Ionization potential of ^{9}Be calculated including nuclear motion and relativistic corrections

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(Received 6 March 2007; revised manuscript received 2 April 2007; published 31 May 2007)

Variational calculations employing explicitly correlated Gaussian functions have been performed for the ground states of ^{9}Be and ^{9}Be$^+$ including the nuclear motion [i.e., without assuming the Born-Oppenheimer (BO) approximation]. An approach based on the analytical energy gradient calculated with respect to the Gaussian exponential parameters was employed, leading to energies of the two systems noticeably improved over those found in the recent paper of Pachucki and Komasa [Phys. Rev. A **73**, 052502 (2006)]. The non-BO wave functions were used to calculate the α^2 relativistic corrections ($\alpha=e^2/\hbar c$). With those corrections and the α^3 and α^4 corrections taken from Pachucki and Komasa, a new value of the ionization potential (IP) of ^{9}Be was determined. It agrees very well with the most recent experimental IP.

DOI: 10.1103/PhysRevA.75.052510 PACS number(s): 31.15.Pf, 31.25.Nj, 31.30.Jv

I. INTRODUCTION

In recent work [1] Pachucki and Komasa reported new variational Born-Oppenheimer (BO) calculations of the two lowest electronic states of *S* symmetry of the Be atom. They also calculated the corrections due to the finite mass of the nucleus, as well as α^2 and α^3 relativistic and QED corrections, and the estimated α^4 correction. In their conclusions, they stated that the main source of error in their estimation of the ionization potential and the lowest transition energy lies in the inaccuracy of their nonrelativistic BO wave functions. Those functions were expanded in terms of four-electron explicitly correlated Gaussian functions whose parameters were variationally optimized. In this work, we make two improvements in the calculation of the nonrelativistic energy of ^{9}Be and ^{9}Be$^+$. First, in our approach we do not assume the BO approximation, and we consider all particles (the electrons and the nucleus) forming the Be atom and the Be cation on equal footing. Second, we use the analytically calculated gradient of the energy with respect to the Gaussian exponential parameters in the variational optimizations of the wave functions. These two features have allowed us to improve the theoretical prediction of the ionization energy of Be. Furthermore, the non-BO wave functions obtained in the present calculations have been used to calculate the α^2 relativistic corrections. Since the non-BO wave functions have been used, those corrections include not only terms due to the motion of the electrons around the center of mass of the atom, but also terms due the motion of the nucleus.

This work features an approach that can be extended to atoms with more than four electrons. This capability does not seem to be possible for the approach that has previously been successfully applied to perform very accurate calculations for the helium and lithium atoms, and which is based on expanding the wave function of the system in terms of Slater-type or Hylleraas-type explicitly correlated functions [2–6]. As demonstrated in the recent work by Morton *et al.* [2], one can achieve an accuracy of the predicted ionization and transition energies that, in some cases, exceeds the accuracy of the present-day experiment by systematically including relativistic and QED corrections to the nonrelativistic energies of the ground and excited states of the helium atom. The new frontier is now to search for an approach that produces results of similar accuracy for larger atoms. One such approach is to use Gaussian-type explicitly correlated functions [7,8]. In this work we test this possibility by performing very accurate calculations of the ionization energy of Be.

Gaussians, in general, are less effective than Slater-type functions in describing the cusp and long-range behaviors of the wave function, but their use leads to much easier integrals that, for a one-center expansion of the wave function, can be analytically calculated using standard procedures. Also, the expression for the total energy can be analytically differentiated easily with respect to the Gaussian exponential parameters, and the energy gradient can be calculated. The use of the gradient significantly improves the efficiency of the variational optimization of the wave function.

In recent years we have used various types of Gaussian basis functions in very accurate atomic and molecular calculations. In those calculations we have employed an approach departing from the Born-Oppenheimer approximation, whose development has been carried out in our research group [9–14]. If the BO approximation is not assumed, the motions of the electrons and the nuclei are treated on equal footing, and since these motions are highly correlated (coupled), one has to use basis functions that explicitly depend on the distances between the particles (nuclei and electrons) in expanding the wave function. The explicitly correlated Gaussians are such functions.

