Testing quantum electrodynamics in the lowest singlet states of beryllium atom

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High-precision results are reported for the energy levels of 2^1S and 2^1P states of the beryllium atom. Calculations are performed using fully correlated Gaussian basis sets and taking into account the relativistic, quantum electrodynamics (QED), and finite nuclear mass effects. Theoretical predictions for the ionization potential of the beryllium ground state $75\,192.699(7)\ \mathrm{cm}^{-1}$ and the $2^1P \to 2^1S$ transition energy $42\,565.441(11)\ \mathrm{cm}^{-1}$ are compared to the known but less accurate experimental values. The accuracy of the four-electron computations approaches that achieved for the three-electron atoms, which enables determination of the nuclear charge radii and precision tests of QED.

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Spectroscopic standards for the energy transitions of the beryllium atom have been established many years ago (1962) in the experiments by Johansson. In most cases the accuracy of the wavelength measurements of 0.01-0.02 Å [1] has been reached. The only more precise beryllium energy level determination comes from the experiment by Bozman *et al.* [2] in which the transition energy of $21\,978.925\ \mathrm{cm}^{-1}$ between the ground and the $2\,^3P_1$ state accurate to about $0.01\ \mathrm{cm}^{-1}$ (0.002 Å) has been measured [3]. Seaton, through a fit to a collection of excited states data, has determined the ionization potential (IP) of the ground state to be $75\,192.56(10)\ \mathrm{cm}^{-1}$ [4]. Later, this quantity has been improved by Beigang *et al.*, who obtained $75\,192.64(6)\ \mathrm{cm}^{-1}$ [5]. Contemporary high precision calculations [6, 7] are in good agreement with the rather old experimental IP values. Nevertheless, the precision of the data available for beryllium is far from being satisfactory compared to the exquisite accuracy of the modern atomic spectroscopy. The level of the absolute precision achieved in modern measurements for three-electron systems [8, 9] is as many as four orders of magnitude higher than that obtained in the case of beryllium. As it has been shown for two- and three-electron atoms, the availability of such accurate data, in connection with good understanding of the underlying atomic theory, opens up access to such interesting applications like the determination of the nuclear charge radius or precision tests of the quantum electrodynamics (QED).

Remarkable advances in theoretical methods make it possible to approach the spectroscopic accuracy for the energies and transition frequencies of few-electron atoms. This challenge requires precise treatment of the electron correlations as well as inclusion of relativistic and quantum electrodynamic effects. The concise approach, which accounts for all the effects beyond the nonrelativistic approximation, is based on the expansion of the energy levels in the fine structure constant α (see Eq. (1) below). This method has been successfully applied in recent years to light atomic and molecular systems [10–13]. The frontiers in this field of research have been established by the calculation of higher order $(m\,\alpha^6)$ corrections to helium energy levels [14] and of $m\,\alpha^7$ corrections to helium fine structure [15].

Up to now, the precision of theoretical predictions for the beryllium states with the non-vanishing angular momentum has been severely limited by the accuracy of the lowest-order relativistic $(m\,\alpha^4)$ and QED $(m\,\alpha^5)$ corrections. The most accurate calculations including the relativistic corrections was performed 20 years ago by Chung and Zhu [16] at the full-core plus correlation level of theory, whereas the QED effects have merely been approximated from hydrogenic formulas [17, 18]. This approach has turned out to be unsatisfactory for it has led to a significant discrepancy between theoretical predictions and experimental excitation energies. For instance, the theoretical result [16] is by $3.45\ \mathrm{cm}^{-1}$ higher than the experimental wavelength value $2\,349.329(10)$ Å of the $2^1P \to 2^1S$ transition energy measured with $0.18\ \mathrm{cm}^{-1}$ uncertainty [1]. The fact that the theoretical excitation energy is higher than the experimental value may indicate that correlation effects have not been incorporated satisfactorily. Such a disagreement can only be resolved in an unequivocally more accurate computation of nonrelativistic energies as well as the relativistic and QED effects using the explicitly correlated wave functions. Recent nonrelativistic calculations of low-lying P- and D-states with the relative precision of an order of 10^{-10}-10^{-11} [19, 20] represent a step in this direction.

