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Nonrelativistic energy levels of D₂

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Nonrelativistic energies of the deuterium molecule, accurate to $10^{-7} - 10^{-8} \text{ cm}^{-1}$ for all levels located up to 8000 cm^{-1} above the ground state, are presented. The employed nonadiabatic James-Coolidge wave functions with angular factors enable the high accuracy to be reached regardless of vibrational or rotational quantum number. The derivative of the energy with respect to the deuteron-to-electron mass ratio is supplied for each level, which makes the results independent of the future changes in this physical parameter and will enable its determination from sufficiently accurate experimental data.

Introduction

The deuterium molecule has been extensively studied spectroscopically for almost as long as the hydrogen molecule.^{1–3} Recently, the ionization potential of ortho- (total nuclear spin $I = 0, 2$) and para-D₂ ($I = 1$) have been determined with precision of tens of MHz by combining the measured frequencies of transitions via an intermediate $EF^1\Sigma_g^+$ state^{4,5} and the calculated Rydberg-states binding energies.⁶ Using extremely accurate theoretical data for D₂⁺^{7–9} and the deuterium atom², the dissociation energy of the ortho- and para-D₂ states as well as the separation energy of these states have been determined⁵ with precision higher than 10^{-3} cm^{-1} (30 MHz).

Although only weak electric quadrupole and magnetic dipole transitions⁷ within the manifold of rovibrational states are allowed, a selection of transition energies have been directly acquired using various experimental techniques.^{11–18} Specifically, accurate absorption line positions and intensities for the 2-0 vibrational band have been determined experimentally.¹⁹ Nowadays, a relative accuracy of $5 \cdot 10^{-8}$ has been achieved in the measurements of the transition energies in D₂.

Theoretical energy separation (ionization, dissociation, transition energy) is composed of several additive components. For a light molecule, such as D₂, these components can be well described in the framework of the nonrelativistic quantum electrodynamic theory (NRQED)²⁰ by the following expansion of the total energy in powers of the fine structure constant α ($\approx 1/137$)

$$E(\alpha) = \sum_{i=2}^{\infty} \alpha^i E^{(i)}. \quad (1)$$

The higher the expected accuracy, the more (smaller and smaller)

components of this series must be involved. Furthermore, the higher the expected accuracy, the more accurate the required calculation of the involved components. In particular, the leading term of the expansion (1), which represents the nonrelativistic energy, is by far the most dominant, and its accuracy can directly limit the accuracy of the total energy $E(\alpha)$. For example, attaining the 1 MHz ($\sim 3 \cdot 10^{-5} \text{ cm}^{-1}$) accuracy for the dissociation energy of D₂ requires 10 significant figures of the nonrelativistic component to be known. A common procedure of decomposing the nonrelativistic energy into the clamped nuclei, adiabatic, and nonadiabatic components can hardly enable such an accuracy. However, for systems like deuterium molecule, the nonrelativistic energy can also be calculated directly, i.e. without expansion in a mass parameter. Such pioneering calculations were performed by Kołos and Wolniewicz in 1964.²¹ Much later, variational calculations for rotationless levels were performed using nonadiabatic, explicitly correlated Gaussian (naECG) functions reaching the accuracy of 10^{-5} cm^{-1} .^{22–24} To complete this historical sketch, we mention also the calculations of the leading order nonadiabatic corrections to the Born-Oppenheimer energy by Wolniewicz in 1995²⁵ as well as the application of the nonadiabatic perturbation theory (NAPT)²⁶ to the determination of these corrections for all bound rovibrational levels of D₂ using explicitly correlated Gaussians (ECG)²⁷ and later using James-Coolidge (JC) wave functions.²⁸ In this work, we present the results of another approach to the nonrelativistic energy, which employs nonadiabatic James-Coolidge (naJC) basis functions. This variational and fully nonadiabatic method enables an accuracy of $10^{-7} - 10^{-8} \text{ cm}^{-1}$ to be obtained for the dissociation energy of an energy level and, in contrast to the aforementioned variational calculations, is not limited to the rotationless states. At this level of accuracy the rovibrational energies as well as intervals between them become sensitive to the uncertainty in the deuteron-to-electron mass ratio μ_d . For instance, the change of μ_d by its current uncertainty ($1.3 \cdot 10^{-7}$) results in a change in the vibrational 2-0 excitation en-

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ergy by $1.0 \cdot 10^{-7} \text{ cm}^{-1}$, while the achieved numerical uncertainty is at the level of 10^{-8} cm^{-1} ,