The most recent development of our non-BO approach using Gaussians in very accurate atomic calculations has been the addition of procedures for calculating relativistic corrections in the order of α^2 [15–19]. The corrections include the mass-velocity and Darwin terms, as well as terms due to magnetic orbit-orbit and Fermi contact interactions. In this work we use those procedures.

II. METHOD USED IN THE CALCULATIONS

We consider a system of N particles with masses M_i and charges Q_i $(i=1,\ldots,N)$. In the first step we transform the total nonrelativistic Hamiltonian of the system by separating the center-of-mass motion, thereby reducing the N-particle problem to an n-pseudoparticle problem $(n=N-1)$ described by the internal Hamiltonian H_{int}. In this transformation the laboratory Cartesian coordinate system is replaced by a system whose first three coordinates are the laboratory coordinates of the center of mass, $\mathbf{r}_0$, and the remaining $3n$ coordinates are the Cartesian coordinates in the internal coordinate system whose origin is placed at the nucleus (called the reference particle). The other particles (electrons) are referred to the reference particle using the Cartesian position vectors $\mathbf{r}_i$. The internal Hamiltonian $H_{\rm int}$ is

$$H_{\rm int} = -\frac{1}{2}\left(\sum_{i=1}^{n}\frac{1}{\mu_i}\nabla_{\mathbf{r}_i}^2 + \sum_{i=1}^{n}\sum_{j\neq i}^{n}\frac{1}{M_1}\nabla_{\mathbf{r}_i}\cdot\nabla_{\mathbf{r}_j}\right) + \sum_{i=1}^{n}\frac{q_0 q_i}{r_i} + \sum_{i=1}^{n}\sum_{i<j}^{n}\frac{q_i q_j}{r_{ij}}. \tag{1}$$

The separation of the internal Hamiltonian and the Hamiltonian of the motion of the center of mass is exact. The internal Hamiltonian (1) describes n pseudoparticles with charges $q_i=Q_{i+1}$ and reduced masses $\mu_i=M_1M_{i+1}/(M_1+M_{i+1})$ moving in the central potential of the charge of the reference particle. For Be, the reference particle is the nucleus with the charge $q_0=Q_1=+4$. In this case $N=5$ and the number of pseudoparticles is four $(n=4)$.

^{9}Be is a system that consists of five fermions: four electrons with spin 1/2 and the nucleus with spin 3/2. To describe the relativistic effects in this system, we use the Dirac-Breit Hamiltonian in the Pauli approximation, which suffices for light atoms where the velocities of the electrons are relatively small [18–21]. In the atomic Dirac-Breit-Pauli Hamiltonian, the Darwin correction describing the interaction of the nucleus (with charge Q, spin I, and mass M) with an electron has the following form [22]:

$$\frac{2\pi}{3}\frac{Q}{M^2}(g-1)I(1+\zeta)\delta(\mathbf{r}),$$

where g is the g factor (for the ^{9}Be nucleus it is equal to 0.785 07), and

$$\zeta = \begin{cases} 0 & \text{for an integer spin} \\ \dfrac{1}{4I} & \text{for a half-integer spin.} \end{cases}$$

In the Pauli approximation for states with the S symmetry (these are the states considered in this work for ^{9}Be and ^{9}Be$^+$) and after transformation to the internal coordinate system, the Dirac-Breit-Pauli Hamiltonian has the following form:

$$H_{\rm int}^{\rm rel} = H_{\rm MV} + H_{\rm D} + H_{\rm OO} + H_{\rm SS}, \tag{2}$$

where the mass-velocity term:

$$H_{\rm MV} = -\frac{1}{8}\left[\frac{1}{m_0^3}\left(\sum_{i=1}^{4}\nabla_{\mathbf{r}_i}\right)^4 + \sum_{i=1}^{4}\frac{1}{m_i^3}\nabla_{\mathbf{r}_i}^4\right],$$

the Darwin term:

$$H_{\rm D} = -\frac{\pi}{2}\left(\sum_{i=1}^{4}\frac{1}{m_i^2}q_0 q_i\delta^3(r_i) + \sum_{i=1}^{4}\sum_{j=1,j\neq i}^{4}\frac{1}{m_i^2}q_i q_j\delta^3(r_{ij})\right) + \frac{7\pi}{6}(g-1)\sum_{i=1}^{4}\frac{1}{m_0^2}q_0 q_i\delta^3(r_i),$$

the orbit-orbit term:

$$H_{\rm OO} = -\frac{1}{2}\sum_{i=1}^{4}\frac{q_0 q_i}{m_0 m_i}\left(\frac{1}{r_i}\nabla_{\mathbf{r}_i}\cdot\nabla_{\mathbf{r}_i} + \frac{1}{r_i^3}\mathbf{r}_i\cdot(\mathbf{r}_i\cdot\nabla_{\mathbf{r}_i})\nabla_{\mathbf{r}_i}\right) - \frac{1}{2}\sum_{i=1}^{4}\sum_{j=1,j\neq i}^{4}\frac{q_0 q_i}{m_0 m_i}\left(\frac{1}{r_i}\nabla_{\mathbf{r}_i}\cdot\nabla_{\mathbf{r}_j} + \frac{1}{r_i^3}\mathbf{r}_i\cdot(\mathbf{r}_i\cdot\nabla_{\mathbf{r}_i})\nabla_{\mathbf{r}_j}\right) + \frac{1}{2}\sum_{i=1}^{3}\sum_{j>i}^{4}\frac{q_i q_j}{m_i m_j}\left(\frac{1}{r_{ij}}\nabla_{\mathbf{r}_i}\cdot\nabla_{\mathbf{r}_j} + \frac{1}{r_{ij}^3}\mathbf{r}_{ij}\cdot(\mathbf{r}_{ij}\cdot\nabla_{\mathbf{r}_i})\nabla_{\mathbf{r}_j}\right),$$

and the spin-spin term:

$$H_{\rm SS} = -\frac{8\pi}{3}\sum_{i=1}^{4}\frac{q_0 q_i}{m_0 m_i}(\mathbf{S}_0\cdot\mathbf{S}_i)\delta^3(r_i) - \frac{8\pi}{3}\sum_{j=1}^{4}\sum_{i>j}^{4}\frac{q_i q_j}{m_i m_j}(\mathbf{S}_i\cdot\mathbf{S}_j)\delta^3(r_{ij}),$$

and where in atomic units $q_0=4$, $q_1=q_2=q_3=q_4=-1$, and $m_0=16\,424.2037$, $m_1=m_2=m_3=m_4=1$. In this work we do not consider the electron-nucleus spin-spin interaction because it has a negligibly small effect in comparison with the electron-electron spin-spin interaction.

The general form of the basis function used in this work to calculate states of S symmetry for ^{9}Be and ^{9}Be$^+$ is

$$\phi_k = \exp[-\mathbf{r}'\cdot(L_k L_k'\otimes I_3)\cdot\mathbf{r}], \tag{3}$$

where $\otimes$ is the Kronecker product symbol, $\mathbf{r}$ is the vector of the internal Cartesian coordinates of the four pseudoparticles (for ^{9}Be $\mathbf{r}$ is a 12×1 vector; for Be$^+$ $\mathbf{r}$ it is a 9×1 vector), L_k is the lower triangular matrix of nonlinear variation parameters (for Be L_k is a 4×4 rank-4 matrix and for Be$^+$ L_k is a 3×3 rank-3 matrix), and I_3 is the 3×3 identity matrix. The prime stands for a matrix or vector tranposition. To ensure the proper permutational symmetry of the two electrons, the appropriate symmetry projections are applied to the basis functions. For more details about basis functions (3), transformation to the internal frame, and other technical information, we refer the reader to Refs. [9,10,17].

The wave functions for the ground states of ^{9}Be and ^{9}Be$^+$ have been obtained using the variational method by minimizing the energy with respect to the linear expansion coefficients and with respect to the nonlinear parameters of the

TABLE I. Nonrelativistic and relativistic total ground-state energies of the beryllium atom and beryllium cation and the leading relativistic α^2-dependent corrections: mass-velocity (E_{MV}), Darwin (E_D), spin-spin (E_{SS}), and orbit-orbit (E_{OO}). All numbers are in a.u.