In this paper, we present the first complete and highly accurate treatment of the leading relativistic $(m\,\alpha^4)$ and QED $(m\,\alpha^5)$ effects for a four electron atomic P-state. Moreover, we significantly improved numerical results for relativistic and QED effects for the 2^1S state, which permitted us to push the accuracy of the theoretical predictions of the $2^1P \to 2^1S$ transition energy beyond the experimental uncertainty. Additionally, in combination with the previously reported very accurate data on beryllium cation [11], we obtained an improved ionization potential with the accuracy an order of magnitude higher than that of the available experimental values.

In our approach, we expand the total energy not only in the fine structure constant $\alpha \approx 1/137$ but also in the ratio of the reduced electron mass to the nuclear mass $\eta = -\mu/m_N = -m/(m+m_N) \approx 1/16424$. This way we reduce the isotope dependence to the prefactors only. In terms of these two parameters, the energy levels can be represented as the following expansion

$$E = \; m\,\alpha^2\left[\mathcal{E}^{(2,0)}+\eta\,\mathcal{E}^{(2,1)}\right]+m\,\alpha^4\,\mathcal{E}^{(4,0)} \\ +m\,\alpha^5\,\mathcal{E}^{(5,0)}+m\,\alpha^6\,\mathcal{E}^{(6,0)}+\ldots\,. \tag{1}$$

Each dimensionless coefficient $\mathcal{E}^{(m,n)}$ is calculated separately as an expectation value of the corresponding operator with the nonrelativistic wave function. The leading contribution $\mathcal{E}^{(2,0)} \equiv \mathcal{E}_0$ is an eigenvalue of the Schrödinger equation with the clamped nucleus Hamiltonian

$$\mathcal{H}_0\Psi \;=\; \mathcal{E}_0\Psi, \quad \mathcal{H}_0=\sum_a\frac{p_a^2}{2}-\sum_a\frac{Z}{r_a}+\sum_{a>b}\frac{1}{r_{ab}}. \tag{2}$$

The key to obtaining high-precision results is the use of a very accurate trial wave function Ψ, which contains all the inter particle distances explicitly incorporated. We express Ψ as a linear combination of N four-electron basis functions ψ_i

$$\Psi \;=\; \sum_i^N c_i\,\psi_i, \qquad \psi_i=\mathcal{A}[\phi_i(\vec r_1,\vec r_2,\vec r_3,\vec r_4)\,\chi]\,, \tag{3}$$

where $\mathcal{A}$ is the antisymmetry projector, $\chi = \frac{1}{2}\,(\uparrow_1\downarrow_2-\downarrow_1\uparrow_2)\,(\uparrow_3\downarrow_4-\downarrow_3\uparrow_4)$ is the singlet spin function constructed using electron spinors. The spatial function ϕ is the explicitly correlated Gaussian (ECG) function for S- and P-state, respectively

$$\phi_S \;=\; \exp\big[-\sum_a w_a\,r_a^2-\sum_{a<b}u_{ab}\,r_{ab}^2\big], \tag{4}$$

$$\vec\phi_P \;=\; \vec r_1\,\exp\big[-\sum_a w_a\,r_a^2-\sum_{a<b}u_{ab}\,r_{ab}^2\big]. \tag{5}$$

The main advantage of these Gaussian functions is the availability of analytical forms of the integrals required for matrix elements of the Hamiltonian $\mathcal{H}_0$

$$f(n_1,\ldots,n_{10}) \;=\; \int\ldots\int\frac{d^3r_1}{\pi}\ldots\frac{d^3r_4}{\pi}\,r_1^{n_1}\ldots r_4^{n_4} \\ \times r_{12}^{n_5}\ldots r_{34}^{n_{10}}\,\exp\big[-\sum_a\alpha_a\,r_a^2-\sum_{a<b}\beta_{ab}\,r_{ab}^2\big]\,. \tag{6}$$