Theory

The nonrelativistic Hamiltonian of the molecular system composed of two electrons (1,2) and two nuclei (A,B) reads

$$\hat{H} = -\frac{1}{2M_A}\nabla_A^2 - \frac{1}{2M_B}\nabla_B^2 - \frac{1}{2m_e}\nabla_1^2 - \frac{1}{2m_e}\nabla_2^2 + \frac{Z_A Z_B}{r_{AB}} + \frac{1}{r_{12}} - \frac{Z_A}{r_{1A}} - \frac{Z_A}{r_{2A}} - \frac{Z_B}{r_{1B}} - \frac{Z_B}{r_{2B}}. \quad (2)$$

The wave function of the state with the rotational quantum number J (and its projection M on the laboratory z-axis) accounts for the coupling between the nuclear and electronic angular momenta and is built of components representing electronic symmetry Σ , Π , Δ , and so on

$$\Psi^{J,M} = \Psi_{\Sigma}^{J,M} + \Psi_{\Pi}^{J,M} + \Psi_{\Delta}^{J,M} + \dots \quad (3)$$

Each component $\Psi_{\Lambda}^{J,M}$ is factored into a spatial 'electronic' function Φ_{Λ}^J , the electronic angular factor $1, \rho^i, (\rho^i \rho^{j'})^{(2)}, \dots$, the nuclear angular part containing the spherical harmonic Y_M^J , and the nuclear radial part containing powers of the internuclear distance R . In particular,

$$\Psi_{\Sigma}^{J,M} = Y_M^J \Phi_{\Sigma}^J, \quad \text{for } J \geq 0 \quad (4)$$

$$\Psi_{\Pi}^{J,M} = \sqrt{\frac{2}{J(J+1)}} R \rho^i (\nabla_R^i Y_M^J) \Phi_{\Pi}^J, \quad \text{for } J \geq 1 \quad (5)$$

$$\Psi_{\Delta}^{J,M} = \sqrt{\frac{4}{(J-1)J(J+1)(J+2)}} R^2 (\rho^i \rho^{j'})^{(2)} \times (\nabla_R^i \nabla_R^j Y_M^J) \Phi_{\Delta}^J, \quad \text{for } J \geq 2 \quad (6)$$

where the following symbols are used

$$(\rho^i \rho^{j'})^{(2)} \equiv \frac{1}{2} (\rho^i \rho^{j'} + \rho^j \rho^{i'}) - (\delta^{ij} - n^i n^j) \vec{\rho} \cdot \vec{\rho}', \quad (7)$$

$\vec{\rho}, \vec{\rho}' \equiv \vec{\rho}_1$ or $\vec{\rho}_2$, $n^i \equiv R^i/R$ and $\rho_a^i = (\delta^{ij} - n^i n^j) r_{ab}^j$. The functions Φ_{Λ}^J are expanded in the basis of four-particle nonadiabatic James-Coolidge (naJC) functions

$$\Phi_{\Lambda}^J = R^J \sum_{\{k\}} c_{\{k\}} (1 + \mathcal{P}_{12}) \phi_{\Lambda\{k\}}^J \quad (8)$$

$$\phi_{\{k\}} = e^{-\alpha R - \beta(\zeta_1 + \zeta_2)} R^{k_0} r_{12}^{k_1} \eta_1^{k_2} \eta_2^{k_3} \zeta_1^{k_4} \zeta_2^{k_5} \quad (9)$$

with $\zeta_1 = r_{1A} + r_{1B}$, $\eta_1 = r_{1A} - r_{1B}$, $\zeta_2 = r_{2A} + r_{2B}$, $\eta_2 = r_{2A} - r_{2B}$, and $\vec{R} = \vec{r}_{AB}$. The α and β in Eq. (9) denote nonlinear variational parameters, common for the whole set of basis functions called 'sector', and k_i are non-negative integers collectively denoted as $\{k\}$. If needed, two or more sectors (with different pairs $\alpha^{(i)}$ and $\beta^{(i)}$) can be used. In Eq. (8), $c_{\{k\}}$ are linear variational parameters and \mathcal{P}_{12} is the electron exchange operator.

The components $\Psi_{\Lambda}^{J,M}$ are mutually orthogonal which enables a perturbative scheme of solving the Schrödinger equation to be

applied. This feature is particularly profitable when large basis sets are in use. Technical details concerning evaluation of matrix elements in the naJC basis, the procedure of solving the generalized symmetric eigenvalue problem, as well as the optimization of the nonlinear parameters, the interested reader will find in Refs. 29 and 30. Here, we shall concentrate on the numerical results and their accuracy.

