Lowest Excitation Energy of ^{9}Be

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Variational calculations employing explicitly correlated Gaussian functions and explicitly including the nuclear motion [i.e., without assuming the Born-Oppenheimer (BO) approximation] have been performed to determine the lowest singlet transition energy in the ^{9}Be atom. The non-BO wave functions were used to calculate the α^2 relativistic corrections ($\alpha = 1/137.035\,999\,679$). With those corrections and with the α^3 and α^4 QED corrections determined previously by others, we obtained 54 677.35 cm^{-1} for the $3^1S \rightarrow 2^1S$ transition energy. This result falls within the error bracket for the experimental transition of 54 677.26(10) cm^{-1}. This is the first time an electronic transition of Be has been calculated from first principles with the experimental accuracy.

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The theoretical calculations on two- and three-electron atomic systems using Slater-type or Hylleraas-type explicitly correlated functions have achieved a very high level of precision matching and, in some instances, have exceeded the precision of the experiment [1–5]. Thus the challenge in very accurate atomic calculations is now shifted to achieving a similar level of accuracy in calculations on atoms with more than three electrons. Though the Slater-type or Hylleraas-type functions very effectively describe the most important features of atomic wave functions, in cases with more than three electrons they lead to difficulties in calculating the Hamiltonian matrix elements, which have not been resolved. In such a situation there has been a search for alternative basis functions for atomic calculations that are efficient in describing atomic states yet easy to use in practical implementations. One of the bases that has been tested are explicitly correlated Gaussian functions (ECGF). The simplicity of the matrix with these types of functions has motivated their use in atomic and molecular calculations since they were first introduced to the field by Boys [6] in the 1960s. However, since Gaussians, in general, are less effective than Slaters or Hylleraas-type functions in describing the cusp and long-range behaviors of the wave function, their use in calculations aiming at a sub-wave-number precision in determining atomic transition energies has not been fully successful. For example, the recent work of Pachucki and Komasa [7] on the lowest transition energy of the berillum atom showed that, despite including several thousand Gaussian in the basis set, the results are still short of the experimental transition by about 0.2 cm^{-1} [8].

In recent years we have also used various types of ECGFs in very accurate variational atomic and molecular calculations performed with an approach where the Born-Oppenheimer (BO) approximation is not assumed [9–14]. Without the BO approximation, the calculations treat the motions of the electrons and the nuclei on equal footing. Hence, the effect of the finite masses of the nuclei (the nucleus for an atomic system) is automatically included in the total energy, and it is not added as a perturbation as is usually done in precise atomic calculations, including those of Pachucki and Komasa for Be [7].

There are three differences in the present calculations in comparison to the standard approach used by others including Pachucki and Komasa. First, our approach includes putting the nuclear motion on equal footing with the electronic motion (the non-BO approach). Second, we use the analytical gradient of the energy calculated with respect to the Gaussian exponential parameters in the variational optimizations of the wave functions. Third, the non-BO wave functions are used to calculate the α^2 relativistic corrections with the algorithms we have recently developed [15–19]; thus those corrections explicitly include the nuclear effects in addition to the electronic effects.

In our view, the significance of this work lies in showing that, with the above-described new features of the method, one can achieve in the calculations employing correlated Gaussians on a four-electron system an accuracy similar to that achieved before in the calculations for two- and three-electron atoms using Slater-type or Hylleraas-type explicitly correlated functions [1–5]. Thus the frontier of very accurate atomic calculations can now be extended, and such quantities as ionization potentials, electron affinities, and transition energies can be determined with the accuracy matching the accuracy of the present day experiment.

^{9}Be is a system consisting of five fermions, four electrons, and the nucleus with spin $3/2$. Let us start with the nonrelativistic Hamiltonian for ^{9}Be after the motion of the center-of-mass motion has been separated out. With this separation, the five-particle problem is reduced to a four-particle problem described by the internal Hamiltonian, H_{int} [9,10]. In our approach we use Cartesian coordinates to describe the internal states of the system. The origin of the internal coordinate system 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, $H_{\rm int}$, for ^{9}Be is

