2)	−1.111931605329(9)	554.136254(10)	−0.0000789497696(6)
11.0	−0.5556089487667(2)	−1.111328746937(7)	381.542549572(6)	−0.0000100772184(5)
12.0	−0.5556073253122(2)	−1.111109129406(5)	282.851826(4)	0.0000087934349(3)
13.0	−0.55559657674945(8)	−1.111045458700(3)	220.9128920(10)	0.0000113611384(2)
14.0	−0.55558598493495(7)	−1.111038377196(3)	178.4156600(3)	0.00000954233391(9)
15.0	−0.55557766341943(4)	−1.111048403025(2)	147.17447(2)	0.00000712825429(4)
16.0	−0.55557158647196(3)	−1.1110613254747(7)	123.129210(2)	0.00000511546683(2)
17.0	−0.55556725402419(2)	−1.1110727609832(3)	104.088093(8)	0.000003632180311287(10)
18.0	−0.55556417668809(2)	−1.1110818270817(2)	88.737289(7)	0.000002584794136(3)
19.0	−0.55556197917279(2)	−1.1110887305460(2)	76.208782(3)	0.000001854094711(6)
20.0	−0.555560395394540(9)	−1.111093917775096(3)	65.886691(2)	0.000001343650688(8)

Table A82: Same as for Table A1, but for $2\,^3\Delta_u$.

$2\,^3\Delta_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.0200029371587427(5)	–	5.4064900(5)	–
0.01	97.98025840474(10)	95.9610342638(7)	5.400(3)	−9999.94825457(5)
0.05	17.986020408(3)	15.98347201(2)	5.35(6)	−399.7713762(3)
0.1	8.001754864(7)	6.04261212(4)	5.45(8)	−99.6089760(3)
0.15	4.690941918(4)	2.79059065(2)	5.80(2)	−43.94195454(9)
0.2	3.051376349(3)	1.21799384(2)	6.08(2)	−24.42379428(7)
0.3	1.446625504(2)	−0.245415237(7)	6.79(3)	−10.46222082(2)
0.4	0.6792416918(7)	−0.876167368(4)	7.618(9)	−5.586626880(7)
0.5	0.2450071597(3)	−1.185670396(2)	8.730(2)	−3.351369432(3)
0.6	−0.0248235704(2)	−1.3443628501(10)	9.9345(5)	−2.157859516(2)
0.7	−0.20263113416(9)	−1.4241349329(8)	11.291(6)	−1.4555323780(8)
0.8	−0.32448726218(9)	−1.4597982005(7)	12.821(6)	−1.0135295952(7)
0.9	−0.41027862788(8)	−1.4698028255(8)	14.529(7)	−0.7213839664(7)
1.0	−0.47179553320(8)	−1.4645646166(9)	16.429(8)	−0.5209735504(7)
1.1	−0.51642228284(9)	−1.4502397144(10)	18.537(8)	−0.3794501353(7)
1.2	−0.54898626128(4)	−1.430592101(2)	20.871(10)	−0.2771829823(7)
1.3	−0.57275381512(9)	−1.407981096(2)	23.456(2)	−0.2019026664(8)
1.4	−0.58999832516(4)	−1.383911556(2)	26.313(3)	−0.1456535042(8)
1.5	−0.6023397673(2)	−1.359353625(2)	29.467(5)	−0.1031160600(9)
1.6	−0.6109557277(2)	−1.334935108(2)	32.942(3)	−0.0706397832(10)
1.7	−0.6167169077(2)	−1.311060594(3)	36.78(2)	−0.0456628114(10)
1.8	−0.62027662088(3)	−1.287987021(3)	41.04(2)	−0.026352100(2)
1.9	−0.6221313547(3)	−1.265872604(3)	45.787(3)	−0.011373629(2)
2.0	−0.6226626335(3)	−1.244809063(3)	51.003(2)	0.000258102(2)
2.1	−0.6221665036(2)	−1.224843164(4)	56.793(3)	0.009280877(2)
2.2	−0.62087464802(2)	−1.205991277(4)	63.226(4)	0.016253645(2)
2.3	−0.6189697346(3)	−1.188249319(4)	70.370(9)	0.021604413(2)
2.4	−0.6165967213(4)	−1.171599594(5)	78.319(6)	0.025664104(2)
2.5	−0.61387128547(7)	−1.156015509(5)	87.1906(8)	0.028690825(2)
2.6	−0.61088617795(6)	−1.141464851(6)	97.076(6)	0.030887502(2)
2.7	−0.60771606041(6)	−1.127912049(6)	108.134(6)	0.032414841(2)
2.8	−0.6044212223(5)	−1.115319740(7)	120.517(7)	0.033400966(2)
2.9	−0.60105045996(5)	−1.103649837(7)	134.403(9)	0.033948649(2)
3.0	−0.5976433263(4)	−1.092864268(7)	149.997(10)	0.034140795(2)
3.1	−0.5942318977(4)	−1.082925462(9)	167.549(3)	0.034044624(3)
3.2	−0.59084217558(5)	−1.073796685(9)	187.340(4)	0.033714896(3)
3.3	−0.58749520168(5)	−1.065442268(9)	209.722(8)	0.033196405(3)
3.4	−0.58420795369(5)	−1.057827768(10)	235.06(2)	0.032525923(3)
3.5	−0.58099406834(5)	−1.050920110(10)	263.844(10)	0.031733722(3)
3.6	−0.57786442972(2)	−1.04468773(2)	296.612(9)	0.030844758(3)
3.7	−0.57482765208(5)	−1.03910076(2)	334.041(7)	0.029879607(4)
3.8	−0.57189048062(5)	−1.03413128(2)	376.915(8)	0.028855179(4)
3.9	−0.56905812924(5)	−1.02975372(2)	426.20(2)	0.027785267(3)
4.0	−0.56633457162(4)	−1.02594540(2)	483.089(2)	0.026680935(4)
4.1	−0.5637228009(10)	−1.02268747(2)	548.99(3)	0.025550764(4)
4.2	−0.5612250713(10)	−1.01996620(2)	625.75(3)	0.024400938(4)
4.3	−0.558843142(2)	−1.01777514(3)	715.52(3)	0.023235150(6)
4.4	−0.556578541(2)	−1.01611839(4)	821.03(3)	0.022054247(7)

4.5	−0.55443288138(7)	−1.01501597(4)	945.54(4)	0.020855510(8)
4.6	−0.552408279(3)	−1.01451236(5)	1092.89(4)	0.019631347(10)
4.7	−0.550507937(3)	−1.01469059(6)	1267.09(5)	0.01836708(2)
4.8	−0.548737024(3)	−1.01569440(8)	1471.16(5)	0.01703743(2)
4.9	−0.547103972(4)	−1.01776075(10)	1703.80(6)	0.01560147(2)
5.0	−0.5456222913(2)	−1.0212544(2)	1951.02(7)	0.01399804(3)
5.1	−0.5443125008(3)	−1.026654426(4)	2168.1587(8)	0.0121510932(5)
5.2	−0.5432019101(4)	−1.034332090(7)	2251.1194(10)	0.010013794(2)
5.3	−0.5423163386(5)	−1.043882162(10)	2030.4070(10)	0.007688776(2)
5.4	−0.5416582835(5)	−1.05337508(2)	1366.2142(8)	0.005544720(2)
5.5	−0.54118535897(9)	−1.060094589(9)	320.3920(6)	0.004050205(2)
5.6	−0.5408201582(6)	−1.062687141(7)	−848.8310(4)	0.0033844956(10)
5.7	−0.5404869603(5)	−1.061821924(5)	−1887.7004(3)	0.0033599994(7)
5.8	−0.5401373893(5)	−1.059039050(4)	−2669.3601(3)	0.0036613326(4)
5.9	−0.5397523584(4)	−1.055687939(3)	−3180.5427(2)	0.0040367420(3)
6.0	−0.53933231324(3)	−1.0525829857(9)	−3466.8979(2)	0.00434694015(9)
6.5	−0.53707110149(2)	−1.0459742782(6)	−3331.4207(2)	0.00433352690(6)
7.0	−0.535168928190(10)	−1.0476915121(5)	−2647.22195(9)	0.00323519204(6)
7.5	−0.533822550330(8)	−1.0512176861(5)	−2017.61725(8)	0.00219032194(5)
8.0	−0.532932119480(8)	−1.0545192649(5)	−1489.29614(7)	0.00141812176(5)
8.5	−0.532362013692(8)	−1.0570804210(5)	−1066.85193(7)	0.00089924781(4)
9.0	−0.532001768368(7)	−1.0588980901(4)	−745.18404(6)	0.00056727185(4)
9.5	−0.531774019695(7)	−1.0601259994(4)	−510.55708(5)	0.00036021474(4)
10.0	−0.531628435154(7)	−1.0609329979(4)	−345.09012(5)	0.00023238724(3)
11.0	−0.531470123399(6)	−1.0617949711(3)	−153.75884(4)	0.00010411597(3)
12.0	−0.531395443869(5)	−1.0621590777(3)	−64.80720(4)	0.00005265084(2)
13.0	−0.531355299016(5)	−1.0623125574(3)	−20.85826(4)	0.00003061851(2)
14.0	−0.531330336053(4)	−1.0623737718(2)	0.88590(4)	0.000020492880(2)
15.0	−0.531312811720(4)	−1.0624003621(2)	10.63407(3)	0.000015017422(9)
16.0	−0.531299677372(3)	−1.0624158907(2)	14.54654(3)	0.000011466501(7)
17.0	−0.53128955193(2)	−1.0624276037(2)	15.79426(3)	0.000008911773(6)
18.0	−0.531281644216(3)	−1.06243745234(10)	15.80708(2)	0.000006990894(4)
19.0	−0.531275421228(3)	−1.06244598589(9)	15.22318(2)	0.000005518767(4)
20.0	−0.531270496395(2)	−1.06245342067(7)	14.34616(2)	0.000004378607(3)

Table A83: Same as for Table A1, but for $3\,^3\Delta_u$.

$3\,^3\Delta_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.0138906838155497(3)	–	3.2684586(8)	–
0.01	97.9863706646(5)	95.973258786(4)	3.2687(4)	−9999.9482544(3)
0.05	17.99213269(2)	15.99569665(9)	3.297(2)	−399.771375(2)
0.1	8.00786718(4)	6.0548369(2)	3.384(3)	−99.608975(2)
0.15	4.69705428(4)	2.8028156(2)	3.515(3)	−43.9419533(9)
0.2	3.05748876(3)	1.2302189(2)	3.682(3)	−24.4237929(5)
0.3	1.45273807(2)	−0.23318959(8)	4.107(3)	−10.4622191(2)
0.4	0.685354452(3)	−0.86394100(2)	4.635(2)	−5.58662476(4)
0.5	0.251120150(2)	−1.17344318(2)	5.265(2)	−3.35136696(2)
0.6	−0.018710314(2)	−1.332134638(9)	5.986(2)	−2.15785668(2)
0.7	−0.1965175762(5)	−1.411905576(5)	6.74(4)	−1.455529177(5)
0.8	−0.3183733651(9)	−1.447567537(7)	7.720(2)	−1.013526008(7)
0.9	−0.404164352(2)	−1.45757068(2)	8.741(4)	−0.72137997(2)
1.0	−0.4656808360(2)	−1.452330787(2)	9.885(3)	−0.520969115(2)
1.1	−0.5103071188(2)	−1.438003987(2)	11.148(3)	−0.379445226(2)
1.2	−0.5428705811(3)	−1.418354235(2)	12.547(4)	−0.277177561(2)
1.3	−0.5666375654(3)	−1.395740825(3)	14.094(4)	−0.201896688(2)
1.4	−0.5838814477(3)	−1.371668580(3)	15.803(4)	−0.145646918(2)
1.5	−0.5962221986(3)	−1.347107609(3)	17.705(4)	−0.103108808(2)
1.6	−0.6048373977(4)	−1.322685677(4)	19.7861(7)	−0.070631801(2)
1.7	−0.6105977400(4)	−1.298807321(4)	21.4(4)	−0.045654024(2)
1.8	−0.6141565310(5)	−1.275729425(5)	24.636(9)	−0.026342424(2)
1.9	−0.6160102490(5)	−1.253610139(5)	27.44(4)	−0.011362969(3)
2.0	−0.6165404084(6)	−1.232541110(6)	30.57(4)	0.000269854(3)
2.1	−0.6160430437(6)	−1.212569015(7)	34.06(3)	0.009293844(3)
2.2	−0.6147498251(7)	−1.193710124(7)	37.92(4)	0.016267966(3)
2.3	−0.6128434054(7)	−1.175960240(8)	42.259(3)	0.021620248(3)
2.4	−0.6104687255(8)	−1.159301529(9)	47.033(7)	0.025681634(4)
2.5	−0.6077414435(9)	−1.143707244(10)	52.376(2)	0.028710257(4)
2.6	−0.6047542881(9)	−1.12914499(2)	58.339(8)	0.030909073(4)
2.7	−0.6015818955(10)	−1.11557898(2)	64.97(5)	0.032438820(4)
2.8	−0.5982845264(10)	−1.10297160(2)	72.46(5)	0.033427663(4)
2.9	−0.594910944(2)	−1.09128447(2)	80.893(7)	0.033978419(4)
3.0	−0.591500663(2)	−1.08047919(2)	90.32(3)	0.034174045(5)
3.1	−0.588085716(2)	−1.07051778(2)	100.99(2)	0.034081825(5)
3.2	−0.584692054(2)	−1.06136302(2)	113.05(2)	0.033756589(5)
3.3	−0.581340661(2)	−1.05297870(2)	126.70(2)	0.033243218(5)
3.4	−0.578048446(2)	−1.04532971(2)	142.220(2)	0.032578583(5)
3.5	−0.574828967(2)	−1.03838218(2)	159.88(2)	0.031793072(5)
3.6	−0.571693019(2)	−1.03210363(3)	180.07(3)	0.030911780(5)
3.7	−0.568649109(2)	−1.02646308(3)	203.24(2)	0.029955443(5)
3.8	−0.565703858(2)	−1.02143132(3)	229.91(2)	0.028941156(6)
3.9	−0.562862339(2)	−1.01698128(3)	260.76(2)	0.027882923(6)
4.0	−0.560128360(2)	−1.01308860(3)	296.62(3)	0.026792030(6)
4.1	−0.557504726(2)	−1.00973263(4)	338.53(3)	0.025677274(7)
4.2	−0.554993486(2)	−1.00689800(4)	387.80(4)	0.024544992(8)
4.3	−0.552596186(3)	−1.00457741(5)	446.10(4)	0.023398827(9)
4.4	−0.550314168(3)	−1.00277635(5)	515.51(5)	0.022239088(10)

4.5	$-0.548148960(3)$	$-1.00152181(7)$	$598.58(4)$	$0.02106136(2)$
4.6	$-0.546102879(4)$	$-1.00087870(8)$	$698.07(5)$	$0.01985371(2)$
4.7	$-0.544180025(4)$	$-1.0009819(2)$	$816.11(6)$	$0.01859110(3)$
4.8	$-0.542388083(6)$	$-1.0020994(2)$	$950.73(9)$	$0.01722433(4)$
4.9	$-0.540741664(7)$	$-1.0047493(3)$	$1084.92(9)$	$0.01566000(5)$
5.0	$-0.53926793(2)$	$-1.0098416(7)$	$1153.4(2)$	$0.0137388(2)$
5.1	$-0.538011562(7)$	$-1.0183961(2)$	$973.95(4)$	$0.01129943(4)$
5.2	$-0.537018090(9)$	$-1.0293351(3)$	$251.49(4)$	$0.00859636(4)$
5.3	$-0.536264444(10)$	$-1.0369413(2)$	$-981.61(4)$	$0.00671463(2)$
5.4	$-0.535623036(9)$	$-1.03701510(3)$	$-2100.95(4)$	$0.006339069(2)$
5.5	$-0.534967735(7)$	$-1.03237217(3)$	$-2664.83(3)$	$0.006829687(7)$
5.6	$-0.534256245(5)$	$-1.02726386(4)$	$-2743.35(3)$	$0.007365824(8)$
5.7	$-0.533504346(4)$	$-1.02358183(3)$	$-2563.04(2)$	$0.007618745(6)$
5.8	$-0.532742439(3)$	$-1.02154790(3)$	$-2279.371(8)$	$0.007575340(5)$
5.9	$-0.531996845(2)$	$-1.02089845(2)$	$-1961.418(5)$	$0.007304277(4)$
6.0	$-0.531287199(3)$	$-1.02139241(4)$	$-1628.691(4)$	$0.006863664(8)$
6.5	$-0.5288103574(3)$	$-1.04234278(2)$	$550.8415(6)$	$0.002350451(2)$
7.0	$-0.528871363(8)$	$-1.0683622(2)$	$1526.12(5)$	$-0.00151707(2)$
7.5	$-0.52967112981(9)$	$-1.070450074(2)$	$1127.7077(5)$	$-0.0014810420(2)$
8.0	$-0.53029637849(5)$	$-1.0687751634(4)$	$799.3609(3)$	$-0.00102280080(4)$
8.5	$-0.53071038893(8)$	$-1.0669795932(7)$	$580.6234(4)$	$-0.00065397827(6)$
9.0	$-0.53096999340(6)$	$-1.0655567568(5)$	$433.9929(3)$	$-0.00040186334(4)$
9.5	$-0.53112704163(4)$	$-1.0645206448(4)$	$334.0754(3)$	$-0.00023858542(3)$
10.0	$-0.53121863177(2)$	$-1.06379611019(8)$	$264.94184(8)$	$-0.000135884666(6)$
11.0	$-0.531295431753(6)$	$-1.06297006623(5)$	$180.70620(6)$	$-0.000034472975(4)$
12.0	$-0.531308992240(5)$	$-1.06260792904(5)$	$131.68657(5)$	$0.000000837953(3)$
13.0	$-0.531302051582(4)$	$-1.06246710374(4)$	$97.26417(4)$	$0.000010538417(3)$
14.0	$-0.531290936650(4)$	$-1.06242929274(3)$	$72.98299(4)$	$0.000010898611(2)$
15.0	$-0.531281024435(3)$	$-1.06243003137(2)$	$56.70616(4)$	$0.0000088011665(10)$
16.0	$-0.531273347667(3)$	$-1.06244094086(2)$	$45.49577(4)$	$0.0000066096545(6)$
17.0	$-0.531267651376(2)$	$-1.062452598588(9)$	$37.32628(4)$	$0.0000048649508(4)$
18.0	$-0.531263464297(2)$	$-1.062462525001(6)$	$31.09463(4)$	$0.0000035779774(2)$
19.0	$-0.5312603759944(9)$	$-1.062470409947(4)$	$26.19586(4)$	$0.00000264958115(10)$
20.0	$-0.5312580787056(7)$	$-1.062476531526(3)$	$22.26884(3)$	$0.00000198129426(5)$

Table A84: Same as for Table A1, but for $4\,^3\Delta_u$.