Results

In order to establish a reliable uncertainty estimation for calculated rovibrational energies we performed a detailed convergence study for individual levels. The size of the basis set was successively increased under the control of the 'shell' parameter Ω . For k_0 fixed at an optimal k_0^{\max} value we included all the basis functions satisfying the condition $\sum_{i=1}^5 k_i \leq \Omega$. Observation of the convergence of energy with Ω allowed the numerical uncertainty and the number of significant digits to be determined. Sample results of such a study for the ground level energy are shown in Table 1. The energy converges regularly with increasing Ω , enabling a firm extrapolation to the infinite basis set size. In general, the energy with 13 stable figures was obtained for all the levels considered here.

Table 1 Convergence of the lowest eigenvalue $E_{0,0}$ (in a.u.) for D_2 with the growing basis set size K . A two-sector wave function was used with optimal $\alpha^{(1)} = \alpha^{(2)} \equiv \alpha$, $\beta^{(1)}$ and $\beta^{(2)}$ parameters. k_0^{\max} powers were fixed at 38 and 21 for sector 1 and 2, respectively.

Ω	α	$\beta^{(1)}$	$\beta^{(2)}$	K	$E_{0,0}$
9	17.96	0.870	2.306	33733	-1.167 168 809 240 572
10	17.95	0.910	2.690	49959	-1.167 168 809 276 440
11	18.02	0.932	3.088	71736	-1.167 168 809 282 247
12	18.06	0.959	3.519	100772	-1.167 168 809 283 632
13	18.06	0.990	3.910	138348	-1.167 168 809 283 929
14	18.06	1.019	4.314	186660	-1.167 168 809 284 013
∞				∞	-1.167 168 809 284 05(4)

Table 2 contains the final nonrelativistic energies for the rovibrational levels (v, J) located up to ca. 8000 cm^{-1} above the ground level. For each level, the corresponding dissociation energy

$$D_{v,J} = 2\mathcal{R} (2E(D) - E_{v,J}),$$

where $2E(D) = -m_e m_d / (m_e + m_d)$, is also supplied. The deuteron-to-electron mass ratio ($m_d/m_e = 3670.482 967 85(13)$) was taken from the 2014 CODATA³¹ compilation while the Rydberg constant ($\mathcal{R} = 109737.31568153(10) \text{ cm}^{-1}$) from Ref. ? as more accurate than the CODATA value ($109737.31568508(65) \text{ cm}^{-1}$). Additionally, this table contains derivatives of the energy with respect to the deuteron-to-electron mass ratio $\mu_d = m_d/m_e$. Knowledge of their values allows the energy results to be corrected later by prospective revisions of μ_d . These derivatives will also be useful in selecting the transitions that are the most sensitive to μ_d variations.

As already mentioned in the Introduction, results of nonadiabatic calculations for rotationless ($J = 0$) energy levels of D_2 exist in literature. The new data reported in this work enable an as-

Table 2 Nonrelativistic eigenvalue ($E_{v,J}$) and dissociation energy ($D_{v,J}$) of the rovibrational energy levels of D_2 located up to ca. 8000cm^{-1} above the ground level. The uncertainties assigned to $E_{v,J}$ and $D_{v,J}$ are due to the numerical convergence only and do not account for uncertainties transferred from the fundamental constants (e.g. $D_{v,J} \delta \mathcal{R} / \mathcal{R} \approx 2 \times 10^{-7} \text{cm}^{-1}$). The last column contains derivatives of the nonrelativistic energy with respect to the deuteron-to-electron mass ratio, μ_d