Among all the integrals represented by the above formula we can distinguish two subsets used in our calculations. The first subset contains the "regular" integrals with the non-negative even integers n_i such that $\sum_i n_i \le \Omega_1$, where the shell parameter $\Omega_1 = 0,2,4,\ldots$. The second subset permits a single odd index $n_i \ge -1$ for which $\sum_i n_i \le \Omega_{1/r}$ ($\Omega_{1/r} = -1,1,3,\ldots$) and is related to the components of the Coulomb potential. To systematize the use of the ECG basis sets we re-derived the recurrence scheme for the generation of both the classes of integrals from the master expression [21, 22]. An advantage of such approach is the possibility of a gradual extension of calculation to the states with higher angular momenta. The sets of integrals employed in a specific case can be characterized using the Ω shell parameters. For instance, the matrix elements of the nonrelativistic Hamiltonian require integrals with $\Omega_1 = 2$, $\Omega_{1/r} = -1$ for S-states (Eq. (4)), and $\Omega_1 = 4$, $\Omega_{1/r} = 1$ for P-states (Eq. (5)). If, additionally, gradients with respect to the nonlinear parameters are to be used, both shell parameters have to be increased by two.

To control the uncertainty of our results we performed the calculations with several basis sets successively increasing their size by a factor of two. From the analysis of convergence we obtained the extrapolated nonrelativistic energies and mean values of the operators presented in Table I. The largest wave functions optimized variationally were composed of 4096 and 6144 terms for the S- and P-state, respectively, leading to the nonrelativistic energies $\mathcal{E}^{(2,0)}(2^1S) = -14.667\,356\,494\,9$ and $\mathcal{E}^{(2,0)}(2^1P) = -14.473\,451\,33\,4$. These upper bounds improve slightly those obtained by Adamowicz *et al.* [7, 19].

The other coefficients of expansion (1) are calculated as mean values with the nonrelativistic wave function Ψ. The nonrelativistic finite mass correction is given by $\mathcal{E}^{(2,1)} = \mathcal{E}^{(2,0)} - \sum_{a<b}\langle\vec p_a\cdot\vec p_b\rangle$. In order to calculate the leading relativistic corrections $\mathcal{E}^{(4,0)} = \langle\mathcal{H}^{(4,0)}\rangle$ we consider the Breit-Pauli Hamiltonian [23], which for the states with vanishing spin can be effectively replaced by the form

$$\mathcal{H}^{(4,0)} \;=\; \sum_a\left[-\frac{\vec p_a^{\,4}}{8}+\frac{\pi\,Z\,\alpha}{2}\,\delta^3(r_a)\right] \\ +\sum_{a<b}\left[\pi\,\delta^3(r_{ab})-\frac{1}{2}\,p_a^i\left(\frac{\delta^{ij}}{r_{ab}}+\frac{r_{ab}^i\,r_{ab}^j}{r_{ab}^3}\right)p_b^j\right]. \tag{7}$$

Since the ECG basis does not reproduce the cusps of the wave function, a slow convergence becomes evident for relativistic matrix elements of the Dirac δ and the kinetic energy operator p_a^4. To speed up the convergence, the singular operators can be transformed into their equivalent forms, whose behavior is less sensitive to the local properties of the wave function. For the Dirac δ expectation value, such a prescription has been proposed by Drachman [24]. For example, from direct calculation with the basis size of 4096 for S-state, we get $\langle\delta(r_a)\rangle = 35.366\,89\ldots$, while using the Drachman regularization approach we improve the convergence by three orders of magnitude (see Table I). Regularization methods have also been applied for the beryllium ground state in the former paper [6], nonetheless the present results are more accurate by 2 orders of magnitude due to the better optimized wave function. For P-states, the expectation values of the relativistic and QED operators as well as of the Bethe logarithm have been unavailable in literature to date. Analogous calculations of relativistic terms in the ECG basis have been performed only for P-states of the four-body positronium molecule [25]. Methods for evaluation of additional integrals "$1/r^2$" and "$1/(r_a r_b)$" of the form (6) required for the regularized operators of the Breit-Pauli Hamiltonian have been developed, resulting in computationally tractable recursive expressions derived from corresponding master integrals. These have been presented in the original paper only for three-body systems [22].