$4\,^3\Delta_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.4656774229394(8)	−1.4523210696(2)	1.78896(6)	−0.52096622373(7)
1.1	−0.5103033999491(4)	−1.43799299519(5)	2.11776(5)	−0.37944199571(3)
1.2	−0.5428665200(3)	−1.41834176045(5)	2.48760(3)	−0.277173935(2)
1.3	−0.5666331188324(2)	−1.39572661879(2)	2.90146(3)	−0.201892600860(5)
1.4	−0.5838765663278(9)	−1.371652350139(5)	3.36264(3)	−0.145642298203(3)
1.5	−0.59621682514(2)	−1.34708901189(7)	3.87468(8)	−0.10310357440(3)
1.6	−0.604831466269(2)	−1.322664309214(8)	4.44163(8)	−0.070625860422(4)
1.7	−0.610591174779(3)	−1.29878271374(2)	5.06771(9)	−0.045647273051(9)
1.8	−0.614149245096(3)	−1.275701028799(5)	5.7576(2)	−0.0263347436709(4)
1.9	−0.616002142990(2)	−1.253577314225(3)	6.5167(2)	−0.0113542253923(2)
2.0	−0.616531368371(2)	−1.232503111160(2)	7.3504(2)	0.000279812788(2)
2.1	−0.616032939692(2)	−1.212524974281(4)	8.2653(3)	0.0093051929066(5)
2.2	−0.61473850844886(4)	−1.1936590300821(6)	9.2681(3)	0.0162809030980(3)
2.3	−0.612830706224(3)	−1.17590091261(5)	10.3668(2)	0.02163499993(2)
2.4	−0.6104544496025(9)	−1.15923259155(2)	11.5691(5)	0.025698461522(7)
2.5	−0.6077253686434(5)	−1.1436270864(2)	12.8852(6)	0.02872946036(6)
2.6	−0.6047361597718(2)	−1.1290517254(2)	14.3250(7)	0.03093099777(7)
2.7	−0.601561422072(2)	−1.11547039697(3)	15.9002(8)	0.032463869323(10)
2.8	−0.598261372583(2)	−1.10284509650(4)	17.6234(9)	0.03345630310(2)
2.9	−0.594884724227(3)	−1.09113697664(5)	19.5095(5)	0.03401119718(2)
3.0	−0.591470932110(3)	−1.08030705103(6)	21.574(4)	0.03421160440(2)
3.1	−0.5880519591951(2)	−1.0703166520(5)	23.83399(2)	0.0341249247(2)
3.2	−0.584653673209(4)	−1.06112771402(8)	26.302(7)	0.03380613512(3)
3.3	−0.581296958392(5)	−1.05270294251(10)	29.00(2)	0.03330029523(3)
3.4	−0.5779986054032(2)	−1.0450058940(8)	31.99628(2)	0.0326445050(3)
3.5	−0.574772027348(6)	−1.0380010039(2)	35.2604(5)	0.03186944309(4)
3.6	−0.571627838762(6)	−1.0316535849(2)	38.84473(10)	0.03100058129(4)
3.7	−0.568574326218(7)	−1.0259297958(2)	42.7846(5)	0.03005915045(5)
3.8	−0.565617832512(8)	−1.0207966085(2)	47.1180(2)	0.02906290960(5)
3.9	−0.562763071899(9)	−1.0162217709(3)	51.8896(3)	0.02802676228(5)
4.0	−0.560013389993(9)	−1.0121737736(3)	57.14927(9)	0.02696325160(6)
4.1	−0.557370979154(10)	−1.0086218260(3)	62.95249(4)	0.02588295911(6)
4.2	−0.5548370579458(9)	−1.005535844(3)	69.36257(7)	0.0247948268(5)
4.3	−0.552412021607(2)	−1.002886441(3)	76.4515(4)	0.0237064192(6)
4.4	−0.550095568874(2)	−1.000644952(3)	84.30216(3)	0.0226241332(6)
4.5	−0.547886809796(3)	−0.998783449(4)	93.00691(6)	0.0215533713(7)
4.6	−0.54578435798(2)	−0.9972747804(5)	102.67307(8)	0.02049868165(10)
4.7	−0.5437864101127(4)	−0.9960926300(6)	113.42316(6)	0.01946387027(10)
4.8	−0.541890815335(6)	−0.995211569(5)	125.3983(2)	0.0184520963(8)
4.9	−0.540095135976(7)	−0.994607126(5)	138.7623(2)	0.0174659483(9)
5.0	−0.53839670161(3)	−0.99425558842(7)	153.7050509(3)	0.0165075038(2)

Table A85: Same as for Table A1, but for $5\,^3\Delta_u$.

$5\,^3\Delta_u$				
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46199405632(2)	−1.4449547956(8)	6.3688(5)	−0.5209666831(6)
1.1	−0.50662008322(2)	−1.4306269534(8)	7.1812(6)	−0.3794425345(5)
1.2	−0.53918326291(2)	−1.4109760382(10)	8.0805(6)	−0.2771745938(7)
1.3	−0.562949935582(4)	−1.388361315(2)	9.0750(7)	−0.2018934187(7)
1.4	−0.580193474761(10)	−1.364287596(2)	10.1743(8)	−0.1456433193(8)
1.5	−0.592533848059(9)	−1.339724970(2)	11.3892(9)	−0.1031048495(9)
1.6	−0.601148631892(9)	−1.315301178(2)	12.7319(10)	−0.0706274468(10)
1.7	−0.606908517393(7)	−1.291420734(3)	14.217(2)	−0.045649235(2)
1.8	−0.610466805856(6)	−1.268340489(3)	15.860(2)	−0.026337154(2)
1.9	−0.612319970810(5)	−1.246218559(4)	17.679(2)	−0.011357167(2)
2.0	−0.612849520971(3)	−1.225146550(4)	19.696(2)	0.000276246(2)
2.1	−0.6123514848044(10)	−1.205171092(5)	21.935(2)	0.009300894(2)
2.2	−0.6110575252239(9)	−1.186308399(5)	24.423(3)	0.016275750(2)
2.3	−0.609150286863(3)	−1.168554210(6)	27.191(3)	0.021628853(2)
2.4	−0.606774701298(5)	−1.151890615(6)	30.276(3)	0.025691161(3)
2.5	−0.604046415838(4)	−1.136290780(7)	33.718(3)	0.028720820(3)
2.6	−0.601058146852(8)	−1.121722202(8)	37.567(4)	0.030920804(3)
2.7	−0.5978845165470(10)	−1.108148981(4)	41.877(4)	0.0324518711(10)
2.8	−0.594585769043(3)	−1.095533351(6)	46.712(4)	0.033442210(2)
2.9	−0.591210648913(3)	−1.083836770(7)	52.147(5)	0.033994665(2)
3.0	−0.5877986486409(10)	−1.073020617(9)	58.270(5)	0.034192227(3)
3.1	−0.5843817756362(6)	−1.063046679(9)	65.183(6)	0.034102217(3)
3.2	−0.58098595080(2)	−1.05387745(2)	73.007(6)	0.033779515(4)
3.3	−0.577632122414(3)	−1.045476358(9)	81.886(7)	0.033269057(3)
3.4	−0.574337159471(6)	−1.037807855(9)	91.990(8)	0.032607783(3)
3.5	−0.571114571361(8)	−1.030837556(9)	103.527(9)	0.031826168(3)
3.6	−0.567975092602(5)	−1.024532313(9)	116.746(10)	0.030949409(3)
3.7	−0.5649271614974(7)	−1.018860347(9)	131.95(2)	0.029998372(3)
3.8	−0.561977315474(6)	−1.013791436(10)	149.53(2)	0.028990315(3)
3.9	−0.55913052290(2)	−1.009297236(10)	169.94(2)	0.027939438(3)
4.0	−0.55639046780(3)	−1.00535182(2)	193.79(2)	0.026857280(3)
4.1	−0.55375980370(5)	−1.00193257(2)	221.82(2)	0.025752936(3)
4.2	−0.55124039433(7)	−0.99902181(5)	255.02(3)	0.024633090(10)
4.3	−0.54883356640(9)	−0.99660971(2)	294.63(3)	0.023501725(4)
4.4	−0.5465404108(2)	−0.99469971(7)	342.24(4)	0.02235934(2)
4.5	−0.5443622180(2)	−0.99331960(4)	399.74(5)	0.021201075(7)
4.6	−0.54230118536(10)	−0.99254459(5)	469.03(5)	0.020012562(10)
4.7	−0.5403617867(2)	−0.99254992(8)	550.29(6)	0.01876035(2)
4.8	−0.5385536440(2)	−0.9937340(2)	635.37(7)	0.01736943(3)
4.9	−0.5368978445(2)	−0.9969884(3)	682.18(8)	0.01567496(5)
5.0	−0.5354385201(7)	−1.0039345(5)	530.32(10)	0.01338850(9)

Table A86: Same as for Table A1, but for $6\,^3\Delta_u$.

$6\,^3\Delta_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46199182388324(7)	−1.444948415989(7)	1.18595430(7)	−0.520964768221(3)
1.1	−0.50661764837236(5)	−1.430619737581(4)	1.40122536(6)	−0.379440400759(2)
1.2	−0.53918060171895(3)	−1.410967842710(3)	1.64332351(7)	−0.2771721993926(7)
1.3	−0.56294702029999(3)	−1.388351984247(2)	1.91424002(8)	−0.2018907258815(6)
1.4	−0.58019027324829(4)	−1.364276941407(2)	2.21615694(10)	−0.1456402820788(5)
1.5	−0.59253032333924(3)	−1.339712770540(2)	2.554(2)	−0.1031014159072(5)
1.6	−0.6011447414404(3)	−1.315287175633(2)	2.9227896(2)	−0.0706235579698(6)
1.7	−0.6069042124214(8)	−1.291404626556(5)	3.3330071(6)	−0.045644824537(2)
1.8	−0.6104620304776(7)	−1.268321924600(5)	3.66(6)	−0.026332146469(2)
1.9	−0.6123146610844(2)	−1.246197127035(2)	4.2831006(4)	−0.0113514762453(9)
2.0	−0.6128436037911(3)	−1.225121771869(3)	4.8302936(5)	0.0002827178600(8)
2.1	−0.6123448766141(3)	−1.205142409980(3)	5.4310942(6)	0.009308258693(2)
2.2	−0.6110501305240(3)	−1.186275163295(4)	6.0901762(8)	0.016284135343(2)
2.3	−0.6091419964691(4)	−1.168515660350(5)	6.8127085(9)	0.021638405473(2)
2.4	−0.6067653903006(4)	−1.151845864440(6)	7.604415(2)	0.025702048401(2)
2.5	−0.6040359412010(5)	−1.136238787179(7)	8.471641(2)	0.028733238089(3)
2.6	−0.60104634456714(4)	−1.121661747991(8)	8.6(9)	0.030934977363(3)
2.7	−0.59787119828967(4)	−1.108078624869(9)	10.461618(2)	0.032468063596(3)
2.8	−0.59457071802584(4)	−1.095451400433(10)	11.600914(3)	0.033460727007(4)
2.9	−0.59119361508918(4)	−1.08374121313(2)	0(2)	0.034015867948(4)
3.0	−0.58777934273805(5)	−1.07290905992(2)	14.216803(3)	0.034216541852(4)
3.1	−0.5843598618137(10)	−1.06291625350(2)	15.716327(9)	0.034130151654(5)
3.2	−0.58096103759191(6)	−1.05372470716(2)	17.361162(4)	0.033811677507(5)
3.3	−0.57760375154070(7)	−1.04529709973(2)	19.166459(4)	0.033306182834(5)
3.4	−0.57430479114628(8)	−1.03759695834(2)	21.149240(5)	0.032650771752(5)
3.5	−0.5710775658863(2)	−1.03058868642(2)	23.328627(5)	0.031876127243(5)
3.6	−0.567932686220(2)	−1.02423755708(2)	51.452277(10)	0.031007726490(5)
3.7	−0.564878434079(2)	−1.01850968629(3)	56.73208(2)	0.030066805909(5)
3.8	−0.561921147032(2)	−1.01337199696(3)	31.275734(6)	0.029071130818(5)
3.9	−0.559065533442(2)	−1.00879218135(3)	34.486252(7)	0.028035611676(5)
4.0	−0.556314932306(2)	−1.00473866785(3)	38.032791(8)	0.026972799190(6)
4.1	−0.553671528573(2)	−1.00118059580(3)	41.955394(8)	0.025893283254(6)
4.2	−0.551136532534(2)	−0.99808780114(3)	46.299732(9)	0.024806015220(6)
4.3	−0.548710330185(2)	−0.99543081456(3)	51.118068(9)	0.023718568794(6)
4.4	−0.546392610033(2)	−0.99318087293(3)	56.470417(10)	0.022637351621(6)
4.5	−0.544182470825(3)	−0.99130994451(4)	62.3(9)	0.021567777141(7)
4.6	−0.542078513730(3)	−0.98979076764(4)	69.06491(2)	0.020514404309(7)
4.7	−0.540078921920(3)	−0.98859690311(4)	76.48054(2)	0.019481051220(8)
4.8	−0.538181529875(3)	−0.98770280030(5)	84.78226(2)	0.018470887385(8)
4.9	−0.536383884384(3)	−0.98708387856(5)	94.09922(2)	0.017486508207(9)
5.0	−0.534683298880(4)	−0.98671662767(6)	104.58541(2)	0.016529994018(10)

Table A87: Same as for Table A1, but for $1\,^1\Phi_g$.