(v,J)	$E_{v,J}/\text{hartree}$	$D_{v,J}/\text{cm}^{-1}$	$\frac{\partial E_{v,J}}{\partial \mu_d} \cdot 10^6$
(0,0)	-1.16716880928405(4)	36749.09098981(1)	-1.02
(0,1)	-1.16689643235976(4)	36689.31116476(1)	-1.10
(0,2)	-1.16635293028883(4)	36570.02624810(1)	-1.24
(0,3)	-1.16554078662744(4)	36391.78131740(1)	-1.46
(0,4)	-1.16446367747261(4)	36155.38318270(1)	-1.75
(0,5)	-1.1631264144511(2)	35861.88787401(4)	-2.10
(0,6)	-1.1615348720091(2)	35512.58468327(4)	-2.52
(0,7)	-1.1596959015498(2)	35108.97731963(4)	-3.00
(0,8)	-1.1576172352765(1)	34652.76280556(2)	-3.53
(0,9)	-1.1553073827533(2)	34145.80877452(4)	-4.12
(0,10)	-1.1527755231827(2)	33590.12982860(4)	-4.75
(0,11)	-1.1500313962527(2)	32987.86358223(4)	-5.43
(0,12)	-1.1470851941469(1)	32341.24696114(2)	-6.15
(0,13)	-1.1439474569694(3)	31652.59325079(6)	-6.90
(0,14)	-1.1406289734489(3)	30924.27030346(6)	-7.67
(0,15)	-1.1371406883765(3)	30158.68022309(6)	-8.48
(0,16)	-1.1334936178335(2)	29358.24076011(4)	-9.30
(1,0)	-1.15352889637999(5)	33755.47613337(1)	-2.81
(1,1)	-1.15326613332580(4)	33697.80630891(1)	-2.88
(1,2)	-1.15274182922909(5)	33582.73486056(1)	-3.01
(1,3)	-1.15195840834627(5)	33410.79385111(1)	-3.22
(1,4)	-1.15091945841430(4)	33182.77069778(1)	-3.49
(1,5)	-1.1496296743731(2)	32899.69582080(5)	-3.83
(1,6)	-1.1480947866696(2)	32562.82690789(5)	-4.22
(1,7)	-1.1463214767099(2)	32173.63035820(5)	-4.67
(1,8)	-1.1443172823321(1)	31733.76053594(2)	-5.18
(1,9)	-1.1420904963122(2)	31245.03749510(5)	-5.73
(1,10)	-1.1396500608929(2)	30709.42383109(5)	-6.33
(1,11)	-1.1370054611617(2)	30129.00127998(5)	-6.97
(1,12)	-1.1341666198321(1)	29505.94762567(2)	-7.64
(2,0)	-1.14043169661532(4)	30880.97304313(1)	-4.44
(2,1)	-1.14017837963564(5)	30825.37639239(1)	-4.51
(2,2)	-1.13967293901077(5)	30714.44499757(1)	-4.64
(2,3)	-1.13891774189684(5)	30548.69838939(1)	-4.83
(2,4)	-1.13791629102280(5)	30328.90532798(1)	-5.09
(2,5)	-1.1366731692039(2)	30056.07162503(5)	-5.41
(2,6)	-1.1351939687289(2)	29731.42464607(5)	-5.78
(2,7)	-1.1334852082000(2)	29356.39505891(5)	-6.21
(2,8)	-1.1315542397072(1)	28932.59646078(2)	-6.68
(2,9)	-1.1294091493442(2)	28461.80354412(5)	-7.20
(3,0)	-1.1278676783515(5)	28123.48976624(9)	-5.94

assessment of the quality of the results obtained in the past using other methods. In particular, Table 3 presents such a comparison with the variational method of nonadiabatic explicitly correlated Gaussians (naECG) and with the second-order nonadiabatic perturbation theory (NAPT) employing James-Coolidge basis functions. As one can infer from the data, the previously reported energies reached an accuracy of up to 10^{-5}cm^{-1} . It is also evident that the energy error of these two methods grows with increasing vibrational quantum number. This growth is more pronounced in the case of the variational ECG method as illustrated in Figure 1.

The same conclusion can be drawn for H_2 and HD molecules.^{29,30}

The accuracy of the NAPT results for $D_{v,J}$ is limited to $10^{-4} - 10^{-5} \text{cm}^{-1}$ by the lack of the higher order terms. Although the general expressions for the third- and fourth-order NAPT corrections are known²⁸ no direct calculations of these terms have been performed. Hence, the numerical values of the higher order NAPT corrections are unknown. The results reported in this work correspond to the NAPT expansion summed up to infinity, which gives the opportunity to estimate the value of the sum of the higher or-

Table 3 Comparison of the best previous literature data with the non-relativistic dissociation energy $D_{v,J}$ obtained in this work for the lowest rotationless ($J = 0$) levels of D_2

