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Ground-state energy of beryllium atom with parameter perturbation method*

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We present a perturbation study of the ground-state energy of the beryllium atom by incorporating double parameters in the atom's Hamiltonian. The eigenvalue of the Hamiltonian is then solved with a double-fold perturbation scheme, where the spin–spin interaction of electrons from different shells of the atom is also considered. Calculations show that the obtained ground-state energy is in satisfactory agreement with experiment. It is found that the Coulomb repulsion of the inner-shell electrons enhances the effective nuclear charge seen by the outer-shell electrons, and the shielding effect of the outer-shell electrons to the nucleus is also notable compared with that of the inner-shell electrons.

Keywords: parameter perturbation method, double-fold perturbation scheme, ground-state energy

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1. Introduction

Perturbation theory is widely used for solving a Schrödinger equation that has no exact analytical solution.[1–6] It is well-known that the accuracy of the calculated energies from perturbation theory depends on the magnitude of the perturbation term in the Hamiltonian of the Schrödinger equation. Recently, Zhang *et al.*[7,8] proposed a parameter perturbation method to minimize the influence of the perturbation term and this method gives a good estimate of the ground-state energy for the helium-like atom. To be clear, they reconstruct the non-perturbation and perturbation terms in the Hamiltonian by introducing one parameter in the Hamiltonian, and then deduce the ground state energy with the parameter. Employing the property that the ground-state energy of the system has a minimum energy, the ground-state energy is determined by minimizing it with the parameter.

Although the parameter perturbation method is successful in dealing with the ground-state helium-like atom that has two identical electrons lying in the same orbit, this method needs to be developed to study those atoms with electrons distributed in different orbits, and the spin–spin interaction of electrons from different shells of the atom needs to be properly included. As a first attempt, we proposed the double-parameter perturbation method to study the ground states of lithium-like atoms,[9] which are the simplest multi-shell atoms with three electrons in two different orbits. Calculations show that the double-parameter perturbation method is superior to the one-parameter perturbation method in that it can not only give a ground-state energy in better agreement with experiment, but can also be utilized to study the shielding effect of electrons in different shells of atoms to the nucleus.

In previous work, the shielding effect of inner K-shell electrons in atoms to the nucleus has been thoroughly studied.[1] However, the influence of inner-shell electrons to outer-shell electrons and the shielding effect of outer-shell electrons to the nucleus are not so clear. To elucidate these problems, the beryllium (Be) atom[10] is a simplest representative system studied, since it has just two electrons in the inner K shell and two electrons in the outer L shell. Because of the relative complexity of the Be atom, we employ the double-parameter double-fold perturbation scheme to investigate the ground state of this atom, wherein the spin–spin interaction of electrons from different shells of the atom is elaborately incorporated according to both the Pauli exclusion principle and the exchange symmetry of identical particles.

2. Theory and methods

2.1. Reconstruction of the Hamiltonian

The non-relativistic Hamiltonian of the Be atom, in atomic units, reads

$$H = \sum_{i=1}^{4}\left(-\frac{1}{2}\nabla_i^2 - \frac{Z}{r_i}\right) + \sum_{j>i=1}^{4}\frac{1}{r_{ij}}, \tag{1}$$

where Z is the charge of the nucleus, r_i is the distance between the electron i and the nucleus, and r_{ij} is the distance between the electron i and the electron j. Here, $i = 1,2$ denote the inner K-shell electrons and $i = 3,4$ denote the outer L-shell electrons.

According to the parameter perturbation method, the Hamiltonian can be rewritten as

$$H = H_{\rm a} + H_{\rm b} + H', \tag{2}$$

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where

$$H_{\rm a} = -\frac{1}{2}\nabla_1^2 - \frac{1}{2}\nabla_2^2 - \sigma_{\rm a}\left(\frac{1}{r_1}+\frac{1}{r_2}\right)+\frac{1}{r_{12}}, \tag{3}$$

$$H_{\rm b} = -\frac{1}{2}\nabla_3^2 - \frac{1}{2}\nabla_4^2 - \sigma_{\rm b}\left(\frac{1}{r_3}+\frac{1}{r_4}\right)+\frac{1}{r_{34}}, \tag{4}$$

$$H' = -(Z-\sigma_{\rm a})\left(\frac{1}{r_1}+\frac{1}{r_2}\right)-(Z-\sigma_{\rm b})\left(\frac{1}{r_3}+\frac{1}{r_4}\right) + \left(\frac{1}{r_{13}}+\frac{1}{r_{14}}\right)+\left(\frac{1}{r_{23}}+\frac{1}{r_{24}}\right), \tag{5}$$

where $\sigma_{\rm a}$ and $\sigma_{\rm b}$ are two parameters reflecting the shielding effects of the electrons in different shells to the nucleus. H' is taken as the perturbation term of H, and in the sub-Hamiltonian $H_{\rm a}$ and $H_{\rm b}$, $1/r_{12}$ and $1/r_{34}$ are taken as the perturbation terms of $H_{\rm a}$ and $H_{\rm b}$, respectively.