$$H_{\rm int} = -\frac{1}{2}\left(\sum_{i=1}^{4} \frac{1}{\mu_i}\nabla^2_{\mathbf{r}_i} + \sum_{i=1}^{4}\sum_{j\neq i}^{4} \frac{1}{M_1}\nabla_{\mathbf{r}_i}\cdot\nabla_{\mathbf{r}_j}\right) + \sum_{i=1}^{4} \frac{Q_0Q_i}{r_i} + \sum_{i=1}^{3}\sum_{j<i}^{4} \frac{Q_iQ_j}{r_{ij}}, \qquad (1)$$

where $Q_0 = +4$ is the nuclear charge, $Q_1 = Q_2 = Q_3 = Q_4 = -1$ are charges of the electrons, $\mu_i = M_0M_i/(M_0 + M_i)$, $i = 1, \ldots, 4$ are the reduced masses, M_0 is the mass of the nucleus ($M_0 = 16424.2037$ a.u.), and $M_i = 1$ a.u., $i = 1, \ldots, 4$ are the electron masses. The separation of the internal Hamiltonian and the Hamiltonian of the motion of the center-of-mass is exact. The internal Hamiltonian (1) describes the motion of four pseudoparticles (pseudoelectrons) in the central potential of the charge of the nucleus.

To account for the relativistic effects in ^{9}Be, we use the Dirac-Breit Hamiltonian in the Pauli approximation, which suffices for light atoms where the velocities of the electrons are relatively small [20,21]. In this approximation, for states with the S symmetry (these are the states considered in this work for ^{9}Be) and after the transformation to the internal coordinate system, the Dirac-Breit-Pauli Hamiltonian has the following form [15]:

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

where the mass-velocity term

$$H_{\rm MV} = -\frac{1}{8}\left[\frac{1}{M_0^3}\left(\sum_{i=1}^{4}\nabla_{\mathbf{r}_i}\right)^4 + \sum_{i=1}^{4}\frac{1}{M_i^3}\nabla^4_{\mathbf{r}_i}\right],$$

the Darwin term

$$H_D = -\frac{\pi}{2}\left[\sum_{i=1}^{4} \frac{1}{M_i^2}Q_0Q_i\delta^3(r_i) + \sum_{i=1}^{4}\sum_{j=1,j\neq i}^{4} \frac{1}{M_i^2}Q_iQ_j\delta^3(r_{ij})\right] + \frac{14\pi}{3}\sum_{i=1}^{4}\frac{1}{M_0^2}Q_0Q_i\delta^3(r_i),$$

the orbit-orbit term

$$H_{\rm OO} = -\frac{1}{2}\sum_{i=1}^{4}\sum_{j=1}^{4}\frac{Q_0Q_i}{M_0M_i}\left[\frac{1}{r_i}\nabla_{\mathbf{r}_i}\cdot\nabla_{\mathbf{r}_j} + \frac{1}{r_i^3}\mathbf{r}_i\cdot(\mathbf{r}_i\cdot\nabla_{\mathbf{r}_i})\nabla_{\mathbf{r}_j}\right] + \frac{1}{2}\sum_{i=1}^{3}\sum_{j>i}^{4}\frac{Q_iQ_j}{M_iM_j}\left[\frac{1}{r_{ij}}\nabla_{\mathbf{r}_i}\cdot\nabla_{\mathbf{r}_j} + \frac{1}{r_{ij}^3}\mathbf{r}_{ij}\cdot(\mathbf{r}_{ij}\cdot\nabla_{\mathbf{r}_i})\nabla_{\mathbf{r}_j}\right],$$

and the spin-spin term is

$$H_{\rm SS} = -\frac{8\pi}{3}\sum_{i=1}^{4}\frac{Q_0Q_i}{M_0M_i}(\mathbf{S}_0\cdot\mathbf{S}_i)\delta^3(r_i) - \frac{8\pi}{3}\sum_{i=1}^{3}\sum_{j>i}^{4}\frac{Q_iQ_j}{M_iM_j} \times (\mathbf{S}_i\cdot\mathbf{S}_j)\delta^3(r_{ij}).$$

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 gyromagnetic ratio (for the ^{9}Be nucleus it is equal to 0.78507). Parameter ζ is equal to zero for an integer spin and $1/(4I)$ for a half-integer spin. In this work we do not consider the electron-nucleus spin-spin interaction, because it is negligibly small in comparison with the electron-electron spin-spin interaction.