The calculation of the leading QED corrections is the main challenge of this work. It is particularly laborious because we deal with the states of the non-vanishing angular momentum.

TABLE I: Expectation values of various operators with nonrelativistic wave function for 2^1S and 2^1P states of beryllium atom.

Operator	2^1S	2^1P
$\mathcal{H}_0$	$-14.667\,356\,498(3)$	$-14.473\,451\,37(4)$
$\vec{p}_a \cdot \vec{p}_b$	$0.460\,224\,112(8)$	$0.434\,811\,25(13)$
p_a^4	$2\,165.630\,1(9)$	$2\,133.321\,1(12)$
$\delta(r_a)$	$35.369\,002\,6(6)$	$34.897\,914\,6(8)$
$\delta(r_{ab})$	$1.605\,305\,33(9)$	$1.567\,943\,6(2)$
$p_a^i\big(\frac{\delta^{ij}}{r_{ab}}+\frac{r_{ab}^i r_{ab}^j}{r_{ab}^3}\big)p_b^j$	$1.783\,648\,19(15)$	$1.624\,185\,8(5)$
$P(r_{ab}^{-3})$	$-7.326\,766(3)$	$-7.097\,15(8)$
$\ln k_0$	$5.750\,46(2)$	$5.752\,32(8)$

The explicit form of the $m\,\alpha^5$ terms is given by [26, 27]

$$\mathcal{E}^{(5,0)} = \frac{4\,Z}{3}\left[\frac{19}{30}+\ln(\alpha^{-2})-\ln k_0\right]\sum_a\langle\delta^3(r_a)\rangle \qquad (8)$$
$$+\left[\frac{164}{15}+\frac{14}{3}\ln\alpha\right]\sum_{a<b}\langle\delta^3(r_{ab})\rangle-\frac{7}{6\,\pi}\sum_{a<b}\left\langle P\left(\frac{1}{r_{ab}^3}\right)\right\rangle.$$

This expression contains two highly nontrivial terms: the Bethe logarithm $\ln k_0$ and the so-called Araki-Sucher distribution $P(r_{ab}^{-3})$. In ECG basis, the latter exhibits exceptionally slow convergence when evaluated directly from its definition. The regularization is in this case mandatory if one aims at a high accuracy of the final results. For this purpose we extended the original Drachman's idea and obtained the following regularized form for the distribution [28]

$$\left\langle P\left(\frac{1}{r_{ab}^3}\right)\right\rangle = \sum_c\left\langle\vec{p}_c\,\frac{\ln r_{ab}}{r_{ab}}\,\vec{p}_c\right\rangle \qquad (9)$$
$$+\left\langle 4\pi\,(1+\gamma)\,\delta(r_{ab})+2\,(\mathcal{E}_0-V)\,\frac{\ln r_{ab}}{r_{ab}}\right\rangle.$$

As we can see, new classes of the integrals containing factors of the form "$\ln r/r$", "$\ln r/r^2$", "$\ln r_a/(r_a r_b)$" arise. With the master integral, such integrals can be expressed analytically in terms of elementary and Clausen functions.