R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
		$1\,^1\Phi_g$		
0.0	−2.02000071089858471(1)	–	1.4044136	–
0.01	97.98026065229(4)	95.9610387603(3)	1.40491(2)	−9999.94825443(2)
0.05	17.986022689(5)	15.98347664(4)	1.41551(2)	−399.7713747(5)
0.1	8.001757228(5)	6.04261707(3)	1.44408(2)	−99.6089739(3)
0.15	4.690944419(4)	2.79059613(3)	1.48486(2)	−43.94195138(10)
0.2	3.051379028(2)	1.21799999(2)	1.53445(3)	−24.42379033(4)
0.3	1.4466286553(7)	−0.245407304(4)	1.65162(4)	−10.462215383(9)
0.4	0.67924545612(9)	−0.8761571126(6)	1.78444(3)	−5.5866200622(10)
0.5	0.24501167300(2)	−1.18565729095(10)	1.9275(3)	−3.3513612739(2)
0.6	−0.02481817450(2)	−1.34434636284(9)	2.07768(4)	−2.1578500231(2)
0.7	−0.202624721746(3)	−1.4241145201(7)	2.2338(2)	−1.4555215378(7)
0.8	−0.324479697169(2)	−1.4597732986(5)	2.3954(2)	−1.0135173802(5)
0.9	−0.410269771048(2)	−1.4697728480(4)	2.5626(2)	−0.7213703398(3)
1.0	−0.471785241159(2)	−1.4645289484(3)	2.7362(2)	−0.5209584661(2)
1.1	−0.516410407148(2)	−1.4501977062(3)	2.9172(2)	−0.3794335380(2)
1.2	−0.548972647468(2)	−1.4305430635(3)	3.1074(2)	−0.2771648071(2)
1.3	−0.572738301733(2)	−1.4079242927(3)	3.3088(2)	−0.2018828378(2)
1.4	−0.589980742602(2)	−1.3838461943(3)	3.5240(2)	−0.1456319351(2)
1.5	−0.602319936689(2)	−1.3592788483(3)	3.7564(2)	−0.1030926499(2)
1.6	−0.610933459043(2)	−1.3348499848(3)	4.0100(2)	−0.0706144167(2)
1.7	−0.616691999088(3)	−1.3109641026(4)	4.2893(2)	−0.0456353555(2)
1.8	−0.620248855993(3)	−1.2878780350(4)	4.6001(2)	−0.0263224016(2)
1.9	−0.622100500664(3)	−1.2657498749(5)	4.9489(2)	−0.0113415124(2)
2.0	−0.622628438589(3)	−1.2446712000(5)	5.3435(2)	0.0002928386(2)
2.1	−0.622128694291(3)	−1.2246886054(6)	5.7930(2)	0.0093184682(3)
2.2	−0.620832925877(3)	−1.2058182621(7)	6.3080(2)	0.0162943590(3)
2.3	−0.618923772129(4)	−1.1880558539(8)	6.9007(2)	0.0216485610(3)
2.4	−0.616546157515(4)	−1.1713834058(10)	7.5855(2)	0.0257120456(4)
2.5	−0.613815720701(4)	−1.155773998(2)	8.3786(2)	0.0287429774(4)
2.6	−0.610825167540(4)	−1.141195028(2)	9.2991(2)	0.0309443489(4)
2.7	−0.607649107462(4)	−1.127610460(2)	10.3688(2)	0.0324769462(5)
2.8	−0.604347768880(4)	−1.114982375(2)	11.61259(10)	0.0334689866(5)
2.9	−0.600969877222(4)	−1.103272022(2)	13.05932(8)	0.0340233560(5)
3.0	−0.597554901390(4)	−1.092440522(2)	14.74179(5)	0.0342230937(6)
3.1	−0.594134819585(4)	−1.082449328(3)	16.69759(3)	0.0341355844(6)
3.2	−0.590735516382(4)	−1.073260512(3)	18.969626(10)	0.0338157877(7)
3.3	−0.587377894736(4)	−1.064836936(3)	21.60690(5)	0.0333087437(7)
3.4	−0.584078766099(4)	−1.057142330(3)	24.66536(9)	0.0326515301(7)
3.5	−0.580851566733(4)	−1.050141334(3)	28.2088(2)	0.0318747999(8)
3.6	−0.577706937097(4)	−1.043799489(4)	32.3101(2)	0.0310039959(8)
3.7	−0.574653192800(4)	−1.038083220(4)	37.0521(3)	0.0300603152(8)
3.8	−0.571696709320(4)	−1.032959804(4)	42.5297(3)	0.0290614776(9)
3.9	−0.568842237817(4)	−1.028397346(4)	48.8512(4)	0.0280223410(9)
4.0	−0.566093165761(4)	−1.024364752(5)	56.1403(5)	0.0269553950(10)
4.1	−0.56345173323(7)	−1.020831717(2)	64.5395(2)	0.0258711584(3)
4.2	−0.560919213324(8)	−1.0177687401(2)	74.21112(2)	0.02477849680(3)
4.3	−0.55849606426(7)	−1.015147128(2)	85.3426(2)	0.0236848837(3)
4.4	−0.55618205758(7)	−1.012939044(2)	98.1511(3)	0.0225966071(3)

4.5	−0.553976388313(4)	−1.011117568(2)	112.8875(3)	0.0215189354(3)
4.6	−0.55187777003(8)	−1.009656784(2)	129.8438(4)	0.0204562512(3)
4.7	−0.54988451766(8)	−1.008531900(2)	149.3617(4)	0.0194121565(3)
4.8	−0.54799462163(8)	−1.007719389(2)	171.8426(5)	0.0183895530(3)
4.9	−0.54620581464(9)	−1.007197193(2)	197.7611(6)	0.0173907014(3)
5.0	−0.544515633620(6)	−1.006944965(2)	227.6815(7)	0.0164172605(4)
5.5	−0.53745169841(2)	−1.009193370(2)	466.6326(8)	0.0119472775(3)
6.0	−0.53248424182(3)	−1.017252940(7)	999.878(3)	0.00795259087(9)
6.5	−0.52960054618(2)	−1.037603520(2)	2050.55248(4)	0.0033227034(3)
7.0	−0.529133668331(6)	−1.063785059(2)	2063.5749(2)	−0.0007882461(3)
7.5	−0.529737835301(5)	−1.069267328(2)	1301.0201(2)	−0.0013055543(2)
8.0	−0.530315564838(4)	−1.068455174(2)	831.6977(2)	−0.0009780056(2)
8.5	−0.53071710645(2)	−1.0668892857(9)	557.0363(2)	−0.00064177327(8)
9.0	−0.530973140359(4)	−1.0655270792(7)	385.6317(2)	−0.00039786650(6)
9.5	−0.531128722299(3)	−1.0645015268(6)	273.6424(2)	−0.00023621918(5)
10.0	−0.53121917871(2)	−1.0637748(2)	198.30(9)	−0.000133647(9)
11.0	−0.531293942136(5)	−1.06294953(9)	111.7(2)	−0.000032876(6)
12.0	−0.531306698843(2)	−1.06260356(7)	70.13(10)	0.000000820(4)
13.0	−0.531300340018(3)	−1.06247576(5)	49.26(8)	0.000009609(2)
14.0	−0.5312901353089(6)	−1.06243871(3)	38.02(7)	0.000010111(2)
15.0	−0.531280818245(2)	−1.06243583(3)	31.27(6)	0.0000083872(9)
16.0	−0.531273420417(2)	−1.06244381(2)	26.70(5)	0.0000064398(6)
17.0	−0.531267826205(2)	−1.062453805(10)	23.27(4)	0.0000048147(3)
18.0	−0.5312636596801(2)	−1.062462895(10)	20.49(4)	0.0000035792(4)
19.0	−0.5312605582656(2)	−1.062470374(8)	18.17(4)	0.0000026708(3)
20.0	−0.5312582359376(2)	−1.062476306(7)	16.19(4)	0.0000020084(3)

Table A88: Same as for Table A1, but for $2\,^1\Phi_g$.

$2\,^1\Phi_g$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.01388934538731322(3)	–	0.8985799(7)	–
0.01	97.98637201788(6)	95.9732614919(4)	0.898951(7)	−9999.94825438(3)
0.05	17.992134051(4)	15.99569935(3)	0.905903(10)	−399.7713750(3)
0.1	8.007868591(6)	6.05483979(4)	0.9246(2)	−99.6089739(3)
0.15	4.697055774(5)	2.80281882(3)	0.9516(3)	−43.9419515(2)
0.2	3.057490371(3)	1.23022262(2)	0.98484(7)	−24.42379059(6)
0.3	1.4527399616(7)	−0.233184829(4)	1.06387(5)	−10.462215840(9)
0.4	0.6853567069(2)	−0.8639348723(9)	1.15465(3)	−5.586620715(2)
0.5	0.25112284869(6)	−1.1734353637(3)	1.253719(6)	−3.3513621221(4)
0.6	−0.01870709322(3)	−1.3321248240(2)	1.35929(4)	−2.1578510626(2)
0.7	−0.196513755(3)	−1.4118937(3)	1.47039(5)	−1.4555232(4)
0.8	−0.31836886056(5)	−1.4475529(2)	1.58731(3)	−1.0135190(3)
0.9	−0.40415908315(7)	−1.4575528852(4)	1.70997(3)	−0.7213719099(3)
1.0	−0.46567471824(4)	−1.45230972(8)	1.83878(3)	−0.52096029(9)
1.1	−0.51030006442(4)	−1.43797918(9)	1.974702(8)	−0.37943551(9)
1.2	−0.54286249891(3)	−1.41832522(4)	2.118809(2)	−0.27716685(4)
1.3	−0.56662836003(6)	−1.3957071745(10)	2.272502(10)	−0.2018849651(8)
1.4	−0.58387101883(7)	−1.3716298697(9)	2.437550(4)	−0.1456341659(8)
1.5	−0.59621044039(3)	−1.347063332(2)	2.61608(2)	−0.1030949674(8)
1.6	−0.60482419797(6)	−1.322635279(2)	2.810668(8)	−0.0706168021(10)
1.7	−0.61058297899(3)	−1.298750197(2)	3.024353(9)	−0.0456377878(8)
1.8	−0.61414008050(3)	−1.2756649053(10)	3.26073(2)	−0.0263248580(6)
1.9	−0.61599197089(5)	−1.2535381(6)	3.5236(5)	−0.0113443(4)
2.0	−0.61652015315(4)	−1.232459483(2)	3.819204(10)	0.0002904115(7)
2.1	−0.61602064883(4)	−1.212477492(7)	4.15198(3)	0.009316098(4)
2.2	−0.61472511280(4)	−1.193607646(7)	4.52909(3)	0.016292081(4)
2.3	−0.61281618030(4)	−1.175845608(7)	4.95830(3)	0.021646414(4)
2.4	−0.61043877185(5)	−1.159173374(7)	5.44857(3)	0.025710071(4)
2.5	−0.60770852173(5)	−1.14356405(6)	6.01023(6)	0.02874120(3)
2.6	−0.60471813097(6)	−1.12898486(5)	6.65530(5)	0.03094284(2)
2.7	−0.60154220361(6)	−1.115399787(5)	7.39750(3)	0.032475785(2)
2.8	−0.59824096209(6)	−1.102770923(4)	8.25256(3)	0.033468215(2)
2.9	−0.5948631253(2)	−1.091059429(5)	9.23859(3)	0.034023042(2)
3.0	−0.59144815462(5)	−1.080226359(2)	10.37635(6)	0.0342233166(4)
3.1	−0.58802802026(6)	−1.070233112(2)	11.68963(9)	0.0341364287(5)
3.2	−0.58462859768(6)	−1.061041680(2)	13.2057(2)	0.0338173486(5)
3.3	−0.58127077978(6)	−1.052614840(3)	14.9558(2)	0.0333111272(6)
3.4	−0.57797136688(5)	−1.044916232(3)	16.9756(2)	0.0326548536(6)
3.5	−0.57474378285(5)	−1.037910388(3)	19.3062(3)	0.0318791936(7)
3.6	−0.57159865442(5)	−1.031562734(3)	21.9945(3)	0.0310096042(7)
3.7	−0.56854428203(4)	−1.025839562(4)	25.0946(4)	0.0300672978(7)
3.8	−0.56558702433(4)	−1.020708006(4)	28.6686(5)	0.0290700112(8)
3.9	−0.56273161393(4)	−1.016136008(4)	32.7881(6)	0.0280326205(8)
4.0	−0.55998141784(4)	−1.01209231(2)	37.535(3)	0.026967631(4)
4.1	−0.55733865368(5)	−1.0085463779(8)	43.0096(2)	0.0258855926(2)
4.2	−0.55480457007(5)	−1.0054685366(8)	49.3190(2)	0.0247953818(2)
4.3	−0.55237959847(5)	−1.0028298609(9)	56.5965(2)	0.0237044968(2)
4.4	−0.55006348183(5)	−1.0006022892(9)	64.9965(3)	0.0226192442(2)

4.5	−0.54785538476(6)	−0.998937614(9)	74.7018(9)	0.0215449079(2)
4.6	−0.54575398915(6)	−0.9972729403(10)	85.9332(4)	0.0204858778(2)
4.7	−0.54375757834(6)	−0.9961201372(10)	98.9527(4)	0.0194457488(2)
4.8	−0.54186411293(6)	−0.995276752(2)	114.0819(5)	0.0184273905(3)
4.9	−0.54007130096(7)	−0.994720959(2)	131.7154(6)	0.0174329883(3)
5.0	−0.53837666558(6)	−0.9944330672(10)	152.3452(5)	0.0164640528(2)
5.5	−0.5312860427(2)	−0.996595489(4)	329.571(2)	0.0119957448(6)
6.0	−0.5263714295(5)	−1.00834125(2)	793.242(3)	0.007400268(3)
6.5	−0.524682454(2)	−1.04765326(3)	−604.268(3)	0.000263330(3)
7.0	−0.5240980215(9)	−1.0330771546(6)	−1740.715(2)	0.0021598407(4)
7.5	−0.5229454714(4)	−1.029453435(2)	−1306.9467(4)	0.00219166770(10)
8.0	−0.5219975528(7)	−1.031262696(5)	−939.2329(3)	0.0015915512(4)
8.5	−0.5213382632(2)	−1.033574278(2)	−676.18356(8)	0.0010708527(2)
9.0	−0.5209010560(2)	−1.035486370(2)	−480.3716(2)	0.0007017491(2)
9.5	−0.5206158686(2)	−1.036895926(2)	−334.2670(2)	0.0004564011(2)
10.0	−0.5204302506(4)	−1.037882760(4)	−227.3472(4)	0.0002977742(3)
11.0	−0.5202278192(3)	−1.039007800(3)	−97.6152(4)	0.0001316217(2)
12.0	−0.5201352974(3)	−1.039512118(3)	−36.4244(4)	0.0000632064(2)
13.0	−0.5200887993(2)	−1.039739524(2)	−9.3027(4)	0.00003369808(8)
14.0	−0.5200627937(2)	−1.0398464465(9)	2.2407(4)	0.00001993864(5)
15.0	−0.52004672769(9)	−1.0398996486(7)	6.9592(4)	0.00001292045(3)
16.0	−0.52003594429(7)	−1.0399280587(6)	8.6003(3)	0.00000898936(3)
17.0	−0.52002825910(6)	−1.0399450715(5)	8.8578(3)	0.00000655569(2)
18.0	−0.52002256922(5)	−1.0399565000(4)	8.5443(3)	0.00000492436(2)
19.0	−0.52001825111(5)	−1.0399647696(3)	8.0239(2)	0.00000377540(2)
20.0	−0.52001491423(4)	−1.0399710067(3)	7.4485(2)	0.000002941090(9)

Table A89: Same as for Table A1, but for $1\,^3\Phi_g$.

R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
		$1\,^3\Phi_g$		
0.0	−2.02000071089858471(1)	–	1.4040013	–
0.01	97.98026065231(5)	95.9610387606(4)	1.404491(3)	−9999.94825440(3)
0.05	17.986022684(2)	15.98347661(2)	1.41505(3)	−399.7713752(2)
0.1	8.001757227(3)	6.04261706(2)	1.44361(2)	−99.6089740(2)
0.15	4.690944418(3)	2.79059613(2)	1.484358(9)	−43.94195139(8)
0.2	3.0513790279(7)	1.217999989(5)	1.53393(5)	−24.42379033(2)
0.3	1.4466286553(2)	−0.245407304(2)	1.650998(8)	−10.462215383(3)
0.4	0.67924545608(8)	−0.8761571128(6)	1.783686(6)	−5.5866200623(10)
0.5	0.24501167293(4)	−1.1856572912(3)	1.926481(7)	−3.3513612741(4)
0.6	−0.024818174559(4)	−1.3443463632(2)	2.07652(2)	−2.1578500235(3)
0.7	−0.202624721835(2)	−1.4241145204(7)	2.23241(5)	−1.4555215380(7)
0.8	−0.324479697276(2)	−1.4597732990(5)	2.39372(5)	−1.0135173804(5)
0.9	−0.410269771177(2)	−1.4697728485(3)	2.56061(5)	−0.7213703401(3)
1.0	−0.471785241314(2)	−1.4645289490(3)	2.73375(4)	−0.5209584663(2)
1.1	−0.516410407332(2)	−1.4501977069(2)	2.91431(4)	−0.3794335383(2)
1.2	−0.548972647684(2)	−1.4305430644(3)	3.10389(5)	−0.2771648075(2)
1.3	−0.572738301986(2)	−1.4079242937(2)	3.30466(3)	−0.20188283820(10)
1.4	−0.589980742896(2)	−1.3838461955(2)	3.51922(3)	−0.14563193546(10)
1.5	−0.602319937028(2)	−1.3592788497(3)	3.75086(3)	−0.1030926504(2)
1.6	−0.610933459431(2)	−1.3348499864(3)	4.00352(3)	−0.0706144172(2)
1.7	−0.616691999530(2)	−1.3109641044(3)	4.28193(2)	−0.0456353561(2)
1.8	−0.620248856493(3)	−1.2878780370(3)	4.59168(2)	−0.0263224022(2)
1.9	−0.622100501227(3)	−1.2657498773(4)	4.939401(7)	−0.0113415130(2)
2.0	−0.622628439218(3)	−1.2446712026(5)	5.3328446(4)	0.0002928379(2)
2.1	−0.622128694991(3)	−1.2246886082(6)	5.781084(8)	0.0093184675(2)
2.2	−0.620832926651(4)	−1.2058182652(6)	6.29471(2)	0.0162943582(3)
2.3	−0.618923772982(4)	−1.1880558574(7)	6.88602(3)	0.0216485603(3)
2.4	−0.616546158449(4)	−1.1713834096(9)	7.56923(5)	0.0257120448(4)
2.5	−0.613815721719(4)	−1.1557740022(10)	8.36080(7)	0.0287429765(4)
2.6	−0.610825168645(4)	−1.141195032(2)	9.27967(8)	0.0309443481(4)
2.7	−0.607649108655(4)	−1.127610465(2)	10.34766(10)	0.0324769454(5)
2.8	−0.604347770163(4)	−1.114982380(2)	11.5898(2)	0.0334689857(5)
2.9	−0.600969878595(4)	−1.103272027(2)	13.0348(2)	0.0340233552(5)
3.0	−0.597554902852(4)	−1.092440527(2)	14.7156(2)	0.0342230929(6)
3.1	−0.594134821136(4)	−1.082449333(3)	16.6697(2)	0.0341355836(6)
3.2	−0.590735518019(4)	−1.073260518(3)	18.9401(3)	0.0338157868(6)
3.3	−0.587377896456(4)	−1.064836942(3)	21.5759(3)	0.0333087429(7)
3.4	−0.584078767897(4)	−1.057142336(3)	24.6329(4)	0.0326515294(7)
3.5	−0.580851568604(4)	−1.050141340(3)	28.1751(4)	0.0318747992(8)
3.6	−0.577706939031(4)	−1.043799495(4)	32.2753(4)	0.0310039953(8)
3.7	−0.574653194791(4)	−1.038083226(4)	37.0164(5)	0.0300603147(8)
3.8	−0.571696711355(4)	−1.032959810(4)	42.4934(5)	0.0290614772(9)
3.9	−0.568842239883(4)	−1.028397351(4)	48.8145(6)	0.0280223408(9)
4.0	−0.566093167843(4)	−1.024364756(5)	56.1037(6)	0.0269553950(10)
4.1	−0.56345173531(7)	−1.020831720(2)	64.5035(2)	0.0258711586(3)
4.2	−0.560919215381(9)	−1.0177687428(2)	74.17613(2)	0.02477849714(3)
4.3	−0.55849606627(7)	−1.015147130(2)	85.3091(3)	0.0236848843(3)
4.4	−0.55618205951(7)	−1.012939044(2)	98.1198(3)	0.0225966080(3)

