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Testing quantum electrodynamics in the lowest singlet states of the beryllium atom

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High-precision results are reported for the energy levels of the $2\,^1S$ 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) cm^{-1} and the $2\,^1P \to 2\,^1S$ transition energy 42 565.441(11) cm^{-1} are compared to 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 were established many years ago in 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 cm^{-1} between the ground and the $2\,^3P_1$ state that is accurate to about 0.01 cm^{-1} (0.002 Å) has been measured [3]. Seaton, through a fit to a collection of excited-state data, determined the ionization potential (IP) of the ground state to be 75 192.56(10) cm^{-1} [4]. Later, this quantity was improved by Beigang *et al.*, who obtained 75 192.64(6) 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 superior accuracy of modern atomic spectroscopy. The level of absolute precision achieved in modern measurements for three-electron systems [8,9] is as many as four orders of magnitude higher than that obtained for the case of beryllium. As it has been shown for two- and three-electron atoms, the availability of such accurate data, in connection with a good understanding of the underlying atomic theory, opens up access to interesting applications such as 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 the helium fine structure [15].

Up to now, the precision of theoretical predictions for the beryllium states with a nonvanishing 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 were performed 20 years ago by Chung and Zhu [16] at the full-core plus correlation level of theory, whereas the QED effects have been merely 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 3.45 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 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 a relative precision of an order of 10^{-10}–10^{-11} [19,20] represent a step in this direction.

In this Rapid Communication, we present a 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 improve the numerical results for relativistic and QED effects for the $2\,^1S$ state, which permit 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 data on beryllium cation [11], we obtain an improved ionization potential with an accuracy that is 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, $\eta = -\mu/m_N = -m/(m+m_N) \approx 1/16\,424$. 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:

$$E = m\alpha^2[\mathcal{E}^{(2,0)} + \eta\mathcal{E}^{(2,1)}] + m\alpha^4\mathcal{E}^{(4,0)} + m\alpha^5\mathcal{E}^{(5,0)} + m\alpha^6\mathcal{E}^{(6,0)} + \cdots. \quad (1)$$

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 a clamped nucleus Hamiltonian,

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

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

$$\Psi = \sum_i^N c_i\psi_i, \quad \psi_i = \mathcal{A}[\phi_i(\vec{r}_1,\vec{r}_2,\vec{r}_3,\vec{r}_4)\chi], \quad (3)$$

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

$$\phi_S = \exp\left[-\sum_a w_a r_a^2 - \sum_{a<b} u_{ab} r_{ab}^2\right], \quad (4)$$

$$\vec{\phi}_P = \vec{r}_1 \exp\left[-\sum_a w_a r_a^2 - \sum_{a<b} u_{ab} r_{ab}^2\right]. \quad (5)$$

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

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

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 $\sum_i n_i \leqslant \Omega_1$, where the shell parameter $\Omega_1 = 0, 2, 4, \ldots$. The second subset permits a single odd index $n_i \geqslant -1$ for which $\sum_i n_i \leqslant \Omega_{1/r}$ ($\Omega_{1/r} = -1,1,3,\ldots$) and is related to the components of the Coulomb potential. To systematize the use of the ECG basis sets we rederive the recurrence scheme for the generation of both classes of integrals from the master expression [21,22]. An advantage of such an approach is the possibility of a gradual extension of the calculation to states with higher angular momenta. The sets of integrals employed in a specific case can be characterized by 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 the S states [Eq. (4)] and $\Omega_1 = 4$, $\Omega_{1/r} = 1$ for the 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 2.

TABLE I. Expectation values of various operators with a nonrelativistic wave function for the $2\,^1S$ and $2\,^1P$ states of the 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)
$p_a^i\left(\frac{\delta^{ij}}{r_{ab}} + \frac{r_{ab}^i r_{ab}^j}{r_{ab}^3}\right)p_b^j$	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)

To control the uncertainty of our results we perform the calculations with several basis sets, successively increasing their size by a factor of 2. From the analysis of convergence we obtain 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 states, 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 states with a vanishing spin can be effectively replaced by the form

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

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 a basis size of 4096 for the S state, we get $\langle\delta(r_a)\rangle = 35.366\,89\ldots$, and while using the Drachman regularization approach we improve the convergence by four 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 two 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. Analogous calculations of relativistic terms in the ECG basis have been performed only for the P states of the four-body positronium molecule [25]. Methods for the 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 the 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 Rapid Communication. It is particularly laborious because we deal with the states of the nonvanishing angular momentum. The explicit form of the $m\alpha^5$ terms is given by [26,27]

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

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 the ECG basis, the latter exhibits exceptionally slow convergence when evaluated directly from its definition. The regularization is in this case mandatory if one aims for a high accuracy of the final results. For this purpose we extend Drachman's original idea and obtain the following regularized form for the distribution [28]:

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

As we can see, different classes of the integrals containing factors of the form $\ln r/r$, $\ln r/r^2$, and $\ln r_a/(r_a r_b)$ 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 ECG functions have been presented in the former work devoted to the lithium atom [29] and later on applied to the beryllium ground state [6],

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

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 ^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 $\langle\vec{P}(\mathcal{H}_0 - \mathcal{E}_0)^{-1}\vec{P}\rangle = 3Z/2$. This value is useful in judging the completeness of the virtual states and the estimation of uncertainties.

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

Operator	$2\,^1P$-$2\,^1S$	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)

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]:

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

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 a higher charge of the beryllium nucleus, that the neglected terms contribute less than 20% to the overall $m\alpha^6$ correction.

Except for $\mathcal{E}^{(6,0)}$, all the coefficients of the expansion (1) were evaluated in their full form, i.e., no approximation was introduced nor any physical effect of given order were 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 the α and η contributions, namely, $m\alpha^2\eta^2$ and $m\alpha^4\eta$, are estimated to be less than 0.001 cm^{-1} to both the transition energy and ionization potential, and thus they are negligible when compared to the present uncertainty of 0.01 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 $E(\text{Be}^+) = -14.325\,836\,7$ a.u. calculated with Hylleraas wave functions [11].

The accuracy of 0.011 cm^{-1} for the transition $2\,^1P$-$2\,^1S$ and 0.007 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 the mean values of singular operators, such as the Araki-Sucher term, has been developed [6]. Particularly, an extension of the numerical methods for relativistic and QED corrections on the 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 the electromagnetic field, electron-positron virtual pair creation, and the retardation of the electron-electron interaction. The results of Table II show clearly that taking into account such energetically subtle QED effects is unavoidable in order 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) 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 a beryllium atom. At this level of accuracy we are able to resolve the $2\,^1P$-$2\,^1S$ line discrepancy of 3.45 cm^{-1} between the experiment [16] and theory, in favor of the latter. Although the available semiempirical 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 more accurate measurements.

The uncertainty of our results comes mainly from the neglect of the higher-order relativistic and QED corrections of the order $\alpha^{6,7}$. The evaluation of these terms 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 Rapid Communication allows an application of the ECG functions to the states with a nonvanishing angular momentum. It establishes a framework for highly accurate studies of the fine structure and hyperfine splitting in the beryllium atom. The isotope mass shifts can also be precisely calculated. However, 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. A systematic extension to transition energies involving D states is mandatory to resolve other severe discrepancies between theory and measurements as pointed out by Chung and Zhu [16], such as, e.g., the largest one of 7.38 cm^{-1} for the $3\,^1D$-$2\,^1S$ transition. The methodology presented in this Rapid Communication 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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