The evaluation of the Bethe logarithm is the most time consuming part of the calculations. Formulas for such calculations with the ECG functions have been presented in the former work devoted to lithium atom [29] and later on applied to the beryllium ground state [6]

$$\ln k_0 = \frac{1}{D}\int_0^\infty dt\,\frac{f(t)-f_0-f_2t^2}{t^3} \qquad (10)$$
$$f(t) = -\left\langle\vec{P}\,\frac{\omega}{\mathcal{E}_0-\mathcal{H}_0-\omega}\,\vec{P}\right\rangle,\quad t=\frac{1}{\sqrt{1+2\,\omega}}\,,$$
$$D = 2\pi Z\sum_a\langle\delta^3(r_a)\rangle,\ \vec{P}=\sum_a\vec{p}_a\,,$$
$$f_0 = \langle\vec{P}^2\rangle,\ f_2=-2\,.$$

However, for the 2^1P state such calculations become more sophisticated. Compared to the ground state, which through the momentum operator is coupled only with the virtual ${}^1P$ states, the 2^1P state requires a complete set of the ${}^1S$, ${}^1P^e$, and ${}^1D$ intermediate states. These three types of states can be well represented in the bases ϕ_S, $\epsilon^{ijk}\,r_a^j\,r_b^k\,\phi_S$, and $((r_a^i\,r_b^j+r_a^j\,r_b^i)/2-1/3\,\delta^{ij}\,r_a^k\,r_b^k)\,\phi_S$, respectively. Evaluation of $f(t)/\omega$ in the limit of $\omega=0$ is clearly established numerically from the Thomas-Reiche-Kuhn sum rule for dipole oscillator strengths $\langle\vec{P}\,(\mathcal{H}_0-\mathcal{E}_0)^{-1}\,\vec{P}\rangle=3\,Z/2$. This value is useful in judging the completeness of the virtual states and estimation of uncertainties.

Because of principal difficulties, the $m\,\alpha^6$ corrections in their full form were evaluated only for two electron atoms [14]. Therefore, for the four-electron beryllium atom we use the following approximate formula based on the hydrogen atom theory [30]

$$\mathcal{E}^{(6,0)} \approx \pi\,Z^2\left[\frac{427}{96}-2\ln(2)\right]\sum_a\langle\delta^3(r_a)\rangle. \qquad (11)$$

This approximation includes the dominating electron-nucleus one-loop radiative correction and neglects the two-loop radiative, electron-electron radiative, and the higher order relativistic corrections. On the basis of the experience gained in helium calculations [14], we estimate, considering higher charge of the beryllium nucleus, that the neglected terms contribute less than 20% to the overall $m\,\alpha^6$ correction.

TABLE II: Components of the 2^1P-2^1S transition energy and the ionization potential (IP) for ^{9}Be atom in cm^{-1}. CODATA [32] inverse fine structure constant $\alpha^{-1}=137.035\,999\,074(44)$ and the nuclear mass $m_N({}^9\mathrm{Be})=9.012\,182\,20(43)$ u [31].

Operator	2^1P-2^1S	$\mathrm{IP}(2^1S)$
$m\,\alpha^2$	$42\,557.255(6)$	$75\,190.543(4)$
$m\,\alpha^2\,\eta$	$-2.930\,72$	$-4.675\,65$
$m\,\alpha^4$	$12.167(1)$	$7.414\,0(8)$
$m\,\alpha^5$	$-1.003\,3(14)$	$-0.557\,7(3)$
$m\,\alpha^6$	$-0.045(9)$	$-0.025(5)$
Total	$42\,565.441(11)$	$75\,192.699(7)$
Theory [16]	$42\,568.80$	
Theory [7]		$75\,192.667(19)$
Theory [6]		$75\,192.510(80)$
Experiment [1]	$42\,565.35(18)$	
Experiment [4]		$75\,192.50(10)$
Experiment [5]		$75\,192.64(6)$