4.5	−0.553976390142(5)	−1.0111175651(4)	112.85946(10)	0.02151893670(8)
4.6	−0.55187777172(8)	−1.009656780(2)	129.8195(4)	0.0204562529(3)
4.7	−0.54988451915(8)	−1.008531893(2)	149.3424(4)	0.0194121586(3)
4.8	−0.54799462289(9)	−1.007719379(2)	171.8296(5)	0.0183895556(3)
4.9	−0.54620581561(9)	−1.007197179(2)	197.7558(6)	0.0173907046(4)
5.0	−0.544515634232(8)	−1.006944953(9)	227.684(3)	0.016417263(2)
5.5	−0.53745169574(2)	−1.009193310(2)	466.7247(7)	0.0119472876(3)
6.0	−0.53248423099(3)	−1.0172527689(6)	1000.20982(8)	0.00795261551(8)
6.5	−0.52960051946(3)	−1.037603290(2)	2051.4886(2)	0.0033227305(2)
7.0	−0.52913364740(2)	−1.063785291(2)	2064.7731(2)	−0.0007882852(2)
7.5	−0.529737831222(6)	−1.069267503(2)	1301.9094(2)	−0.0013055788(2)
8.0	−0.530315569154(4)	−1.0684552680(9)	832.36662(8)	−0.00097801621(9)
8.5	−0.530717114160(3)	−1.0668893331(7)	557.57538(5)	−0.00064177702(7)
9.0	−0.53097314901(2)	−1.0655270998(6)	386.09105(3)	−0.00039786686(5)
9.5	−0.531128730658(2)	−1.0645015312(5)	274.04932(2)	−0.00023621788(4)
10.0	−0.531219186208(3)	−1.0637748(2)	198.6(2)	−0.000133644(9)
11.0	−0.531293947446(5)	−1.06294951(9)	112.0(2)	−0.000032874(6)
12.0	−0.531306702176(2)	−1.06260355(7)	70.39(10)	0.000000822(4)
13.0	−0.531300341884(3)	−1.06247575(5)	49.49(9)	0.000009610(3)
14.0	−0.5312901361957(6)	−1.06243871(4)	38.21(7)	0.000010112(2)
15.0	−0.5312808185258(4)	−1.06243583(3)	31.43(6)	0.0000083877(9)
16.0	−0.5312734203530(8)	−1.06244380(2)	26.84(5)	0.0000064400(6)
17.0	−0.5312678259648(6)	−1.062453803(10)	23.39(4)	0.0000048148(4)
18.0	−0.5312636593675(2)	−1.062462894(10)	20.59(5)	0.0000035793(4)
19.0	−0.53126055794024(9)	−1.062470373(9)	18.25(4)	0.0000026707(3)
20.0	−0.5312582356315(6)	−1.062476306(7)	16.25(4)	0.0000020083(3)

Table A90: Same as for Table A1, but for $2\,^3\Phi_g$.

$2\,^3\Phi_g$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.01388934538731322(3)	–	0.8981237(7)	–
0.01	97.98637201784(6)	95.9732614918(4)	0.89843(2)	−9999.94825439(3)
0.05	17.992134053(4)	15.99569936(3)	0.90536(4)	−399.7713749(4)
0.1	8.007868589(5)	6.05483978(3)	0.9240(3)	−99.6089740(2)
0.15	4.697055773(3)	2.80281881(2)	0.9510(3)	−43.94195157(8)
0.2	3.057490371(4)	1.23022263(2)	0.9842(2)	−24.42379059(7)
0.3	1.4527399616(10)	−0.233184829(6)	1.06306(10)	−10.46221584(2)
0.4	0.6853567068(3)	−0.863934872(2)	1.15366(8)	−5.586620715(2)
0.5	0.25112284862(6)	−1.1734353639(3)	1.25251(7)	−3.3513621222(4)
0.6	−0.01870709330(3)	−1.3321248242(2)	1.35786(5)	−2.1578510627(2)
0.7	−0.1965137539(2)	−1.4118937(3)	1.46886(4)	−1.4555232(4)
0.8	−0.31836886068(4)	−1.4475529(2)	1.58542(2)	−1.0135190(3)
0.9	−0.40415908329(6)	−1.4575528857(4)	1.707661(7)	−0.7213719101(2)
1.0	−0.46567471841(6)	−1.45230972(8)	1.83603(2)	−0.52096029(9)
1.1	−0.51030006462(3)	−1.437984(4)	1.97141(2)	−0.37943551(9)
1.2	−0.54286249915(3)	−1.41832522(4)	2.11491(2)	−0.27716685(4)
1.3	−0.56662836026(2)	−1.3957071756(10)	2.267936(3)	−0.2018849655(8)
1.4	−0.58387101914(3)	−1.3716298710(9)	2.4322191(5)	−0.1456341664(8)
1.5	−0.59621044076(3)	−1.347063333(2)	2.609904(5)	−0.1030949679(8)
1.6	−0.60482419839(2)	−1.322635281(2)	2.803561(4)	−0.0706168027(10)
1.7	−0.61058297952(5)	−1.298750199(2)	3.016228(4)	−0.0456377884(8)
1.8	−0.61414008101(3)	−1.2756649076(10)	3.251502(5)	−0.0263248587(6)
1.9	−0.61599197151(3)	−1.25353756(7)	3.51358(2)	−0.01134401(4)
2.0	−0.61652015384(3)	−1.232459486(2)	3.807494(5)	0.0002904107(7)
2.1	−0.6160206497(2)	−1.212477496(7)	4.13891(2)	0.009316097(4)
2.2	−0.6147251138(2)	−1.193607650(7)	4.51458(2)	0.016292080(4)
2.3	−0.61281618122(6)	−1.175845612(7)	4.94227(2)	0.021646413(4)
2.4	−0.61043877286(8)	−1.159173378(7)	5.43095(2)	0.025710070(4)
2.5	−0.60770852284(5)	−1.14356405(6)	5.99098(3)	0.02874120(3)
2.6	−0.60471813217(5)	−1.12898487(5)	6.63435(3)	0.03094284(2)
2.7	−0.60154220490(9)	−1.115399792(5)	7.37481(2)	0.032475784(2)
2.8	−0.59824096348(5)	−1.102770928(4)	8.22812(2)	0.033468214(2)
2.9	−0.59486312673(10)	−1.091059434(5)	9.21240(2)	0.034023041(2)
3.0	−0.59144815620(10)	−1.080226365(2)	10.3481(2)	0.0342233157(4)
3.1	−0.58802802192(5)	−1.070233118(2)	11.6597(3)	0.0341364278(5)
3.2	−0.58462859943(5)	−1.061041686(2)	13.1742(3)	0.0338173478(5)
3.3	−0.58127078162(6)	−1.052614846(2)	14.9227(3)	0.0333111263(6)
3.4	−0.57797136880(5)	−1.044916238(3)	16.9411(4)	0.0326548528(6)
3.5	−0.57474378484(5)	−1.037910394(3)	19.2705(4)	0.0318791930(6)
3.6	−0.57159865648(5)	−1.031562740(3)	21.9577(5)	0.0310096037(7)
3.7	−0.56854428413(4)	−1.025839568(3)	25.0570(5)	0.0300672974(7)
3.8	−0.56558702647(4)	−1.020708012(4)	28.6305(6)	0.0290700109(8)
3.9	−0.56273161610(5)	−1.016136013(4)	32.7499(7)	0.0280326203(8)
4.0	−0.55998142002(2)	−1.01209230023(5)	37.49936(2)	0.02696763494(2)
4.1	−0.55733865584(5)	−1.0085463810(8)	42.9727(2)	0.0258855929(2)
4.2	−0.55480457218(6)	−1.0054685384(9)	49.2836(2)	0.0247953824(2)
4.3	−0.55237960051(6)	−1.0028298611(9)	56.5632(3)	0.0237044977(2)
4.4	−0.55006348376(6)	−1.0006022876(9)	64.9662(3)	0.0226192454(2)

4.5	−0.54785538653(4)	−0.998758683(8)	74.674(2)	0.0215449096(2)
4.6	−0.54575399074(6)	−0.9972729334(10)	85.9120(4)	0.0204858800(2)
4.7	−0.54375757969(6)	−0.996120127(2)	98.9380(4)	0.0194457516(2)
4.8	−0.54186411396(7)	−0.995276737(2)	114.0754(5)	0.0184273940(3)
4.9	−0.54007130160(7)	−0.994720939(2)	131.7192(6)	0.0174329927(3)
5.0	−0.53837666574(8)	−0.994433041(2)	152.3610(7)	0.0164640581(3)
5.5	−0.5312860381(2)	−0.996595394(4)	329.7144(10)	0.0119957604(6)
6.0	−0.5263714100(4)	−1.00834093(2)	793.855(3)	0.007400315(3)
6.5	−0.524682462(2)	−1.047659(3)	−603.90(3)	0.0002625(4)
7.0	−0.5240980613(10)	−1.03307728(5)	−1741.3659(9)	0.002159834(7)
7.5	−0.5229455057(3)	−1.029453421(2)	−1307.624(2)	0.00219167878(9)
8.0	−0.5219975826(3)	−1.031262699(2)	−939.8468(10)	0.0015915582(2)
8.5	−0.52133829005(2)	−1.0335742894(3)	−676.74532(5)	0.00107085773(3)
9.0	−0.52090108068(2)	−1.0354863832(2)	−480.89141(2)	0.00070175313(2)
9.5	−0.5206158917(7)	−1.036895941(7)	−334.753(3)	0.0004564044(6)
10.0	−0.5204302718(3)	−1.037882769(3)	−227.7964(8)	0.0002977774(3)
11.0	−0.5202278372(2)	−1.039007802(3)	−97.9978(6)	0.0001316248(2)
12.0	−0.5201353123(2)	−1.039512111(2)	−36.7422(5)	0.0000632095(2)
13.0	−0.5200888113(2)	−1.039739510(2)	−9.5586(3)	0.00003370098(7)
14.0	−0.52006280288(9)	−1.0398464292(7)	2.0419(2)	0.00001994118(4)
15.0	−0.52004673461(7)	−1.0398996331(5)	6.80898(7)	0.00001292241(3)
16.0	−0.52003594955(5)	−1.0399280471(5)	8.48696(3)	0.00000899075(2)
17.0	−0.52002826318(4)	−1.0399450625(4)	8.77082(2)	0.00000655670(2)
18.0	−0.52002257242(4)	−1.0399564923(3)	8.47692(2)	0.00000492514(2)
19.0	−0.52001825361(3)	−1.0399647628(3)	7.971614(9)	0.000003776021(10)
20.0	−0.52001491618(3)	−1.0399710006(2)	7.408202(7)	0.000002941586(8)

Table A91: Same as for Table A1, but for $1\,^1\Phi_u$.

$1\,^1\Phi_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.031255144381749(1)	–	10.0242694(2)	–
0.01	97.969006228(4)	95.938529907(6)	10.0265(2)	−9999.9482548(6)
0.05	17.974768337(4)	2.01380025(2)	10.0724(2)	−399.7713723(3)
0.1	7.990503118(6)	1.97039358(2)	10.1825(2)	−99.6089674(2)
0.15	4.67969074(2)	2.76809038(8)	10.3164(2)	−43.9419407(4)
0.2	3.040125975(6)	1.844629191(7)	10.4476(2)	−24.423775896(5)
0.3	1.435377438(3)	−0.267903017(5)	10.6322(2)	−10.46219298(2)
0.4	0.6679968825(8)	1.5666389000(5)	10.6355(2)	−5.5865894619(10)
0.5	0.2337665670(2)	−1.2081281176(9)	10.39373(7)	−3.351322503(2)
0.6	−0.0360589992(2)	−1.3667999170(3)	9.8601(2)	−2.157803197735(7)
0.7	−0.21386046443(2)	−1.4465476608(4)	8.9963(2)	−1.4554667599(5)
0.8	−0.33570957143(2)	−1.4821829958(4)	7.7682(2)	−1.0134548162(4)
0.9	−0.42149300671(2)	−1.4921561585(4)	6.1441(2)	−0.7213001612(3)
1.0	−0.48300108593(2)	−1.4868830305(3)	4.0937(2)	−0.5208808586(3)
1.1	−0.527618127935(10)	−1.4725198255(3)	1.5875(2)	−0.3793486996(2)
1.2	−0.560171531512(9)	−1.4528305984(3)	−1.4037(2)	−0.2770729461(2)
1.3	−0.583927657587(9)	−1.4301747388(3)	−4.9086(2)	−0.2017841720(2)
1.4	−0.601159901042(8)	−1.4060571694(3)	−8.95552(10)	−0.1455266910(2)
1.5	−0.613488251553(8)	−1.3814480964(3)	−13.57236(10)	−0.1029810622(2)
1.6	−0.622090308009(7)	−1.3569753798(3)	−18.78653(10)	−0.0704967274(2)
1.7	−0.627836784404(7)	−1.3330436522(2)	−24.62475(9)	−0.04551181378(10)
1.8	−0.631381005140(7)	−1.3099098837(2)	−31.11288(9)	−0.02619326301(9)
1.9	−0.633219466975(7)	−1.2877323065(2)	−38.27574(9)	−0.01120703818(9)
2.0	−0.633733701792(7)	−1.2666026398(2)	−46.13683(8)	0.00043238191(8)
2.1	−0.633219760989(6)	−1.2465676214(2)	−54.71807(8)	0.00946280980(8)
2.2	−0.631909329935(6)	−1.2276435661(2)	−64.03956(8)	0.01644322445(7)
2.3	−0.629985074983(6)	−1.2098263006(5)	−74.1192(2)	0.0218016736(2)
2.4	−0.627591948354(6)	−1.1930979915(5)	−84.9725(2)	0.0258691272(2)
2.5	−0.624845616542(6)	−1.1774318585(2)	−96.61170(7)	0.02890374984(6)
2.6	−0.621838813147(6)	−1.1627954335(5)	−109.0464(2)	0.0311085357(2)
2.7	−0.618646175106(6)	−1.1491528103(5)	−122.2820(2)	0.0326442740(2)
2.8	−0.615327957908(6)	−1.1364661906(5)	−136.3202(2)	0.0336391876(2)
2.9	−0.611932913405(6)	−1.1246969339(5)	−151.1579(2)	0.0341961700(2)
3.0	−0.608500536022(6)	−1.1138062593(2)	−166.78711(7)	0.03439827091(6)
3.1	−0.605062828290(6)	−1.1037557022(5)	−183.1947(2)	0.0343128885(2)
3.2	−0.601645697588(6)	−1.0945073967(5)	−200.3614(2)	0.0339949995(2)
3.3	−0.598270067763(6)	−1.0860242399(5)	−218.2617(2)	0.0334896653(2)
3.4	−0.594952768802(7)	−1.0782699726(6)	−236.8636(2)	0.0328339897(2)
3.5	−0.591707252630(7)	−1.0712092054(6)	−256.1277(2)	0.0320586571(2)
3.6	−0.588544171891(7)	−1.0648074093(6)	−276.0076(2)	0.0311891485(2)
3.7	−0.585471850207(7)	−1.0590308864(6)	−296.4488(2)	0.0302467065(2)
3.8	−0.582496666060(7)	−1.0538467305(6)	−317.3890(2)	0.0292491057(2)
3.9	−0.579623367646(7)	−1.049222787(3)	−338.7581(6)	0.0282112688(5)
4.0	−0.576855332331(8)	−1.0451276074(3)	−360.47622(6)	0.02714576432(6)
4.1	−0.574194781545(4)	−1.04153043380(2)	−382.457708(5)	0.026063202266(4)
4.2	−0.571642959661(4)	−1.03840116230(2)	−404.607126(5)	0.024972561195(3)
4.3	−0.569200283754(4)	−1.03571034011(2)	−426.821556(4)	0.023881448233(2)
4.4	−0.566866469691(4)	−1.033429165276(8)	−448.990566(3)	0.0227963122971(5)