System	Basis size	E_{nonrel}	E_{MV}	E_D	$E_{SS}(e\text{-}e)$	E_{OO}	$\alpha^2 E_{rel}$
$^\infty$Be	3500	−14.6673564044	−270.67823	217.15836	10.09101	−0.89182	-2.3601365×10^{-3}
	4000	−14.6673564232	−270.67430	217.15678	10.09094	−0.89182	-2.3600154×10^{-3}
	4500	−14.6673564360	−270.68155	217.16352	10.09089	−0.89182	-2.3600448×10^{-3}
	5000	−14.6673564456	−270.68163	217.16367	10.09081	−0.89182	-2.3600458×10^{-3}
	5500	−14.6673564527	−270.68192	217.16388	10.09062	−0.89182	-2.3600599×10^{-3}
	6000	−14.6673564586	−270.68119	217.16388	10.09050	−0.89182	-2.3600273×10^{-3}
	6500	−14.6673564631	−270.69105	217.17222	10.09048	−0.89182	-2.3601096×10^{-3}
$^\infty$Be$^+$	2500	−14.3247631657	−268.29522	215.58525	9.93450	−0.90990	-2.3263050×10^{-3}
	3000	−14.3247631687	−268.29784	215.58759	9.93431	−0.90990	-2.3263302×10^{-3}
	3500	−14.3247631708	−268.30100	215.59052	9.93308	−0.90990	-2.3264080×10^{-3}
	4000	−14.3247631724	−268.30116	215.59127	9.93272	−0.90990	-2.3263957×10^{-3}
	4500	−14.3247631735	−268.30772	215.59742	9.93271	−0.90990	-2.3264186×10^{-3}
	5000	−14.3247631744	−268.30788	215.59769	9.93247	−0.90990	-2.3264255×10^{-3}
	5500	−14.3247631749	−268.30766	215.59780	9.93234	−0.90990	-2.3264146×10^{-3}
	6000	−14.3247631754	−268.30768	215.59782	9.93233	−0.90990	-2.3264147×10^{-3}
	6500	−14.3247631757	−268.31010	215.60032	9.93172	−0.90990	-2.3264432×10^{-3}
^{9}Be	2500	−14.6664353592	−270.58956	217.09915	10.08952	−0.91846	-2.3600662×10^{-3}
	3000	−14.6664353966	−270.60975	217.11718	10.08938	−0.91846	-2.3601882×10^{-3}
	3500	−14.6664354225	−270.61126	217.11813	10.08932	−0.91846	-2.3602210×10^{-3}
	4000	−14.6664354412	−270.60734	217.11655	10.08926	−0.91846	-2.3600998×10^{-3}
	4500	−14.6664354540	−270.61458	217.12329	10.08921	−0.91846	-2.3601293×10^{-3}
	5000	−14.6664354637	−270.61467	217.12344	10.08912	−0.91846	-2.3601302×10^{-3}
	5500	−14.6664354707	−270.61495	217.12365	10.08893	−0.91846	-2.3601444×10^{-3}
	6000	−14.6664354766	−270.61423	217.12365	10.08882	−0.91846	-2.3601117×10^{-3}
	6500	−14.6664354811	−270.62409	217.13199	10.08880	−0.91846	-2.3601940×10^{-3}
^{9}Be$^+$	2500	−14.3238634836	−268.22900	215.54544	9.93285	−0.93630	-2.3263924×10^{-3}
	3000	−14.3238634866	−268.23163	215.54778	9.93266	−0.93630	-2.3264176×10^{-3}
	3500	−14.3238634888	−268.23478	215.55071	9.93143	−0.93630	-2.3264954×10^{-3}
	4000	−14.3238634903	−268.23494	215.55146	9.93107	−0.93630	-2.3264830×10^{-3}
	4500	−14.3238634915	−268.24151	215.55761	9.93106	−0.93630	-2.3265060×10^{-3}
	5000	−14.3238634923	−268.24167	215.55787	9.93082	−0.93630	-2.3265128×10^{-3}
	5500	−14.3238634929	−268.24145	215.55799	9.93069	−0.93630	-2.3265019×10^{-3}
	6000	−14.3238634933	−268.24146	215.55801	9.93068	−0.93630	-2.3265020×10^{-3}
	6500	−14.3238634937	−268.24388	215.56051	9.93007	−0.93630	-2.3265304×10^{-3}