The Gaussian basis functions used in this work to calculate the 2^1S and 3^1S states of ^{9}Be are

$$\phi_k = \exp[-\mathbf{r}'(L_kL_k'\otimes I_3)\mathbf{r}], \qquad (3)$$

where $\otimes$ is the Kronecker product symbol, $\mathbf{r}$ is a vector of the internal Cartesian coordinates of the four pseudoparticles (for ^{9}Be $\mathbf{r}$ is a 12×1 vector), L_k is lower triangular matrix of nonlinear variation parameters (for Be L_k is a 4×4 rank 4 matrix), and I_3 is the 3×3 identity matrix. To ensure the proper permutational symmetry of the electrons, the appropriate symmetry projections are applied to the basis functions.

The wave functions and the corresponding energies of the 2^1S and 3^1S states of ^{9}Be have been obtained using the variational method by minimizing the energy

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

with respect to both linear expansion coefficients, c_k, and the nonlinear parameters of the basis functions, i.e., the basis set exponent matrices, L_k. In the above expression, $H(\{L_k\})$ and $S(\{L_k\})$ are the Hamiltonian and overlap matrices, respectively. Both depend on the nonlinear parameters of the basis functions. c is a column vector whose components are c_k. The variational calculations for the 2^1S and 3^1S states have been performed independently and, for each state, a different Gaussian basis set was generated. The use of the analytical gradient in optimizing the basis functions was key in achieving high accuracy and lowering the computational cost.

The results of the calculations are summarized in Tables I and II. The results in Table I show how the total energy of the ground and the first excited singlet state with the S symmetry (the 2^1S and 3^1S states) converges with the number of basis functions. The ground-state results have been taken from our recent work concerning the calculations of the ionization potential of ^{9}Be [23]. For each state two sets of results are presented. The first set consists of finite-mass results corresponding for ^{9}Be obtained using the variational minimization of the total energy with the nonrelativistic internal Hamiltonian (1). The second set of results was obtained by setting the mass of the Be nucleus to infinity. Such calculations are equivalent to calculations

TABLE I. Nonrelativistic energies, leading relativistic corrections, and the total energies for the ground and the first excited S-state of the beryllium atom. MV, D, SS, and OO stand for mass-velocity, Darwin, spin-spin, and orbit-orbit corrections, respectively. $E_{\rm rel} = E_{\rm MV} + E_{\rm D} + E_{\rm SS}(e-e) + E_{\rm OO}$. All quantities are in hartrees.