4.5	−0.564640638988(10)	−1.0315294988(4)	−470.99671(6)	0.02172261760(6)
4.6	−0.562521409943(4)	−1.029983886282(3)	−492.7160563(7)	0.020664985563(3)
4.7	−0.56050697595(3)	−1.0287655903(5)	−514.01922(6)	0.01962731095(10)
4.8	−0.558595173062(4)	−1.02784862562(2)	−534.771834(2)	0.018612858435(6)
4.9	−0.55678353921(3)	−1.0272078067(5)	−554.83632(6)	0.0176243411(2)
5.0	−0.55506936552(2)	−1.0268187882(5)	−574.07231(5)	0.01666398856(7)
5.5	−0.54785365779(2)	−1.027863434(4)	−652.94263(7)	0.0123352513(7)
6.0	−0.54259339941(3)	−1.032109152(6)	−691.5148(3)	0.0088462746(8)
6.5	−0.538872121538(4)	−1.03766180854(5)	−679.84118(2)	0.006166528390(6)
7.0	−0.536309065021(4)	−1.04326905151(5)	−619.11669(2)	0.004192725505(5)
7.5	−0.534583756716(4)	−1.04822199541(4)	−522.59231(2)	0.002792735736(4)
8.0	−0.533443121857(3)	−1.05222641596(4)	−410.40869(2)	0.001832478470(4)
8.5	−0.532698157459(3)	−1.05526672072(3)	−301.39795(2)	0.001191716964(3)
9.0	−0.532214608932(3)	−1.05747608452(3)	−207.534512(10)	0.000772570371(3)
9.5	−0.531900994174(3)	−1.05903565893(3)	−133.324224(10)	0.000501718886(3)
10.0	−0.531696842363(3)	−1.06011651063(3)	−78.164401(9)	0.000327717409(2)
11.0	−0.531474182951(2)	−1.06136161312(2)	−12.328689(7)	0.000144250253(2)
12.0	−0.531373678949(2)	−1.061936381977(10)	16.378487(5)	0.0000675813268(7)
13.0	−0.5313249072835(8)	−1.062202643292(6)	26.738516(3)	0.0000343977904(4)
14.0	−0.5312990421541(6)	−1.062329327219(4)	28.901556(2)	0.0000191969350(2)
15.0	−0.5312840134709(4)	−1.062392839129(3)	27.738573(2)	0.0000116791875(2)
16.0	−0.5312745553792(3)	−1.062427186623(2)	25.4247167(4)	0.00000762025844(4)
17.0	−0.5312682254520(3)	−1.0624474744235(7)	22.87243969(9)	0.00000523391061(2)
18.0	−0.5312637986729(2)	−1.0624605131116(6)	20.4346350(6)	0.00000372690187(5)
19.0	−0.5312606060388(2)	−1.062469487543(2)	18.2274520(9)	0.00000272234389(9)
20.0	−0.5312582520459(2)	−1.062475978723(3)	16.271919(2)	0.0000020262684(2)

Table A92: Same as for Table A1, but for $2\,^1\Phi_u$.

		$2\,^1\Phi_u$		
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.0200029371587427(5)	–	5.7042946(4)	–
0.01	97.98025842757(9)	95.9610343145(7)	5.631(3)	−9999.94825407(6)
0.05	17.986020496(5)	15.98347232(3)	5.736(2)	−399.7713735(5)
0.1	8.001755150(2)	6.042613241(5)	5.8(4)	−99.60897084(9)
0.15	4.690942543(3)	2.79059311(2)	5.869(3)	−43.94194649(7)
0.2	3.0513774442(9)	1.217998177(6)	6.0(2)	−24.42378356(2)
0.3	1.446627938(3)	−0.24540556(2)	6.16(2)	−10.46220479(4)
0.4	0.6792459979(9)	−0.876150220(7)	6.240(2)	−5.58660554(2)
0.5	0.2450138616(7)	−1.185643704(6)	6.212(2)	−3.351342855(10)
0.6	−0.0248139508(7)	−1.344324548(6)	6.046(2)	−2.157827744(8)
0.7	−0.2026180795(6)	−1.424082976(6)	5.719(2)	−1.455495452(7)
0.8	−0.324470259(2)	−1.45973056(2)	5.216(4)	−1.01348755(2)
0.9	−0.4102571668(5)	−1.469717500(6)	4.516(2)	−0.721336852(5)
1.0	−0.4717691084(5)	−1.464459612(5)	3.605(2)	−0.520921395(5)
1.1	−0.5163903918(5)	−1.450113051(5)	2.468(2)	−0.379392971(4)
1.2	−0.5489484043(5)	−1.430441807(5)	1.089(2)	−0.277120832(4)
1.3	−0.5727094946(5)	−1.407805203(5)	−0.549(2)	−0.201835549(4)
1.4	−0.5899470448(5)	−1.383708088(5)	−2.459(2)	−0.145581427(3)
1.5	−0.6022810312(5)	−1.359120593(5)	−4.658(2)	−0.103039021(3)
1.6	−0.6108890387(5)	−1.334670501(5)	−7.159(2)	−0.070557765(3)
1.7	−0.6166417666(4)	−1.310762360(5)	−9.977(2)	−0.045575781(3)
1.8	−0.6201925240(4)	−1.287653055(5)	−13.126(2)	−0.026260004(3)
1.9	−0.6220377920(4)	−1.265500728(5)	−16.620(2)	−0.011276392(3)
2.0	−0.6225590858(4)	−1.244397004(5)	−20.471(2)	0.000360584(2)
2.1	−0.6220524398(4)	−1.224388523(5)	−24.692(2)	0.009388741(2)
2.2	−0.6207495216(4)	−1.205491499(5)	−29.294(2)	0.016367066(2)
2.3	−0.6188329794(9)	−1.18770165(2)	−34.286(3)	0.021723612(4)
2.4	−0.6164477460(9)	−1.171001038(2)	−39.678(3)	0.025789356(4)
2.5	−0.6137094685(9)	−1.15536276(2)	−45.477(3)	0.028822469(4)
2.6	−0.6107108600(9)	−1.14075424(2)	−51.689(3)	0.031025952(4)
2.7	−0.6075265366(9)	−1.12713945(2)	−58.318(3)	0.032560601(4)
2.8	−0.6042167320(10)	−1.11448046(2)	−65.366(3)	0.033554645(4)
2.9	−0.6008301758(10)	−1.10273850(2)	−72.832(3)	0.034110984(4)
3.0	−0.5974063394(10)	−1.09187465(2)	−80.715(3)	0.034312676(4)
3.1	−0.5939772016(10)	−1.08185032(2)	−89.009(3)	0.034227124(4)
3.2	−0.5905686456(10)	−1.07262749(2)	−97.705(3)	0.033909312(4)
3.3	−0.587201570(2)	−1.06416893(2)	−106.793(3)	0.033404307(4)
3.4	−0.5838927796(5)	−1.056438208(6)	−116.259(2)	0.032749221(2)
3.5	−0.5806556998(5)	−1.049399799(6)	−126.0839(10)	0.031974743(2)
3.6	−0.5775009564(5)	−1.043019016(6)	−136.2471(10)	0.031106360(2)
3.7	−0.5744368457(5)	−1.037262002(7)	−146.7233(9)	0.030165322(2)
3.8	−0.5714697181(5)	−1.032095692(7)	−157.4835(9)	0.029169406(2)
3.9	−0.5686042934(6)	−1.027487770(7)	−168.4949(8)	0.028133543(2)
4.0	−0.565843920(2)	−1.02340663(2)	−179.721(2)	0.027070302(4)
4.1	−0.563190794(9)	−1.01982138(10)	−191.5(5)	0.02599029(2)
4.2	−0.560646121(9)	−1.01670168(9)	−202.66(5)	0.02490251(2)
4.3	−0.558210294(8)	−1.01401798(8)	−215.2(3)	0.02381456(2)
4.4	−0.5558829941(7)	−1.011741273(8)	−225.8963(4)	0.022732890(2)

4.5	−0.553663320(2)	−1.00984334(2)	−237.5075(5)	0.021662957(4)
4.6	−0.5515498565(7)	−1.008296539(9)	−249.0338(2)	0.020609386(2)
4.7	−0.54954077(2)	−1.0070741(2)	−260.6(2)	0.01957606(3)
4.8	−0.54763386(2)	−1.00614970(9)	−272.23(9)	0.01856626(2)
4.9	−0.54582665(2)	−1.0054982(2)	−282.7(2)	0.01758266(2)
5.0	−0.544116377(2)	−1.00509521(3)	−293.0299(10)	0.016627510(4)
5.5	−0.5369117709(4)	−1.006018650(5)	−338.280(2)	0.0123281621(7)
6.0	−0.5316469911(3)	−1.010064733(4)	−365.2404(8)	0.0088715415(5)
6.5	−0.52790539698(8)	−1.0153707881(10)	−368.0816(3)	0.0062215394(2)
7.0	−0.52530915845(7)	−1.0207388819(9)	−345.3826(3)	0.00426849071(10)
7.5	−0.52354344064(6)	−1.0255139389(7)	−301.2827(2)	0.00287639231(7)
8.0	−0.5223615610(2)	−1.029425970(2)	−244.4691(2)	0.0019121440(2)
8.5	−0.52157938659(8)	−1.0324476628(10)	−185.03679(4)	0.00126013063(9)
9.0	−0.52106500799(6)	−1.0346832263(7)	−131.02771(3)	0.00082742108(7)
9.5	−0.52072721979(5)	−1.0362877893(5)	−86.713136(2)	0.00054385792(5)
10.0	−0.52050473974(4)	−1.0374166367(4)	−52.97703(2)	0.00035928428(3)
11.0	−0.52025843753(3)	−1.03874243098(4)	−11.87991(4)	0.00016131307(2)
12.0	−0.52014531294(2)	−1.03937193512(4)	6.74734(5)	0.000076557564(2)
13.0	−0.520090104500(7)	−1.03967832617(3)	15.02813(7)	0.000038606372(2)
14.0	−0.52006198413(8)	−1.0398467946(10)	18.6572(4)	0.00001979812(6)
15.0	−0.5200465445(5)	−1.039907613(4)	15.1207(10)	0.0000123649(3)
16.0	−0.520036053(2)	−1.03992977(2)	11.994(3)	0.0000088960(9)
17.0	−0.520028379(3)	−1.03994471(3)	10.208(5)	0.000006590(2)
18.0	−0.520022648(6)	−1.03995592(5)	9.064(9)	0.000004964(4)
19.0	−0.52001830(2)	−1.03996441(8)	8.21(2)	0.000003797(6)
20.0	−0.52001495(3)	−1.0399709(2)	7.51(2)	0.000002946(9)

Table A93: Same as for Table A1, but for $3\,^1\Phi_u$.

$3\,^1\Phi_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.0138906838155497(3)	–	3.482257(7)	–
0.01	97.986370681(2)	95.973258826(10)	3.4844(4)	−9999.9482535(8)
0.05	17.992132738(5)	15.99569678(5)	3.502(2)	−399.7713739(7)
0.1	8.007867339(8)	6.05483748(5)	3.537(8)	−99.6089720(4)
0.15	4.697054638(7)	2.80281698(5)	3.596(8)	−43.9419486(2)
0.2	3.057489402(6)	1.23022148(4)	3.659(8)	−24.4237866(2)
0.3	1.452739489(5)	−0.23318393(4)	3.775(9)	−10.46220969(8)
0.4	0.685356793(2)	−0.863935186(7)	0.438582(5)	−5.586621932(10)
0.5	0.25112279694(8)	−1.1734362453(5)	0.509420(10)	−3.3513636783(5)
0.6	−0.01870731748(4)	−1.3321264083(2)	0.592654(5)	−2.1578529556(2)
0.7	−0.19651418382(2)	−1.411895858(4)	0.68862(8)	−1.45552499(2)
0.8	−0.318369528927(6)	−1.4475561159(5)	0.79820(4)	−1.013521325(3)
0.9	−0.404160021197(4)	−1.457557327(2)	0.92216(2)	−0.72137475971(7)
1.0	−0.4656759562581(3)	−1.45231525301(2)	1.06156(2)	−0.520963340496(6)
1.1	−0.510301631366(2)	−1.437985988285(8)	1.21757(2)	−0.379438841411(4)
1.2	−0.542864422339(2)	−1.418333458893(6)	1.391582(2)	−0.277170511847(3)
1.3	−0.5666306659052(9)	−1.395716919707(5)	1.58514(3)	−0.201888913766(3)
1.4	−0.5838737315725(8)	−1.371641152073(5)	1.799973(9)	−0.145638349234(3)
1.5	−0.5962135825107(6)	−1.347076214617(4)	2.038013(4)	−0.103099366397(2)
1.6	−0.6048277900056(6)	−1.322649813765(4)	2.301439(2)	−0.070621396096(2)
1.7	−0.6105870393691(5)	−1.298766421990(4)	2.59268(9)(2)	−0.045642554854(2)
1.8	−0.6141446252666(5)	−1.275682843380(4)	2.9144903(5)	−0.026329773804(2)
1.9	−0.6159970136702(4)	−1.253557138198(4)	3.2699146(4)	−0.011349005714(2)
2.0	−0.61652570465490(4)	−1.232480847652(4)	3.6623987(4)	0.000285280829(2)
2.1	−0.6160267167971(3)	−1.212500526066(3)	4.0958028(3)	0.009310908347(2)
2.2	−0.6147317016600(3)	−1.193632299059(3)	4.5744619(3)	0.016286865573(2)
2.3	−0.6128232908220(3)	−1.175871799137(9)	5.1032447(9)	0.021641209786(3)
2.4	−0.6104464008034(3)	−1.159200993845(9)	5.6876247(9)	0.025704919901(3)
2.5	−0.6077166614976(3)	−1.143592899373(9)	6.3337520(9)	0.028736169449(3)
2.6	−0.6047267690572(4)	−1.12901484006(2)	7.048544(3)	0.030937960792(4)
2.7	−0.6015513221759(3)	−1.11543069915(2)	7.839771(2)	0.032471090816(4)
2.8	−0.5982505373650(3)	−1.10280246493(2)	8.716188(2)	0.033463789215(4)
2.9	−0.5948731268452(3)	−1.09109128189(2)	9.687634(2)	0.034018955793(4)
3.0	−0.5914585448392(2)	−1.08025815348(2)	10.765180(2)	0.034219645400(4)
3.1	−0.5880387532111(4)	−1.07026439928(2)	11.961290(2)	0.034133260368(4)
3.2	−0.5846396183225(5)	−1.06107193994(2)	13.289987(2)	0.033814780219(4)
3.3	−0.5812820227897(6)	−1.05264346206(2)	14.767063(2)	0.033309267732(4)
3.4	−0.5779827553127(6)	−1.044942500944(9)	16.41030(2)	0.032653826377(3)
3.5	−0.574755226648(5)	−1.0379334687(2)	18.23970(2)	0.03187913846(5)
3.6	−0.571610048592(5)	−1.0315816469(2)	20.27785(2)	0.03101068064(5)
3.7	−0.568555504477(6)	−1.0258531606(3)	22.55017(2)	0.03006968876(6)
3.8	−0.565597933313(7)	−1.0207149413(3)	25.08534(3)	0.02907392773(6)
3.9	−0.562742044941(8)	−1.0161346895(3)	27.91568(3)	0.02803830779(7)
4.0	−0.559991179846(9)	−1.012080843(3)	31.07771(3)	0.0269753793(6)
4.1	−0.55734752449(8)	−1.008522542(3)	34.61275(4)	0.0258957334(7)
4.2	−0.55481229045(9)	−1.005429628(3)	38.56746(4)	0.0248083221(7)
4.3	−0.55238586501(10)	−1.002772630(4)	42.99470(4)	0.0237207210(8)
4.4	−0.5500679377(2)	−1.000522775(4)	47.95445(4)	0.0226393410(8)

4.5	−0.5478576076984(7)	−0.9986520110(4)	53.51492(2)	0.02156960098(7)
4.6	−0.545753476395(6)	−0.99713304872(9)	59.753514(9)	0.02051606610(2)
4.7	−0.54375372595(5)	−0.995939392(2)	66.75866(5)	0.0194825659(3)
4.8	−0.54185618856(5)	−0.995045403(2)	74.63174(5)	0.0184722863(3)
4.9	−0.540058406749(7)	−0.9944263622(2)	83.48892(2)	0.01748784720(3)
5.0	−0.538357686699(8)	−0.9940585473(6)	93.46353(5)	0.01653136523(10)

Table A94: Same as for Table A1, but for $4\,^1\Phi_u$.