basis functions, i.e., the basis set exponent matrices L_k. In the minimization we used the analytically calculated gradient of the Rayleigh quotient,

$$E(\{L_k\},\{c_k\}) = \min_{\{L_k\},\{c_k\}} \frac{c' \cdot H(\{L_k\}) \cdot c}{c' \cdot S(\{L_k\}) \cdot c}$$

with respect to the linear, $\{c_k\}$, and the nonlinear parameters, $\{L_k\}$. In the above expression, $H(\{L_k\})$ and $S(\{L_k\})$ are the Hamiltonian and overlap matrices, respectively. Both are functions of the nonlinear parameters of the basis functions. c is a column vector whose components are c_k. The use of the analytical gradient in the optimizations of the basis function parameters significantly accelerates the optimization process and allows one to achieve high accuracy at a lower computational cost.

III. RESULTS

The results of the calculations are summarized in Tables I and II. In Table I we show how the total energy of Be and Be^+ improves with addition of more functions to the basis set. For each system, two sets of results are presented. The results corresponding to ^{9}Be and $^9Be^+$ have been obtained using the variational minimization of the total energy using the nonrelativistic Hamiltonian (1). We used up to 6500 basis functions for each system. The results shown in Table I correspond to basis sets whose sizes increase incrementally by

TABLE II. Nonrelativistic energies (E_{nonrel}), finite-mass (E_{FM}), α^2 relativistic ($\alpha^2\,E_{\mathrm{rel}}$), and QED corrections ($\alpha^3\,E^{(3)}_{\mathrm{QED}}$ and $\alpha^4\,E^{(4)}_{\mathrm{QED}}$) for Be and Be^+, and the experimental ionization potential values. All numbers are in cm^{-1}.

	Be[a]	Be^{+}[a]	Δ[a]	Be[b]	Be^{+}[b]	Δ[b]
E_{nonrel}	−3218910.521	−3143724.660	−75185.861	−3219112.469(70)	−3143922.112(6)	75190.357(70)
E_{FM}	NA	NA	NA	202.136	197.460	−4.676
$\alpha^2\,E_{\mathrm{rel}}$	−518.003	−510.614	7.388	−518.028(5)	−510.614	7.414(5)
$\alpha^3\,E^{(3)}_{\mathrm{QED}}$				74.576	74.020	−0.557
$\alpha^4\,E^{(4)}_{\mathrm{QED}}$				3.388	3.362	−0.025(5)
E_{tot}[c]	−3219350.559	−3144157.892	75192.667(19)	−3219350.398	−3144157.884	75192.514(80)
Experiment 1[d]			75192.50(10)			
Experiment 2[e]			75192.64(6)			

[a]This work.
[b]Reference [8].
[c]We included QED corrections from [8].
[d]Reference [24].
[e]Reference [25].

500 functions from 2500 to 6500. For each basis set we also performed a calculation with an infinite mass of the Be nucleus. Such calculations are equivalent to calculations where the Born-Oppenheimer approximation is assumed. The calculations where the Be nucleus mass was infinite have been performed with the basis sets taken from the ^{9}Be and $^9Be^+$ calculations, and no additional optimization of the nonlinear parameters was performed. Our previous calculations on atomic systems have shown that adjusting only linear parameters $\{c_k\}$ is sufficient to account for a change of the nuclear mass from its original value of 16 424.2037 a.u. to infinity. The infinite mass energy results obtained in our calculations can be directly compared with the recent BO results of Komasa and Pachucki. Our best result for Be obtained with 6500 basis functions of−14.667 356 463 1 a.u. is noticeably lower than their result of −14.667 355 627 a.u. The improvement is less significant for Be^+. Here our best energy obtained with 6500 basis functions is −14.324 763 175 7 a.u. and their result [23] is −14.324 763 152 a.u.