System	Basis	$E_{\rm nonrel}$	$\alpha^2 E_{\rm MV}$	$\alpha^2 E_{\rm D}$	$\alpha^2 E_{\rm SS}(e\text{-}e)$	$\alpha^2 E_{\rm OO}$	$\alpha^2 E_{\rm rel}$	$E_{\rm nonrel} + \alpha^2 E_{\rm rel}$
$^\infty$Be, 2^1S	1000	−14.667 354 809 6	−0.014 411 215 9	0.011 560 744 8	0.000 537 652 7	−0.000 047 490 8	−0.002 360 309 2	−14.669 715 118 8
	2000	−14.667 356 236 7	−0.014 412 672 4	0.011 562 683 0	0.000 537 375 3	−0.000 047 490 8	−0.002 360 104 9	−14.669 716 341 6
	3000	−14.667 356 378 5	−0.014 413 901 7	0.011 563 926 2	0.000 537 362 6	−0.000 047 490 8	−0.002 360 103 8	−14.6697164823
	4000	−14.667 356 423 2	−0.014 413 773 3	0.011 563 892 5	0.000 537 356 3	−0.000 047 490 8	−0.002 360 015 4	−14.669 716 438 5
	5000	−14.667 356 445 6	−0.014 414 163 4	0.011 564 259 5	0.000 537 349 0	−0.000 047 490 8	−0.002 360 045 8	−14.669 716 491 4
	6000	−14.667 356 458 6	−0.014 414 140 1	0.011 564 270 8	0.000 537 332 9	−0.000 047 490 8	−0.002 360 027 2	−14.669 716 485 8
$^\infty$Be, 3^1S	1000	−14.418 234 396 4	−0.014 292 282 4	0.011 479 239 1	0.000 530 924 1	−0.000 047 933 2	−0.002 330 052 4	−14.420 564 448 8
	2000	−14.418 239 481 7	−0.014 295 697 0	0.011 483 668 4	0.000 530 197 2	−0.000 047 933 0	−0.002 329 764 3	−14.420 569 246 0
	3000	−14.418 240 029 8	−0.014 296 880 1	0.011 485 031 4	0.000 530 101 6	−0.000 047 933 1	−0.002 329 680 2	−14.420 569 710 0
	4000	−14.418 240 169 9	−0.014 298 387 5	0.011 486 533 1	0.000 530 066 3	−0.000 047 933 1	−0.002 329 721 1	−14.420 569 891 0
	5000	−14.418 240 229 8	−0.014 298 894 2	0.011 487 019 3	0.000 530 056 3	−0.000 047 933 1	−0.002 329 751 7	−14.420 569 981 5
	6000	−14.418 240 261 7	−0.014 298 911 2	0.011 487 055 3	0.000 530 028 9	−0.000 047 933 1	−0.002 329 760 0	−14.420 570 021 7
^{9}Be, 2^1S	1000	−14.666 433 828 1	−0.014 407 650 3	0.011 558 603 1	0.000 537 563 0	−0.000 048 909 7	−0.002 360 393 9	−14.668 794 222 0
	2000	−14.666 435 254 8	−0.014 409 107 0	0.011 560 541 2	0.000 537 285 6	−0.000 048 909 4	−0.0023601896	−14.6687954444
	3000	−14.6664353966	−0.0144103357	0.011 561 783 9	0.000 537 273 0	−0.000 048 909 4	−0.002 360 188 2	−14.668 795 584 8
	4000	−14.666 435 441 2	−0.014 410 207 4	0.011 561 750 3	0.000 537 266 6	−0.000 048 909 4	−0.002 360 099 8	−14.668 795 541 0
	5000	−14.666 435 463 7	−0.014 410 597 6	0.011 562 117 3	0.000 537 259 4	−0.000 048 909 4	−0.002 360 130 2	−14.668 795 593 9
	6000	−14.666 435 476 6	−0.014 410 574 2	0.011 562 128 6	0.000 537 243 3	−0.000 048 909 4	−0.002 360 111 7	−14.668 795 588 3
^{9}Be, 3^1S	1000	−14.417 329 172 5	−0.014 288 753 8	0.011 477 117 6	0.000 530 835 9	−0.000 049 340 5	−0.002 330 140 8	−14.419 659 313 3
	2000	−14.417 334 257 4	−0.014 292 166 7	0.011 481 545 9	0.000 530 109 0	−0.000 049 339 7	−0.002 329 851 5	−14.419 664 108 8
	3000	−14.417 334 805 3	−0.014 293 349 1	0.011 482 908 3	0.000 530 013 5	−0.000 049 339 7	−0.0023297669	−14.4196645722
	4000	−14.417 334 945 3	−0.014 294 856 0	0.011 484 409 7	0.000 529 978 2	−0.000 049 339 6	−0.002 329 807 8	−14.419 664 753 0
	5000	−14.417 335 005 1	−0.014 295 362 9	0.011 484 896 0	0.000 529 968 2	−0.000 049 339 6	−0.002 329 838 3	−14.419 664 843 5
	6000	−14.417 335 037 0	−0.014 295 379 8	0.011 484 932 0	0.000 529 940 8	−0.000 049 339 6	−0.002 329 846 6	−14.419 664 883 6

where the Born-Oppenheimer approximation is assumed. The infinite-mass calculations have been performed with the basis sets taken from the finite-mass ^{9}Be calculations, and no additional optimization of the nonlinear parameters was performed. Our previous calculations on atomic systems have shown that adjusting only linear coefficients of the basis functions is sufficient to account for the change of the nuclear mass from a very large finite value (i.e., 16 424.2037 a.u.) to infinity.

The results shown in Table I correspond to basis sets whose sizes have been increased incrementally by 1000 functions from 1000 to 6000. Upon examining the energy convergence, one can see that the ground state converges faster than the first excited state. This can be expected since the excited-state wave function is more difficult to describe than the ground-state wave function due to a radial node.

The infinite-mass energies obtained here can be directly compared with the recent BO results of Komasa and Pachucki. Our best result for Be obtained with 6000 basis functions of −14.667 356 458 6 a.u. is noticeably lower than their result of −14.667 355 748 a.u. However, the

TABLE II. Nonrelativistic energies ($E_{\rm nonrel}$), finite nuclear mass corrections ($E_{\rm FM}$), relativistic ($\alpha^2 E_{\rm rel}$) corrections, QED corrections ($\alpha^3 E_{\rm QED}^{(3)}$ and $\alpha^4 E_{\rm QED}^{(4)}$), and the total energies ($E_{\rm total}$) for the $2^1S^{\rm a}$ and $3^1S^{\rm a}$ states of Be in comparison with the experiment. All energies in hartrees and transition energies in cm^{-1}.