$4\,^1\Phi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.465665506777(5)	−1.452269859(4)	2.5677(7)	−0.520938846(4)
1.1	−0.510288616772(5)	−1.437930479(4)	1.9565(7)	−0.379412042(3)
1.2	−0.542848615368(5)	−1.418266998(4)	1.2071(7)	−0.277141473(3)
1.3	−0.566611845987(4)	−1.395638706(4)	0.3102(7)	−0.201857703(3)
1.4	−0.583851685106(4)	−1.371550424(4)	−0.7432(7)	−0.145605039(3)
1.5	−0.596188103120(4)	−1.346972250(4)	−1.9619(7)	−0.103064029(3)
1.6	−0.604798678774(4)	−1.322531930(4)	−3.3547(7)	−0.070584108(2)
1.7	−0.610554105054(4)	−1.298633979(4)	−4.9302(7)	−0.045603393(2)
1.8	−0.614107684492(4)	−1.275535242(4)	−6.6966(7)	−0.026288818(2)
1.9	−0.615955891101(5)	−1.253393824(4)	−8.6621(7)	−0.011306338(2)
2.0	−0.616480233150(5)	−1.232301309(4)	−10.8343(7)	0.000329579(2)
2.1	−0.615976737534(5)	−1.212304295(4)	−13.2205(7)	0.009356752(2)
2.2	−0.614677064233(5)	−1.193418951(4)	−15.8273(7)	0.016334171(2)
2.3	−0.612763853307(5)	−1.175640954(4)	−18.6608(7)	0.021689892(2)
2.4	−0.610382029787(5)	−1.158952314(4)	−21.7266(7)	0.025754894(2)
2.5	−0.607647232059(5)	−1.143326088(4)	−25.0291(7)	0.028787350(2)
2.6	−0.604652164709(5)	−1.128729641(4)	−28.5720(7)	0.030990265(2)
2.7	−0.601471434740(6)	−1.115126893(4)	−32.3579(7)	0.032524436(2)
2.8	−0.598165266791(6)	−1.102479869(4)	−36.3885(7)	0.033518095(2)
2.9	−0.594782380958(6)	−1.090749743(4)	−40.6639(7)	0.034074145(2)
3.0	−0.591362238996(6)	−1.079897545(4)	−45.1830(6)	0.034275644(2)
3.1	−0.587936809874(6)	−1.069884617(5)	−49.9431(6)	0.034190001(2)
3.2	−0.584531966522(6)	−1.060672894(5)	−54.9401(6)	0.033872200(2)
3.3	−0.581168597471(6)	−1.052225070(5)	−60.1680(6)	0.033367311(2)
3.4	−0.577863496547(6)	−1.044504677(5)	−65.6189(5)	0.032712446(2)
3.5	−0.574630078695(6)	−1.037476115(5)	−71.2832(5)	0.031938298(2)
3.6	−0.571478958794(6)	−1.031104638(5)	−77.1491(4)	0.031070355(2)
3.7	−0.568418421957(6)	−1.025356331(5)	−83.2026(4)	0.030129868(2)
3.8	−0.565454807461(6)	−1.020198068(6)	−89.4280(4)	0.029134618(2)
3.9	−0.562592823660(6)	−1.015597470(6)	−95.8069(3)	0.028099533(2)
4.0	−0.559835807514(6)	−1.011522871(6)	−102.3190(2)	0.027037186(2)
4.1	−0.557185939556(6)	−1.007943287(6)	−108.9417(2)	0.025958193(2)
4.2	−0.554644422885(6)	−1.004828396(6)	−115.65034(6)	0.024871536(2)
4.3	−0.552211633028(6)	−1.002148529(7)	−122.41805(2)	0.023784823(2)
4.4	−0.549887244176(6)	−0.999874673(7)	−129.21613(10)	0.022704503(2)
4.5	−0.547670336198(6)	−0.997978486(7)	−136.0138(2)	0.021636041(2)
4.6	−0.545559485971(6)	−0.996432323(7)	−142.7792(7)	0.020584054(2)
4.7	−0.543552845876(6)	−0.995209264(7)	−149.4767(4)	0.019552431(2)
4.8	−0.541648211749(6)	−0.994283163(7)	−156.0729(5)	0.018544429(2)
4.9	−0.539843082112(3)	−0.99362869(10)	−162.532(2)	0.01756275(2)
5.0	−0.538134710199(5)	−0.993221388(7)	−168.8136(6)	0.016609606(2)

Table A95: Same as for Table A1, but for $5\,{}^1\Phi_u$.

$5\,{}^1\Phi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.4619908992328(10)	−1.444944747994(4)	0.7258089(2)	−0.520962949529(2)
1.1	−0.5066165332647(6)	−1.430615318216(3)	0.8316203(2)	−0.379438410624(2)
1.2	−0.5391792791034(4)	−1.410962605820(2)	0.9495968(2)	−0.277170039678(2)
1.3	−0.5629454733095(3)	−1.388345864531(2)	1.0807830(2)	−0.2018883983941(10)
1.4	−0.580188485192587(5)	−1.364269874353(2)	1.2263535(3)	−0.1456377885480(10)
1.5	−0.5925282776969(3)	−1.339704692337(2)	1.3876270(3)	−0.103098757962(2)
1.6	−0.6011424218459(3)	−1.315278023072(3)	1.5660824(3)	−0.070620737112(2)
1.7	−0.6069016026516(3)	−1.291394336885(3)	1.7633787(4)	−0.045641842107(2)
1.8	−0.6104591144349(3)	−1.268310435368(3)	1.9813767(4)	−0.026329003610(2)
1.9	−0.6123114227736(3)	−1.246184375878(4)	2.2221647(5)	−0.011348173858(2)
2.0	−0.6128400272918(3)	−1.225107696253(4)	2.4880867(5)	0.000286179165(2)
2.1	−0.6123409460502(3)	−1.205126946907(4)	2.7817755(5)	0.009311878663(2)
2.2	−0.6110458300245(3)	−1.186258248932(4)	3.1061891(6)	0.016287914144(2)
2.3	−0.6091373101229(3)	−1.168497229601(5)	3.4646518(6)	0.021642343759(2)
2.4	−0.6067603021026(3)	−1.151825850423(5)	3.8609018(7)	0.025706147409(2)
2.5	−0.6040304349890(4)	−1.136217120624(5)	4.2991432(7)	0.028737499742(2)
2.6	−0.6010404039482(4)	−1.121638356525(5)	4.7841061(8)	0.030939404374(2)
2.7	−0.5978648065543(4)	−1.108053432178(6)	5.3211140(8)	0.032472659604(2)
2.8	−0.5945638580486(4)	−1.095424325286(6)	5.9161593(9)	0.033465496718(2)
2.9	−0.5911862692135(5)	−1.083712168236(7)	6.5759899(10)	0.034020817307(2)
3.0	−0.5877714926437(5)	−1.072877950612(7)	7.308207(2)	0.034221678225(2)
3.1	−0.5843514883635(6)	−1.062882976185(8)	8.121373(2)	0.034135484046(3)
3.2	−0.5809521206568(7)	−1.053689147538(9)	9.025141(2)	0.033817216805(3)
3.3	−0.5775942697969(8)	−1.04525913072(2)	10.030395(2)	0.033311942084(3)
3.4	−0.5742947218445(10)	−1.03755643765(2)	11.149410(2)	0.032656766481(4)
3.5	−0.571066884585(2)	−1.03054545379(2)	12.396046(3)	0.031882375822(4)
3.6	−0.567921366482(2)	−1.02419143095(2)	13.785951(3)	0.031014250559(5)
3.7	−0.564866447119(2)	−1.01846046002(3)	15.336815(4)	0.030073630869(6)
3.8	−0.561908461312(2)	−1.01331943430(3)	17.068652(5)	0.029078286400(7)
3.9	−0.559052114208(3)	−1.00873601118(4)	19.004127(6)	0.028043132624(8)
4.0	−0.556300741047(3)	−1.00467857785(5)	21.168948(7)	0.026980726060(10)
4.1	−0.553656522390(4)	−1.00111622493(6)	23.592313(8)	0.02590166338(2)
4.2	−0.551120663411(4)	−0.99801873057(7)	26.307447(10)	0.02481490387(2)
4.3	−0.548693544120(5)	−0.99535655659(8)	29.35224(2)	0.02372803062(2)
4.4	−0.546374846022(6)	−0.99310085742(9)	32.77001(2)	0.02264746242(2)
4.5	−0.544163659632(7)	−0.9912235018(2)	36.61043(2)	0.02157862611(3)
4.6	−0.542058576415(8)	−0.9896971070(2)	40.93063(2)	0.02052609693(3)
4.7	−0.540057768024(9)	−0.9884950846(2)	45.79659(3)	0.01949371307(3)
4.8	−0.538159055171(10)	−0.9875916977(2)	51.28485(3)	0.01848466929(4)
4.9	−0.53635996801(2)	−0.9869621278(2)	57.48463(3)	0.01750159351(4)
5.0	−0.53465779958(2)	−0.9865825519(3)	64.50052(4)	0.01654660946(4)

Table A96: Same as for Table A1, but for $6\,^1\Phi_u$.

$6\,^1\Phi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.46198438840(2)	−1.44491636(2)	1.8019(2)	−0.520947580(10)
1.1	−0.506608413583(4)	−1.43058058(2)	1.4356(7)	−0.379421593(9)
1.2	−0.539169407701(7)	−1.41092099(2)	0.9824(7)	−0.277151815(9)
1.3	−0.56293371153(2)	−1.38829687(2)	0.4371(8)	−0.201868808(8)
1.4	−0.58017469854(2)	−1.36421302(2)	−0.2061(8)	−0.145616877(8)
1.5	−0.592512336243(10)	−1.33963953(2)	−0.9530(9)	−0.103076570(8)
1.6	−0.601124200284(10)	−1.31520411(2)	−1.8090(9)	−0.070597320(8)
1.7	−0.606880980427(10)	−1.29131127(2)	−2.7798(9)	−0.045617244(8)
1.8	−0.610435975859(10)	−1.26821784(2)	−3.8706(10)	−0.026303274(7)
1.9	−0.612285657117(10)	−1.24608190(2)	−5.0866(10)	−0.011321362(7)
2.0	−0.61281152887(2)	−1.22499501(2)	−6.4327(10)	0.000314022(7)
2.1	−0.61230961429(2)	−1.20500375(2)	−7.9135(10)	0.009340701(7)
2.2	−0.61101156950(2)	−1.18612428(2)	−9.533(2)	0.016317665(6)
2.3	−0.60910003059(2)	−1.16835223(2)	−11.296(2)	0.021672971(6)
2.4	−0.60671991849(2)	−1.15166960(2)	−13.2060(2)	0.025737599(6)
2.5	−0.60398686737(2)	−1.13604942(2)	−15.2650(10)	0.028769725(6)
2.6	−0.60099357745(2)	−1.12145904(2)	−17.4760(10)	0.030972353(6)
2.7	−0.59781465130(2)	−1.10786234(2)	−19.8408(10)	0.032506283(5)
2.8	−0.59451030895(2)	−1.09522133(2)	−22.3603(9)	0.033499747(5)
2.9	−0.59112926581(2)	−1.08349715(2)	−25.0348(9)	0.034055650(5)
3.0	−0.58771097884(2)	−1.07265080(2)	−27.8639(8)	0.034257051(5)
3.1	−0.58428741210(2)	−1.06264362(2)	−30.8453(8)	0.034171357(5)
3.2	−0.58088443350(2)	−1.05343748(2)	−33.9778(7)	0.033853557(5)
3.3	−0.57752292647(2)	−1.04499507(2)	−37.2571(6)	0.033348721(5)
3.4	−0.57421967964(2)	−1.03727988(2)	−40.6786(4)	0.032693963(4)
3.5	−0.57098810271(2)	−1.03025630(2)	−44.2362(2)	0.031919973(5)
3.6	−0.56783880521(2)	−1.02388954(2)	−47.922736(9)	0.031052243(4)
3.7	−0.56478006686(2)	−1.01814565(2)	−51.7302(2)	0.030112021(4)
3.8	−0.56181822150(3)	−1.01299150(2)	−55.6483(5)	0.029117092(4)
3.9	−0.55895797200(3)	−1.00839465(2)	−59.6659(7)	0.028082382(4)
4.0	−0.55620264986(2)	−1.00432343(2)	−63.7705(10)	0.027020466(3)
4.1	−0.55355442998(4)	−1.00074683(2)	−67.9555(5)	0.025941960(4)
4.2	−0.55101451008(4)	−0.99763448(2)	−72.19(2)	0.024855843(4)
4.3	−0.54858326016(5)	−0.99495670(2)	−76.43(3)	0.023769726(3)
4.4	−0.54626034896(6)	−0.99268445(2)	−80.73(3)	0.022690056(3)
4.5	−0.54404485096(7)	−0.99078936(2)	−85.04(2)	0.021622298(3)
4.6	−0.54193533773(8)	−0.98924377(2)	−89.33(2)	0.020571067(3)
4.7	−0.53992995643(10)	−0.98802073(2)	−93.583(7)	0.019540251(3)
4.8	−0.538026497946(10)	−0.987094083(10)	−97.7993(6)	0.018533107(2)
4.9	−0.536222455605(10)	−0.986438476(10)	−101.9153(6)	0.017552334(2)
5.0	−0.534515077968(9)	−0.986029436(9)	−105.991(7)	0.016600144(2)

Table A97: Same as for Table A1, but for $1\,^3\Phi_u$.

$1\,^3\Phi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.031255144381749(1)	–	9.6696396	–
0.01	97.969006203(2)	95.938529859(2)	9.67156(6)	−9999.9482549(4)
0.05	17.974768311(3)	2.01380028(2)	9.71270(7)	−399.7713723(3)
0.1	7.990503092(5)	1.97039361(2)	9.80968(9)	−99.6089674(2)
0.15	4.67969072(2)	2.76809032(8)	9.92381(10)	−43.9419408(4)
0.2	3.040125940(2)	1.844629258(6)	10.02976(10)	−24.42377605(3)
0.3	1.435377404(2)	1.703280494(5)	10.14943(9)	−10.46219303(2)
0.4	0.6679968441(5)	1.56663896130(4)	10.07066(7)	−5.586589517(2)
0.5	0.2337665253(7)	1.4418947630(3)	9.73081(6)	−3.351322581(2)
0.6	−0.0360590474(9)	1.33074100864(6)	9.08366(6)	−2.157803273(2)
0.7	−0.213860522560(5)	−1.4465478341(2)	8.09117(5)	−1.4554668414(2)
0.8	−0.335709638095(4)	−1.4821832003(2)	6.71962(4)	−1.0134549052(2)
0.9	−0.421493082622(3)	−1.4921563967(2)	4.93771(4)	−0.7213002572(2)
1.0	−0.483001171759(3)	−1.4868833045(2)	2.71559(5)	−0.5208809610(2)
1.1	−0.527618224298(3)	−1.4725201371(2)	0.02428(4)	−0.37934880777(10)
1.2	−0.560171638950(3)	−1.4528309491(2)	−3.16460(4)	−0.27707305935(9)
1.3	−0.583927776578(2)	−1.4301751298(2)	−6.87893(3)	−0.20178428970(7)
1.4	−0.601160031992(2)	−1.40605760125(10)	−11.14611(3)	−0.14552681233(7)
1.5	−0.613488394794(2)	−1.38144856932(10)	−15.99299(3)	−0.10298118648(6)
1.6	−0.622090463797(2)	−1.35697589376(10)	−21.44583(2)	−0.07049685385(5)
1.7	−0.627836952914(2)	−1.33304420660(9)	−27.53013(2)	−0.04551194163(5)
1.8	−0.631381186472(2)	−1.30991047756(9)	−34.27049(2)	−0.02619339145(5)
1.9	−0.633219661150(2)	−1.28773293859(9)	−41.69038(2)	−0.01120716647(4)
2.0	−0.633733908758(2)	−1.26660330845(9)	−49.81196(2)	0.00043225453(4)
2.1	−0.633219980617(2)	−1.24656832474(9)	−58.655803(10)	0.00946268405(4)
2.2	−0.631909562031(2)	−1.22764430184(9)	−68.240617(8)	0.01644310101(4)
2.3	−0.629985319280(2)	−1.2098270663(3)	−78.58301(5)	0.02180155315(9)
2.4	−0.627592204528(2)	−1.1930987845(3)	−89.69697(5)	0.02586901024(9)
2.5	−0.624845884209(2)	−1.1774326759(3)	−101.59377(4)	0.02890363701(9)
2.6	−0.621839091869(2)	−1.1627962722(3)	−114.28146(4)	0.03110842751(9)
2.7	−0.618646464398(2)	−1.1491536673(3)	−127.76446(4)	0.03264417094(9)
2.8	−0.615328257241(2)	−1.1364670626(3)	−142.04318(4)	0.03363908996(9)
2.9	−0.611933222213(3)	−1.1246978177(3)	−157.11360(4)	0.03419607819(9)
3.0	−0.608500853706(3)	−1.1138071518(3)	−172.96681(4)	0.03439818522(9)
3.1	−0.605063154225(3)	−1.103756599(3)	−189.5908(2)	0.0343128096(7)
3.2	−0.601646031126(3)	−1.094508298(6)	−206.962(2)	0.033994926(2)
3.3	−0.598270408238(3)	−1.086025140(6)	−225.055(3)	0.033489599(2)
3.4	−0.594953115536(3)	−1.078270869(5)	−243.837(2)	0.032833930(2)
3.5	−0.591707604938(3)	−1.071210094(5)	−263.269(2)	0.032058605(2)
3.6	−0.588544529082(3)	−1.064808288(5)	−283.304(2)	0.031189103(2)
3.7	−0.585472211591(3)	−1.059031753(5)	−303.887(2)	0.030246668(2)
3.8	−0.582497030953(3)	−1.053847582(5)	−324.956(2)	0.029249074(2)
3.9	−0.579623735368(3)	−1.049223619(5)	−346.439(2)	0.0282112440(10)
4.0	−0.576855702214(3)	−1.0451284205(5)	−368.25590(7)	0.02714574600(10)
4.1	−0.57419515294(4)	−1.0415312252(5)	−390.32413(8)	0.0260631904(2)
4.2	−0.57164333192(2)	−1.0384019300(2)	−412.54621(2)	0.02497255567(5)
4.3	−0.56920065625(2)	−1.0357110825(2)	−434.81947(2)	0.02388144883(4)
4.4	−0.56686684183(2)	−1.0334298809(2)	−457.03355(2)	0.02279631882(4)