In Table I we also show the relativistic energy corrections at the order of α^2 calculated in this work and their sum multiplied by α^2 (the entry $\alpha^2\,E_{\mathrm{rel}}$ in the last column in the table). As one can see, the convergence of $\alpha^2\,E_{\mathrm{rel}}$ is quite good, but not as good as for the total nonrelativistic energy. Our α^2 relativistic corrections for ^{9}Be and $^\infty$Be calculated with the 6500-term wave functions of $-2.360\,194\,0\times10^{-3}$ and $-2.360\,109\,6\times10^{-3}$ a.u., respectively, can be compared with the α^2 correction equal to $-2.360\,312\times10^{-3}$ a.u. obtained with the BO wave function reported by Pachucki and Komasa [1]. The values are very similar.

Finally, in Table II we present the calculation of the ionization potential (IP) of Be using the energies obtained in the present calculations, and we compare it both with the calculation performed by Pachucki and Komasa [23] and with the available experimental values. In the first row in the table we list our non-BO total energies of ^{9}Be and $^9Be^+$ and the BO energies of Pachucki and Komasa. The second row contains their finite mass corrections for the two systems. Adding them to the BO energies we get mass-corrected energies that we can directly compare with our non-BO energies. For Be^+ our energy of −3 143 724.660 cm^{-1} agrees well with their energy of −3 143 724.652 cm^{-1}. However, for Be there is an almost 0.2 cm^{-1} difference with our energy equal to −3 218 910.521 cm^{-1} and their energy equal to −3 218 910.333 cm^{-1}. This 0.2 cm^{-1} difference clearly results from the Be BO energy of Pachucki and Komasa not being as well converged as our energy. The difference directly affects the IP calculation, which is described next.

By far the dominant IP contribution comes from the difference of nonrelativistic energies of Be and Be^+. At this level our value is 75 185.861 cm^{-1} and the value of Pachucki and Komasa is 74 185.681 cm^{-1}. Our α^2 relativistic correction to IP differs from their correction by 0.026 cm^{-1}. Since we have not calculated QED corrections of the order of α^3 and α^4 and they did, we used their values to get our final IP estimate. With that, our IP is equal to 75 192.667 cm^{-1}, which can be compared with the final IP of Pachucki and Komasa of 75 192.514 cm^{-1}. The difference between the two values of 0.153 cm^{-1} is significant.

There are two experiments with which we can compare those two values. The earlier experiment of Norcross and Seaton [24] gave the Be IP of 74 192.50(10) cm^{-1}. Nine years later Beigang *et al.* [25] remeasured the Be IP and obtained the value of 75 192.64(6) cm^{-1}. Our result is in better agreement with this latter experiment than with the earlier one. The opposite is the case for the IP obtained by Pachucki and Komasa.

IV. SUMMARY

In this work we have presented a series of calculations leading to the determination of the ionization potential of the Be atom. First we determined the nonrelativistic energies of ^{9}Be and $^9Be^+$ using a variational approach that does not assume the Born-Oppenheimer approximation. In this we differ

with the approach employed earlier by Pachucki and Komasa, where they use the BO energies corrected for the finite mass of the Be nucleus using the perturbation theory. By recalculating the Be and Be^+ energies with the infinite mass of the nucleus we obtained values that we could directly compare to the energies obtained by Pachucki and Komasa. The comparison showed that our nonrelativistic energies are considerably better converged (especially for Be) than theirs. Next we calculated the relativistic corrections of the order of α^2 to the ^{9}Be and $^9Be^+$ energies. To obtain the final estimate for the Be IP we include in our result the QED corrections calculated by Pachucki and Komasa. The value of IP we obtained agrees well with the most recent experimental result obtained by Beigang *et al.* [25].

ACKNOWLEDGMENTS

This work has been supported by the National Science Foundation. We would like to thank Professor Jacek Karwowski, Professor Lutoslaw Wolniewicz, Professor Jacek Komasa, and Professor Krzysztof Pachucki for their valuable suggestions concerning this work. We are grateful to the University of Arizona Center of Computing and Information Technology for the use of their supercomputer resources.

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