Except for $\mathcal{E}^{(6,0)}$, all the coefficients of the expansion (1) are evaluated in complete, i.e. no approximation is introduced nor any physical effect of given order is omitted. Therefore, the uncertainties given in Table II refer to the incompleteness of the basis set. On the basis of our former work [11] on Be$^+$, the higher order in α and η contributions, namely $m\,\alpha^2\eta^2$ and $m\,\alpha^4\eta$ are estimated to be less than $0.001\ \mathrm{cm}^{-1}$ to both the transition energy and ionization potential, and thus they are negligible when compared to the present uncertainty of $0.01\ \mathrm{cm}^{-1}$. We note in passing that in Table II for the values without the uncertainty all the quoted digits are certain. In evaluation of the IP value we used the ground state energy level of the beryllium cation $E(\mathrm{Be}^{+}) = -14.325\,836\,7$ a.u. calculated with Hylleraas wave functions [11].

The accuracy of $0.011\ \mathrm{cm}^{-1}$ for the transition $2^1P - 2^1S$ and $0.007\ \mathrm{cm}^{-1}$ for the ionization energy has been achieved due to the recent progress made in two directions. The first one, essential to reach this accuracy, is the improvement in the optimization process of the nonrelativistic wave functions leading to the overall increase in numerical precision. The second direction is the complete treatment of the leading relativistic and QED effects. More specifically, the approach to effectively calculate the many electron Bethe logarithm and mean values of singular operators, like the Araki-Sucher term, has been developed [6]. Particularly, an extension of the numerical methods for relativistic and QED corrections on P-states of a four-electron system is presented here.

The $m\,\alpha^5$ and $m\,\alpha^6$ terms involve the interaction of the electrons with the vacuum fluctuations of electromagnetic field, the electron-positron virtual pair creation, and the retardation of the electron-electron interaction. Results of Table II show clearly that taking into account such energetically subtle QED effects is unavoidable in to reach the agreement between the experiment and the theory and that it enables testing of QED. For example, the overall contribution of the QED effects to the $2^1P - 2^1S$ transition energy amounts to $1.048(9)\ \mathrm{cm}^{-1}$ and is an order of magnitude higher than the experimental uncertainty. Currently, the accuracy reached by theory for the transition frequencies exceeds by an order of magnitude that of the known measurements for beryllium atom. At this level of accuracy we are able to resolve the $2^1P - 2^1S$ line discrepancy of $3.45\ \mathrm{cm}^{-1}$ between the experiment [16] and theory in favor of the latter. Although, the available semi-empirical results of the ionization energy [5] agree well with the more accurate theoretical results obtained here, we hope that the increased level of accuracy of the theoretical predictions will be a stimulus for new, more accurate measurements.

Uncertainty of our results comes mainly from the neglect of the higher order relativistic and QED corrections of the order $\alpha^{6,7}$. Evaluation of these term sets the direction of our future efforts. Also the numerical accuracy of the nonrelativistic energy has to be improved to achieve further progress in theoretical predictions.

The recursive method of evaluation of the integrals (6) employed in this work allows an application of the ECG functions to the states with non-vanishing angular momentum. It establishes a framework for a high accuracy studies of the fine structure and the hyperfine splitting in the beryllium atom. The isotope mass shifts can also be precisely calculated. However, an accurate experimental data are necessary to enable an extraction of a nuclear-model-independent charge radii from isotope shifts by combining high-accuracy measurements with atomic theory. This is of special interest for the halo nuclei (e.g. ^{11}Be) for which analogous results obtained recently from the $2^2P - 2^2S$ transition in beryllium cation [10, 11] require a confirmation. Systematic extension to transition energies involving D-states is mandatory to resolve other severe discrepancies between theory and measurements pointed out by Chung and Zhu [16] like e.g. the largest one of $7.38\ \mathrm{cm}^{-1}$ for the $3^1D - 2^1S$ transition. To our knowledge, no precise calculations of the Bethe logarithm with such nontrivial angular momentum structures have been performed for any few-electron systems so far (even for helium). The methodology presented in this paper opens up a route towards removing such obstacles and, what is more, is very promising in applications to five- and six-electron systems.

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