4.5	−0.564641010184(4)	−1.0315301862(5)	−479.07127(8)	0.02172262982(10)
4.6	−0.56252177965(4)	−1.0299845444(5)	−500.80885(8)	0.02066500324(10)
4.7	−0.56050734359(2)	−1.0287662175(2)	−522.11708(2)	0.01962733397(4)
4.8	−0.55859553818(2)	−1.0278492219(2)	−542.86231(2)	0.01861288635(4)
4.9	−0.55678390128(2)	−1.0272083706(2)	−562.90703(2)	0.01762437388(4)
5.0	−0.555069724117(5)	−1.026819321(2)	−582.1119(4)	0.0166640254(4)
5.5	−0.547853992970(6)	−1.027863799(4)	−660.6650(10)	0.0123353067(6)
6.0	−0.542593703654(8)	−1.032109356(6)	−698.702(2)	0.0088463419(8)
6.5	−0.538872390465(3)	−1.03766187147(4)	−686.344169(10)	0.006166601455(5)
7.0	−0.536309297103(3)	−1.04326900128(3)	−624.861878(9)	0.004192798989(4)
7.5	−0.534583952898(3)	−1.04822186664(3)	−527.566535(8)	0.002792805221(3)
8.0	−0.533443284961(3)	−1.05222624251(3)	−414.648359(6)	0.001832540926(3)
8.5	−0.532698291425(2)	−1.05526652980(3)	−304.971616(5)	0.001191770947(3)
9.0	−0.532214718070(2)	−1.05747589429(2)	−210.525555(5)	0.000772615761(2)
9.5	−0.531901082632(2)	−1.05903547971(2)	−135.817619(4)	0.000501756374(2)
10.0	−0.531696913839(2)	−1.06011634734(2)	−80.239065(5)	0.000327748034(2)
11.0	−0.531474229405(2)	−1.061361485032(10)	−13.764467(4)	0.0001442703435(8)
12.0	−0.5313737090811(7)	−1.061936285721(7)	15.380349(3)	0.0000675943701(5)
13.0	−0.5313249268428(5)	−1.062202572792(4)	26.038869(2)	0.0000344062226(2)
14.0	−0.5312990548842(4)	−1.062329276477(3)	28.4058044(6)	0.00001920237798(10)
15.0	−0.5312840217927(3)	−1.0623928030517(7)	27.38279543(2)	0.000011682702246(7)
16.0	−0.5312745608524(3)	−1.0624271611879(7)	25.1657628(6)	0.00000762253225(7)
17.0	−0.5312682290794(2)	−1.062447456584(2)	22.681118(2)	0.0000052353867(2)
18.0	−0.5312638010996(3)	−1.062460500634(6)	20.291101(2)	0.0000037278647(4)
19.0	−0.5312606076799(4)	−1.062469478818(9)	18.118121(3)	0.0000027229758(5)
20.0	−0.5312582531696(7)	−1.06247597261(2)	16.187408(4)	0.0000020266862(8)

Table A98: Same as for Table A1, but for $2\,^3\Phi_u$.

$2\,^3\Phi_u$				
R	E	$\langle V \rangle$	$10^6 \cdot \langle \nabla_1 \cdot \nabla_2 \rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.0200029371587427(5)	–	5.4064900(5)	–
0.01	97.9802584074(3)	95.961034275(3)	5.4068(4)	−9999.9482540(2)
0.05	17.986020475(4)	15.98347227(3)	5.427(3)	−399.7713735(4)
0.1	8.001755135(4)	6.04261318(3)	5.477(7)	−99.6089711(3)
0.15	4.690942521(4)	2.79059307(3)	5.557(3)	−43.9419465(2)
0.2	3.051377424(6)	1.21799813(2)	5.623(7)	−24.4237837(2)
0.3	1.446627913(3)	−0.24540561(2)	5.746(2)	−10.46220480(4)
0.4	0.679245966(2)	−0.876150310(10)	5.72(3)	−5.58660560(2)
0.5	0.2450138252(6)	−1.185643805(5)	5.6545(7)	−3.351342910(8)
0.6	−0.0248139931(5)	−1.344324670(5)	5.394(2)	−2.157827806(6)
0.7	−0.2026181282(4)	−1.424083121(4)	4.961(2)	−1.455495521(5)
0.8	−0.3244703148(7)	−1.45973073(2)	4.333(4)	−1.01348763(2)
0.9	−0.4102572302(4)	−1.469717699(4)	3.509(2)	−0.721336932(4)
1.0	−0.4717691800(7)	−1.464459840(8)	2.455(3)	−0.520921480(6)
1.1	−0.5163904720(3)	−1.450113310(4)	1.168(2)	−0.379393060(3)
1.2	−0.5489484936(7)	−1.430442098(8)	−0.375(3)	−0.277120926(5)
1.3	−0.5727095934(3)	−1.407805526(4)	−2.182(2)	−0.201835645(3)
1.4	−0.5899471534(6)	−1.383708444(8)	−4.274(3)	−0.145581527(5)
1.5	−0.6022811499(6)	−1.359120983(7)	−6.660(3)	−0.103039122(4)
1.6	−0.6108891676(6)	−1.334670924(7)	−9.355(3)	−0.070557868(4)
1.7	−0.6166419058(6)	−1.310762816(8)	−12.373(3)	−0.045575885(4)
1.8	−0.6201926735(3)	−1.287653541(4)	−15.724(2)	−0.026260108(2)
1.9	−0.6220379519(6)	−1.265501245(8)	−19.428(3)	−0.011276496(4)
2.0	−0.6225592559(3)	−1.244397549(4)	−23.487(2)	0.000360481(2)
2.1	−0.6220526202(6)	−1.224389096(8)	−27.921(3)	0.009388640(3)
2.2	−0.6207497119(3)	−1.205492096(4)	−32.731(2)	0.016366967(2)
2.3	−0.6188331794(6)	−1.187702272(8)	−37.936(3)	0.021723516(3)
2.4	−0.6164479554(6)	−1.171001680(8)	−43.535(3)	0.025789263(3)
2.5	−0.6137096870(6)	−1.155363425(8)	−49.539(3)	0.028822380(3)
2.6	−0.6107110872(7)	−1.140754921(8)	−55.951(3)	0.031025867(3)
2.7	−0.6075267721(7)	−1.127140140(8)	−62.775(3)	0.032560520(3)
2.8	−0.6042169753(7)	−1.114481158(9)	−70.012(4)	0.033554569(3)
2.9	−0.6008304265(7)	−1.102739204(9)	−77.661(4)	0.034110913(3)
3.0	−0.5974065969(7)	−1.091875364(9)	−85.718(4)	0.034312610(3)
3.1	−0.5939774655(7)	−1.081851035(9)	−94.178(4)	0.034227063(3)
3.2	−0.5905689153(8)	−1.072628210(10)	−103.032(4)	0.033909256(3)
3.3	−0.5872018451(8)	−1.064169640(10)	−112.269(4)	0.033404258(3)
3.4	−0.5838930593(8)	−1.056438918(2)	−121.872(4)	0.032749177(3)
3.5	−0.5806559835(8)	−1.04940050(2)	−131.825(4)	0.031974704(3)
3.6	−0.5775012437(8)	−1.04301971(2)	−142.105(4)	0.031106327(3)
3.7	−0.5744371360(9)	−1.03726268(2)	−152.687(5)	0.030165294(3)
3.8	−0.5714700109(9)	−1.03209639(5)	−163.55(2)	0.029169378(9)
3.9	−0.5686045881(10)	−1.02748842(2)	−174.638(5)	0.028133526(3)
4.0	−0.5658442158(5)	−1.023407263(7)	−185.933(2)	0.027070292(2)
4.1	−0.5631910865(10)	−1.01982196(2)	−197.396(5)	0.025990295(3)
4.2	−0.5606464145(6)	−1.016702252(7)	−208.979(8)	0.024902518(2)
4.3	−0.5582105871(4)	−1.014018524(5)	−220.73(6)	0.0238145697(10)
4.4	−0.5558832901(4)	−1.011741823(6)	−232.44(9)	0.0227328993(10)

4.5	−0.5536636149(7)	−1.009843861(9)	−243.912(2)	0.021662971(2)
4.6	−0.551550150(2)	−1.00829704(2)	−255.448(6)	0.020609403(4)
4.7	−0.5495410583(6)	−1.007074497(8)	−266.8173(3)	0.019576089(2)
4.8	−0.5476341474(5)	−1.006150123(6)	−278.3(2)	0.0185662857(10)
4.9	−0.5458269267(5)	−1.005498634(7)	−289.1(2)	0.017582698(2)
5.0	−0.5441166596(5)	−1.005095601(7)	−299.38(2)	0.016627544(2)
5.5	−0.536912033(2)	−1.00601892(6)	−344.34(3)	0.012328209(8)
6.0	−0.531647227(2)	−1.01006487(6)	−370.84(3)	0.008871597(8)
6.5	−0.52790560250(6)	−1.0153707981(9)	−373.0523(2)	0.0062216011(2)
7.0	−0.52530933295(5)	−1.0207387992(7)	−349.71273(7)	0.00426855239(8)
7.5	−0.5235435851(2)	−1.025513793(2)	−304.9681(5)	0.0028764503(2)
8.0	−0.52236167791(9)	−1.029425791(2)	−247.5454(4)	0.0019121957(2)
8.5	−0.52157947961(7)	−1.0324474750(9)	−187.5679(3)	0.00126017461(8)
9.0	−0.52106508099(5)	−1.0346830467(6)	−133.0902(2)	0.00082745726(6)
9.5	−0.52072727651(4)	−1.0362876264(5)	−88.3840(2)	0.00054388701(4)
10.0	−0.52050478347(6)	−1.037416494(2)	−54.32612(7)	0.00035930737(5)
11.0	−0.52025846285(2)	−1.0387423234(2)	−12.75342(8)	0.00016132748(2)
12.0	−0.52014532668(2)	−1.03937185144(4)	6.19403(7)	0.000076566827(2)
13.0	−0.52009011055(4)	−1.0396782570(2)	14.7125(4)	0.000038612626(3)
14.0	−0.52006198708(8)	−1.0398468167(10)	18.5230(4)	0.00001979696(6)
15.0	−0.5200465490(5)	−1.039907633(4)	15.0051(9)	0.0000123642(3)
16.0	−0.520036057(2)	−1.03992977(2)	11.888(3)	0.0000088965(9)
17.0	−0.520028383(3)	−1.03994471(3)	10.119(5)	0.000006591(2)
18.0	−0.52002264616(2)	−1.0399558723(2)	9.00165(8)	0.000004967778(5)
19.0	−0.52001830(2)	−1.03996441(8)	8.15(2)	0.000003797(6)
20.0	−0.52001496(3)	−1.0399709(2)	7.469(10)	0.000002946(9)

Table A99: Same as for Table A1, but for $3\,^3\Phi_u$.

$3\,^3\Phi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
0.0	−2.0138906838155497(3)	–	3.2684586(8)	–
0.01	97.986370665(2)	95.973258795(9)	3.265(2)	−9999.9482535(6)
0.05	17.992132720(6)	15.99569675(4)	3.273(5)	−399.7713739(6)
0.1	8.007867323(8)	6.05483744(5)	3.29(2)	−99.6089720(4)
0.15	4.697054619(8)	2.80281694(5)	3.33(2)	−43.9419486(2)
0.2	3.057489384(6)	1.23022144(4)	3.38(2)	−24.4237867(2)
0.3	1.452739469(4)	−0.23318398(3)	3.45(2)	−10.46220973(7)
0.4	0.6853567941(10)	−0.863935186(7)	0.438586(7)	−5.58662193(2)
0.5	0.25112279694(8)	−1.1734362453(5)	0.50942(8)	−3.3513636783(5)
0.6	−0.01870731748(4)	−1.3321264083(2)	0.59265(10)	−2.1578529556(2)
0.7	−0.19651418382(2)	−1.411895858(4)	0.68861(8)	−1.45552499(2)
0.8	−0.318369528927(6)	−1.4475561159(5)	0.79820(4)	−1.013521325(3)
0.9	−0.404160021198(4)	−1.457557327(2)	0.92216(2)	−0.72137475971(7)
1.0	−0.4656759562583(3)	−1.45231525302(2)	1.0615524(5)	−0.520963340497(6)
1.1	−0.510301631367(2)	−1.437985988287(8)	1.2175647(2)	−0.379438841412(4)
1.2	−0.542864422339(2)	−1.418333458895(6)	1.3915802(3)	−0.277170511848(3)
1.3	−0.5666306659057(9)	−1.395716919708(5)	1.585137(3)	−0.201888913767(3)
1.4	−0.5838737315730(8)	−1.371641152075(5)	1.799965(2)	−0.145638349235(3)
1.5	−0.5962135825113(6)	−1.347076214620(4)	2.0380027(8)	−0.103099366398(2)
1.6	−0.6048277900063(6)	−1.322649813769(4)	2.3014257(5)	−0.070621396098(2)
1.7	−0.6105870393700(5)	−1.298766421995(4)	2.5926711(5)	−0.045642554856(2)
1.8	−0.6141446252677(5)	−1.275682843386(4)	2.9144716(4)	−0.026329773806(2)
1.9	−0.6159970136714(4)	−1.253557138204(4)	3.2698923(4)	−0.011349005716(2)
2.0	−0.61652570465639(4)	−1.232480847660(4)	3.6623722(4)	0.000285280827(2)
2.1	−0.6160267167988(3)	−1.212500526075(3)	4.0957715(4)	0.009310908344(2)
2.2	−0.6147317016620(3)	−1.193632299070(3)	4.5744249(4)	0.016286865570(2)
2.3	−0.6128232908244(3)	−1.175871799151(9)	5.1032010(10)	0.021641209782(3)
2.4	−0.6104464008062(3)	−1.159200993861(9)	5.6875736(10)	0.025704919897(3)
2.5	−0.6077166615009(3)	−1.143592899391(9)	6.3336922(10)	0.028736169445(3)
2.6	−0.6047267690609(4)	−1.12901484008(2)	7.048472(2)	0.030937960787(4)
2.7	−0.6015513221802(3)	−1.11543069918(2)	7.839690(2)	0.032471090809(4)
2.8	−0.5982505373699(4)	−1.10280246496(2)	8.716095(2)	0.033463789208(4)
2.9	−0.5948731268509(3)	−1.09109128193(2)	9.687525(2)	0.034018955785(4)
3.0	−0.5914585448457(4)	−1.08025815352(2)	10.765055(2)	0.034219645392(4)
3.1	−0.5880387532185(4)	−1.07026439933(2)	11.961146(3)	0.034133260358(4)
3.2	−0.5846396183309(5)	−1.06107194000(2)	13.289822(3)	0.033814780208(4)
3.3	−0.5812820227994(6)	−1.05264346212(2)	14.766873(3)	0.033309267719(4)
3.4	−0.5779827553235(6)	−1.044942501012(8)	16.410081(2)	0.032653826363(3)
3.5	−0.574755226661(5)	−1.0379334688(2)	18.23945(2)	0.03187913844(5)
3.6	−0.571610048607(5)	−1.0315816470(2)	20.27757(3)	0.03101068062(5)
3.7	−0.568555504493(6)	−1.0258531607(3)	22.54985(3)	0.03006968874(6)
3.8	−0.565597933331(7)	−1.0207149414(3)	25.08496(3)	0.02907392771(6)
3.9	−0.562742044961(8)	−1.0161346896(3)	27.91526(4)	0.02803830777(7)
4.0	−0.559991179869(9)	−1.012080843(3)	31.07722(4)	0.0269753793(6)
4.1	−0.55734752451(8)	−1.008522542(3)	34.61219(4)	0.0258957333(7)
4.2	−0.55481229048(9)	−1.005429628(3)	38.56682(5)	0.0248083220(7)
4.3	−0.55238586505(10)	−1.002772630(4)	42.99398(5)	0.0237207210(8)
4.4	−0.5500679377(2)	−1.000522775(4)	47.95364(6)	0.0226393409(8)