Year and method	$D_{v,0}/\text{cm}^{-1}$	Difference
$v = 0$		
This work	36749.09098981(1)	
2018, 2048-term naECG ²⁴	36749.090970	$2.0 \cdot 10^{-5}$
2015, NAPT ²⁸	36749.090976	$1.3 \cdot 10^{-5}$
2011, 10000-term naECG ²³	36749.090974	$1.6 \cdot 10^{-5}$
$v = 1$		
This work	33755.47613337(1)	
2015, NAPT ²⁸	33755.476098	$3.5 \cdot 10^{-5}$
2011, 10000-term naECG ²³	33755.47603	$1.0 \cdot 10^{-4}$
$v = 2$		
This work	30880.97304313(1)	
2015, NAPT ²⁸	30880.972993	$5.0 \cdot 10^{-5}$
2011, 10000-term naECG ²³	30880.97277	$2.7 \cdot 10^{-4}$
$v = 3$		
This work	28123.48976624(9)	
2015, NAPT ²⁸	28123.489708	$5.8 \cdot 10^{-5}$
2011, 10000-term naECG ²³	28123.48930	$4.7 \cdot 10^{-4}$

der (> 2) NAPT terms. A particular numerical value can be easily obtained by subtracting the NAPT energy reported in Ref. 28 from the fully nonadiabatic energy listed in Table 2. A sample of such data collected for $v = 0, 1, 2$, converted to cm^{-1} , and drawn versus $J(J+1)$, is shown in Fig. 2. As can be seen, the missing higher order NAPT remainder changes almost perfectly proportionally to $J(J+1)$.

Conclusions

The nonrelativistic energy is by far the biggest contribution to the dissociation energy of a vibrational state. For a long time, its uncertainty was also greater than or at best comparable with uncertainties carried by relativistic, QED, and higher order corrections. The accuracy achieved presently for the nonrelativistic energy allows its contribution to be practically removed from the overall uncertainty budget. Meanwhile, the nonadiabatic (recoil) contribution to the relativistic correction⁷ in the deuterium molecule has recently been determined,³³ which significantly diminished the uncertainty of this correction. As a result the dominating uncertainty, which limits the present-day accuracy of the theoretical predictions for rovibrational levels of D_2 , comes from the unknown finite mass effects in the $\sim \alpha^5$ QED correction. The nonadiabatic wave functions obtained in the framework of the present project will be employed in future calculations of the relativistic and QED corrections for the rovibrational levels. The ultimate goal of such plans is to achieve an accuracy sensitive to the deuteron-to-electron mass ratio and to the deuteron charge radius.[?]

Conflicts of interest

There are no conflicts of interest to declare.

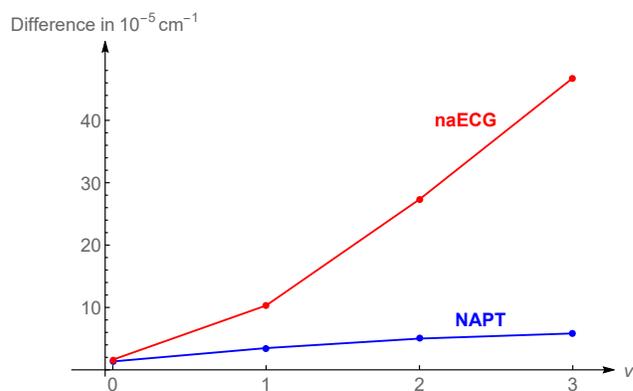


Fig. 1 The difference for the rotationless nonrelativistic energies between the accurate calculations performed here and those obtained using variational naECG method²³ and the second order NAPT³² vs vibrational quantum number v

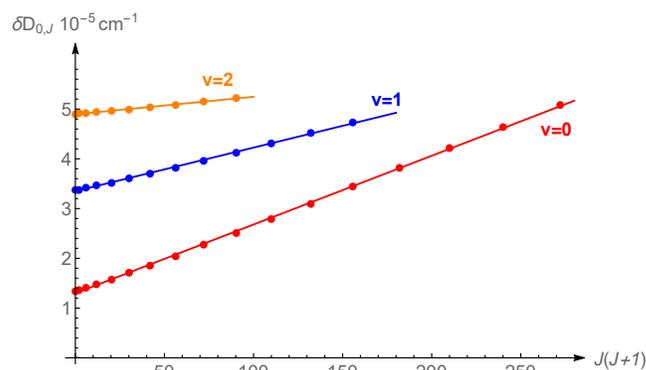


Fig. 2 Dependence of the higher order NAPT remainder $\delta D_{v,J}$ on $J(J+1)$ in the lowest vibrational states ($v = 0, 1, 2$)

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