Quantity	$2^1S^{\rm a}$	$3^1S^{\rm a}$	$\Delta E^{\rm a}$	$2^1S^{\rm b}$	$3^1S^{\rm b}$	$\Delta E^{\rm b}$
$E_{\rm nonrel}$	−14.666 435 477	−14.417 335 037	54 671.227 2(50)	−14.667 355 748	−14.418 236 555	54 675.34(22)
$E_{\rm FM}$	n/a	n/a	n/a	0.000 920 998	0.000 905 240	−3.459(0)
$\alpha^2 E_{\rm rel}$	−0.002 360 112	−0.002 329 847	6.6424(200)	−0.002 360 312	−0.002 331 034	6.43(16)
$\alpha^3 E_{\rm QED}^{(3)}$				0.000 339 785	0.000 337 520	−0.497(1)
$\alpha^4 E_{\rm QED}^{(4)}$				0.000 015 435	0.000 015 330	−0.023(6)
$E_{\rm total}$[c]	−14.668 440 368	−14.419 312 034	54 677.3494(320)	−14.668 439 842	−14.419 309 499	54 677.78(45)
Experiment[d]						54 677.26(10)

[a] This work, computed with 6000 basis functions.

[b] Pachucki and Komasa [7] and private communication.

[c] We included α^3 and α^4 QED corrections from Pachucki and Komasa.

[d] [8].

TABLE III. Convergence of the $3^1S \to 2^1S$ transition energy for Be atom. The results include α^3 and α^4 QED corrections from Pachucki and Komasa.

Basis	ΔE (cm^{-1})
1000	54 678.2721
2000	54 677.4879
3000	54 677.4170
4000	54 677.3677
5000	54 677.3595
6000	54 677.3494

highest improvement was obtained for the first excited states where our infinite-mass energy is $-14.418\,240\,261\,7$ a.u. while their energy was $-14.418\,236\,555$ a.u..

In Table I we also show the relativistic energy corrections in the order of α^2 calculated in this work and their sum multiplied by α^2 (the entry $\alpha^2 E_{\rm rel}$ in the last column in the table). As one can see, the convergence of $\alpha^2 E_{\rm rel}$ is quite good, however not as good as for the total nonrelativistic energy. Our total α^2 relativistic corrections for the two states calculated with the 6000-term wave functions of $-0.002\,360\,112$ a.u. and $-0.002\,329\,847$ a.u., respectively, can be compared with the α^2 corrections of $-0.002\,360\,312$ a.u. and $-0.002\,331\,034$ a.u. obtained with the BO wave functions by Pachucki and Komasa [7]. The values are very similar.

In Table III we present the calculation of the $3^1S \to 2^1S$ transition and a comparison with the results of Pachucki and Komasa [7]. Our final value of the transition energy of 54 677.3494 cm^{-1} was obtained by subtracting our nonrelativistic 2^1S and 3^1S energies obtained with 6000 basis functions, adding the difference between α^2 relativistic corrections of the two states also obtained with the 6000-term wave functions, and adding the α^3 and α^4 QED corrections calculated by Pachucki and Komasa [7] to the result. Our result differs from the result of 54 677.78 cm^{-1} obtained by Pachucki and Komasa [7] by more than 0.4 cm^{-1}. The difference is significant and can be mostly attributed to our nonrelativistic energies of the two states being much better converged than their energies. There is also a smaller contribution to this difference from the improved calculation of the relativistic corrections.

Pachucki and Komasa [7] used the experimental $mP \to nS$ transitions obtained by Johansson [8] to estimate the $3^1S \to 2^1S$ transition. This estimation gave them a value of 54 677.26(10) cm^{-1}. Our result matches this value within the experimental error.

It is interesting to examine the convergence of the transition energy value with the number of the basis functions as shown in Table III. As one can see, the convergence is very good, and the agreement between the calculations and the experiment improves when more functions are added to the basis set. However, at least 6000 functions are needed for the calculations and the experiment to agree within the experimental accuracy. This is the first time such an agreement has been obtained for an electronic transition of the Be atom. However, the calculations also show that a considerable computational effort is required to achieve such a result.

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