4.5	−0.547857607740(5)	−0.9986520113(4)	53.51402(3)	0.02156960094(7)
4.6	−0.54575347645(3)	−0.9971330492(4)	59.75248(3)	0.02051606602(7)
4.7	−0.54375372600(5)	−0.995939393(2)	66.75750(6)	0.0194825658(3)
4.8	−0.54185618862(5)	−0.995045403(2)	74.63044(7)	0.0184722863(3)
4.9	−0.54005840683(7)	−0.994426364(2)	83.48732(8)	0.0174878470(4)
5.0	−0.538357686766(7)	−0.9940585477(6)	93.46193(6)	0.01653136516(10)
5.5	−0.531204805589(2)	−0.995237564(3)	166.47795(3)	0.0122130994(5)
6.0	−0.526010812058(2)	−0.999875034(2)	306.17700(4)	0.0086910984(4)
6.5	−0.52240182955(3)	−1.006907357(2)	594.87904(4)	0.0058302004(3)
7.0	−0.520148334675(9)	−1.0183196182(6)	1204.51984(4)	0.00313957873(8)
7.5	−0.519312197820(6)	−1.0359745500(2)	1677.077636(7)	0.00035331276(2)
8.0	−0.51943186802(2)	−1.0430579754(4)	1260.66730(2)	−0.00052427992(4)
8.5	−0.51969018011(2)	−1.0432976917(4)	847.78109(5)	−0.00046086253(5)
9.0	−0.51987897450(2)	−1.0424276599(5)	573.83997(7)	−0.00029663454(5)
9.5	−0.519993464824(8)	−1.0415955516(2)	391.125933(5)	−0.00016932863(2)
10.0	−0.520055783461(10)	−1.0409764964(2)	267.236170(9)	−0.00008649295(2)
11.0	−0.520095864738(9)	−1.0402801749(2)	125.174264(8)	−0.000008040489(2)
12.0	−0.520090005097(10)	−1.0400059935(2)	59.402272(9)	0.000014501395(10)
13.0	−0.52007294527(2)	−1.0399104045(2)	28.392146(9)	0.00001811431(2)
14.0	−0.52005511963(3)	−1.0398707162(2)	13.27996(5)	0.000017108789(8)
15.0	−0.52004009809(2)	−1.03989101360(3)	10.62611(2)	0.0000126121714(4)
16.0	−0.52002963058(7)	−1.0399216683(7)	9.936(2)	0.00000859955(4)
17.0	−0.52002241327(3)	−1.0399423525(2)	9.0324(3)	0.000006027885(7)
18.0	−0.52001727626(4)	−1.03995607103(5)	8.069(2)	0.00000436007(2)
19.0	−0.52001351494(3)	−1.0399656206(3)	7.1692(4)	0.00000323207(2)
20.0	−0.520010700677(3)	−1.0399725802(4)	6.35214(7)	0.0000024410739(5)

Table A100: Same as for Table A1, but for $4\,^3\Phi_u$.

		$4\,^3\Phi_u$		
R	E	$\langle V\rangle$	$10^6 \cdot \langle\nabla_1 \cdot \nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.465665557927(2)	−1.452270022(3)	1.7475(9)	−0.520938906(3)
1.1	−0.5102886740769(10)	−1.437930664(3)	1.0285(9)	−0.379412105(3)
1.2	−0.5428486791271(9)	−1.418267205(3)	0.1641(9)	−0.277141539(2)
1.3	−0.5666119164557(8)	−1.395638937(3)	−0.8541(9)	−0.201857772(2)
1.4	−0.5838517624952(8)	−1.371550678(3)	−2.0347(9)	−0.145605109(2)
1.5	−0.5961881875959(9)	−1.346972527(3)	−3.3859(9)	−0.103064101(2)
1.6	−0.6047987704567(9)	−1.322532230(3)	−4.9155(9)	−0.070584181(2)
1.7	−0.6105542040152(10)	−1.298634301(3)	−6.6316(9)	−0.045603467(2)
1.8	−0.614107790758(2)	−1.275535587(3)	−8.5417(9)	−0.026288892(2)
1.9	−0.615956004654(2)	−1.253394190(3)	−10.6530(10)	−0.011306411(2)
2.0	−0.616480353926(2)	−1.232301694(3)	−12.9724(10)	0.000329507(2)
2.1	−0.615976865428(2)	−1.212304699(3)	−15.5063(10)	0.009356682(2)
2.2	−0.614677199099(2)	−1.193419373(3)	−18.2607(10)	0.016334102(2)
2.3	−0.612763994962(2)	−1.175641392(3)	−21.2409(10)	0.021689825(2)
2.4	−0.610382178012(3)	−1.158952766(3)	−24.4514(10)	0.0257548293(10)
2.5	−0.607647386605(3)	−1.143326552(3)	−27.8963(10)	0.0287872884(10)
2.6	−0.604652325295(3)	−1.128730116(3)	−31.5784(10)	0.0309902057(10)
2.7	−0.601471601061(3)	−1.115127377(3)	−35.4997(2)	0.0325243797(10)
2.8	−0.598165438521(3)	−1.102480359(3)	−39.661(2)	0.0335180421(9)
2.9	−0.594782557748(3)	−1.090750238(3)	−44.0623(10)	0.0340740957(9)
3.0	−0.591362420482(3)	−1.079898044(4)	−48.702(2)	0.0342755991(9)
3.1	−0.587936995679(4)	−1.069885117(4)	−53.576(2)	0.0341899594(9)
3.2	−0.584532156260(4)	−1.060673394(4)	−58.681(2)	0.0338721621(9)
3.3	−0.581168790747(4)	−1.052225567(4)	−64.010(2)	0.0333672771(9)
3.4	−0.577863692963(4)	−1.044505170(4)	−69.555(2)	0.0327124164(9)
3.5	−0.574630277850(4)	−1.037476602(4)	−75.306(2)	0.0319382725(9)
3.6	−0.571479160284(4)	−1.031105118(4)	−81.251(2)	0.0310703340(9)
3.7	−0.568418625385(4)	−1.025356803(4)	−87.376(2)	0.0301298508(10)
3.8	−0.565455012434(4)	−1.020198529(5)	−93.664(2)	0.0291346041(10)
3.9	−0.562593029789(4)	−1.015597920(5)	−100.099(2)	0.0280995230(10)
4.0	−0.559836014418(4)	−1.011523309(5)	−106.658(2)	0.0270371801(10)
4.1	−0.557186146864(4)	−1.007943710(4)	−113.320(2)	0.0259581913(7)
4.2	−0.554644630235(4)	−1.004828805(6)	−120.060(2)	0.024871537(2)
4.3	−0.552211840070(4)	−1.002148923(6)	−126.851(2)	0.023784827(2)
4.4	−0.549887450572(4)	−0.999875050(6)	−133.665(2)	0.022704512(2)
4.5	−0.547670541622(6)	−0.997978847(6)	−140.471(2)	0.021636053(2)
4.6	−0.545559690114(4)	−0.996432665(6)	−147.236(2)	0.020584068(2)
4.7	−0.543553048439(4)	−0.995209588(6)	−153.927(3)	0.019552449(2)
4.8	−0.541648412448(4)	−0.994283469(6)	−160.509(3)	0.018544449(2)
4.9	−0.539843280685(4)	−0.993628979(6)	−166.946(3)	0.017562772(2)
5.0	−0.538134906379(5)	−0.993221656(7)	−173.201(3)	0.016609631(2)

Table A101: Same as for Table A1, but for $5\,^3\Phi_u$.

		$5\,^3\Phi_u$		
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.4619908992331(10)	−1.444944747995(4)	0.7258039(2)	−0.520962949529(2)
1.1	−0.5066165332650(6)	−1.430615318218(3)	0.8316141(2)	−0.379438410625(2)
1.2	−0.5391792791038(4)	−1.410962605823(2)	0.9495891(2)	−0.277170039679(2)
1.3	−0.5629454733100(3)	−1.388345864534(2)	1.0807734(3)	−0.2018883983952(10)
1.4	−0.5801884851935(3)	−1.364269874356(2)	1.2263417(3)	−0.1456377885494(10)
1.5	−0.5925282776977(3)	−1.339704692342(2)	1.3876126(3)	−0.103098757964(2)
1.6	−0.6011424218469(3)	−1.315278023077(3)	1.5660650(3)	−0.070620737114(2)
1.7	−0.6069016026528(3)	−1.291394336891(3)	1.7633576(4)	−0.045641842109(2)
1.8	−0.6104591144364(3)	−1.268310435375(3)	1.9813514(4)	−0.026329003612(2)
1.9	−0.6123114227753(3)	−1.246184375887(4)	2.2221344(5)	−0.011348173861(2)
2.0	−0.6128400272938(3)	−1.225107696264(4)	2.4880506(5)	0.000286179162(2)
2.1	−0.6123409460526(3)	−1.205126946920(4)	2.7817328(6)	0.009311878659(2)
2.2	−0.6110458300273(3)	−1.186258248948(4)	3.1061387(6)	0.016287914139(2)
2.3	−0.6091373101262(3)	−1.168497229619(5)	3.4645926(7)	0.021642343754(2)
2.4	−0.6067603021064(3)	−1.151825850444(5)	3.8608324(7)	0.025706147404(2)
2.5	−0.6040304349935(4)	−1.136217120649(5)	4.2990622(8)	0.028737499735(2)
2.6	−0.6010404039533(4)	−1.121638356554(5)	4.7840119(9)	0.030939404366(2)
2.7	−0.5978648065601(4)	−1.108053432212(6)	5.3210046(9)	0.032472659596(2)
2.8	−0.5945638580553(4)	−1.095424325325(6)	5.9160326(2)	0.033465496709(2)
2.9	−0.5911862692213(5)	−1.083712168282(6)	6.575844(2)	0.034020817297(2)
3.0	−0.5877714926525(5)	−1.072877950665(7)	7.308038(2)	0.034221678213(2)
3.1	−0.5843514883736(6)	−1.062882976246(8)	8.121179(2)	0.034135484033(3)
3.2	−0.5809521206683(7)	−1.053689147609(9)	9.024918(2)	0.033817216790(3)
3.3	−0.5775942698100(8)	−1.04525913080(2)	10.030139(3)	0.033311942067(3)
3.4	−0.5742947218593(9)	−1.03755643775(2)	11.149118(3)	0.032656766462(4)
3.5	−0.571066884602(2)	−1.03054545390(2)	12.395711(4)	0.031882375801(4)
3.6	−0.567921366501(2)	−1.02419143107(2)	13.785568(4)	0.031014250536(5)
3.7	−0.564866447140(2)	−1.01846046016(3)	15.336379(5)	0.030073630843(6)
3.8	−0.561908461336(2)	−1.01331943446(3)	17.068155(6)	0.029078286371(7)
3.9	−0.559052114235(3)	−1.00873601136(4)	19.003562(7)	0.028043132592(8)
4.0	−0.556300741078(3)	−1.00467857806(5)	21.168306(9)	0.026980726025(10)
4.1	−0.553656522424(4)	−1.00111622516(6)	23.59158(2)	0.02590166334(2)
4.2	−0.551120663449(4)	−0.99801873083(7)	26.30662(2)	0.02481490383(2)
4.3	−0.548693544163(5)	−0.99535655688(8)	29.35131(2)	0.02372803057(2)
4.4	−0.546374846070(6)	−0.99310085774(9)	32.76896(2)	0.02264746236(2)
4.5	−0.544163659686(7)	−0.9912235021(2)	36.60924(3)	0.02157862605(3)
4.6	−0.542058576474(8)	−0.9896971074(2)	40.92929(3)	0.02052609687(3)
4.7	−0.540057768090(9)	−0.9884950851(2)	45.79508(3)	0.01949371300(3)
4.8	−0.538159055243(10)	−0.9875916982(2)	51.28316(4)	0.01848466922(4)
4.9	−0.53635996809(2)	−0.9869621283(2)	57.48274(4)	0.01750159343(4)
5.0	−0.53465779966(2)	−0.9865825524(3)	64.49841(5)	0.01654660938(4)

Table A102: Same as for Table A1, but for $6\,^3\Phi_u$.

$6\,^3\Phi_u$				
R	E	$\langle V\rangle$	$10^6\cdot\langle\nabla_1\cdot\nabla_2\rangle$	$\mathrm{d}E/\mathrm{d}R$
1.0	−0.461984424563(8)	−1.444916481(9)	1.213(4)	−0.520947632(7)
1.1	−0.506608454140(6)	−1.43058072(2)	0.770(4)	−0.379421649(9)
1.2	−0.539169452815(6)	−1.41092115(2)	0.235(4)	−0.277151869(8)
1.3	−0.562933761284(5)	−1.38829704(2)	−0.396(5)	−0.201868857(10)
1.4	−0.580174753158(5)	−1.36421321(2)	−1.129(5)	−0.145616933(8)
1.5	−0.592512395833(5)	−1.33963973(2)	−1.969(5)	−0.103076627(8)
1.6	−0.601124264929(4)	−1.31520434(2)	−2.922(6)	−0.070597378(8)
1.7	−0.606881050174(4)	−1.29131151(2)	−3.992(6)	−0.045617302(8)
1.8	−0.610436050720(4)	−1.26821810(2)	−5.184(6)	−0.026303331(8)
1.9	−0.612285737075(4)	−1.24608217(2)	−6.502(6)	−0.011321419(8)
2.0	−0.612811613883(4)	−1.22499529(3)	−7.949(6)	0.000313971(9)
2.1	−0.612309704272(4)	−1.20500404(2)	−9.536(7)	0.009340651(8)
2.2	−0.611011664347(4)	−1.18612457(2)	−11.260(7)	0.016317616(8)
2.3	−0.609100130168(5)	−1.16835254(2)	−13.125(7)	0.021672923(7)
2.4	−0.606720022640(5)	−1.15166992(2)	−15.135(7)	0.025737553(7)
2.5	−0.603986975906(5)	−1.13604975(2)	−17.293(7)	0.028769681(7)
2.6	−0.600993690184(5)	−1.12145937(2)	−19.601(7)	0.030972311(6)
2.7	−0.597814768000(7)	−1.10786268(2)	−22.060(8)	0.032506243(6)
2.8	−0.594510429392(5)	−1.09522167(2)	−24.670(8)	0.033499710(6)
2.9	−0.591129389750(5)	−1.08349750(2)	−27.431(8)	0.034055615(5)
3.0	−0.587711106031(4)	−1.07265116(2)	−30.343(8)	0.034257018(5)
3.1	−0.584287542231(5)	−1.06264397(2)	−33.404(8)	0.034171329(5)
3.2	−0.580884566320(5)	−1.05343783(2)	−36.611(8)	0.033853532(5)
3.3	−0.577523061702(5)	−1.044995419(5)	−39.960(8)	0.033348698(2)
3.4	−0.574219817013(6)	−1.03728023(2)	−43.445(8)	0.032693942(4)
3.5	−0.570988241929(7)	−1.03025664(2)	−47.062(8)	0.031919955(4)
3.6	−0.567838945997(9)	−1.02388987(2)	−50.802(8)	0.031052228(4)
3.7	−0.56478020886(3)	−1.01814598(3)	−54.656(8)	0.030112010(5)
3.8	−0.56181836452(4)	−1.01299182(2)	−58.616(8)	0.029117083(5)
3.9	−0.55895811576(4)	−1.00839496(2)	−62.673(8)	0.028082376(4)
4.0	−0.556202794173(2)	−1.00432374(2)	−66.809(9)	0.0270204764(3)
4.1	−0.553554574558(2)	−1.000747064(10)	−71.000(4)	0.025941970(2)
4.2	−0.551014654628(2)	−0.997634763(10)	−75.255(4)	0.024855844(2)
4.3	−0.548583404432(2)	−0.994956973(10)	−79.559(9)	0.023769729(2)
4.4	−0.546260492724(2)	−0.992684711(10)	−83.855(4)	0.022690062(2)
4.5	−0.544044993995(2)	−0.990789612(10)	−88.163(4)	0.021622306(2)
4.6	−0.541935479816(2)	−0.989244006(9)	−92.451(4)	0.020571077(2)
4.7	−0.539930097366(2)	−0.988020954(9)	−96.698(3)	0.019540264(2)
4.8	−0.538026637398(2)	−0.987094292(9)	−100.883(3)	0.018533121(2)
4.9	−0.536222593504(2)	−0.986438672(9)	−104.982(3)	0.017552350(2)
5.0	−0.534515214138(3)	−0.986029619(8)	−109.02(2)	0.016600162(2)