2.2. Derivation of ground-state energy with perturbation parameters

In the present work, we first determine the energy eigenvalues and eigenfunctions of $H_{\rm a}$ and $H_{\rm b}$ by using perturbation theory. On the basis of these results, we further deduce the energy eigenvalues and eigenfunctions of H with perturbation theory one more time. This is our so-called double-fold perturbation scheme.

Because the structures of $H_{\rm a}$ and $H_{\rm b}$ are similar to that of helium atom's Hamiltonian, the ground-state energies of $H_{\rm a}$ and $H_{\rm b}$ can be easily determined with perturbation theory as we have done for the helium atom.[1] For simplicity, the first-level approximate perturbation theory is adopted in the following calculation. Since in $H_{\rm a}$ the two electrons included are in the 1s states, the eigenfunction of $H_{\rm a}$ reads

$$\psi_{H_{\rm a}} = \phi_{1,0,0}(\boldsymbol{r}_1,\sigma_{\rm a})\,\phi_{1,0,0}(\boldsymbol{r}_2,\sigma_{\rm a}), \tag{6}$$

where

$$\phi_{1,0,0}(\boldsymbol{r},\sigma) = \frac{1}{\sqrt{\pi}}{\rm e}^{-r\sigma}\sigma^{3/2} \tag{7}$$

is the hydrogen atom eigenfunction in the 1s state. Therefore, the corresponding first-level approximate ground-state energy of $H_{\rm a}$ can be written as

$$E_{H_{\rm a}} = E_{H_{\rm a}}^{(0)} + E_{H_{\rm a}}^{(1)}, \tag{8}$$

with

$$\begin{aligned} E_{H_{\rm a}}^{(0)} &= -2\frac{{\sigma_{\rm a}}^2}{2\times 1^2} = -{\sigma_{\rm a}}^2, \\ E_{H_{\rm a}}^{(1)} &= \iint \psi_{H_{\rm a}}^{*}\frac{1}{r_{12}}\psi_{H_{\rm a}}{\rm d}\boldsymbol{r}_1{\rm d}\boldsymbol{r}_2 \\ &= \iint \phi_{1,0,0}(\boldsymbol{r}_1,\sigma_{\rm a})^2\frac{1}{r_{12}}\phi_{1,0,0}(\boldsymbol{r}_2,\sigma_{\rm a})^2{\rm d}\boldsymbol{r}_1{\rm d}\boldsymbol{r}_2 \\ &= 4\pi\int_0^{\infty}\phi_{1,0,0}(\boldsymbol{r}_1,\sigma_{\rm a})^2 \\ &\quad\times\left[2\pi\int_0^{\infty}\int_0^{\pi}\frac{1}{\sqrt{r_1^2+r_2^2-2r_1r_2\cos\theta_2}} \right. \\ &\quad\left.\times\,\phi_{1,0,0}(\boldsymbol{r}_2,\sigma_{\rm a})^2 r_2^2\sin\theta_2\,{\rm d}r_2\,{\rm d}\theta_2\right]r_1^2\,{\rm d}r_1 \\ &= \frac{5\sigma_{\rm a}}{8}, \end{aligned} \tag{9, 10}$$

where the $\boldsymbol{r}_2$ integral is completed first by fixing $\boldsymbol{r}_1$ as the polar axis, and then the $\boldsymbol{r}_1$ integral is done.[1] As for $H_{\rm b}$, because it contains two electrons in the 2s states, the eigenfunction of $H_{\rm b}$ reads

$$\psi_{H_{\rm b}} = \phi_{2,0,0}(\boldsymbol{r}_3,\sigma_{\rm b})\,\phi_{2,0,0}(\boldsymbol{r}_4,\sigma_{\rm b}), \tag{11}$$

where

$$\phi_{2,0,0}(\boldsymbol{r},\sigma) = \frac{1}{2\sqrt{2\pi}}{\rm e}^{-\frac{r\sigma}{2}}\sigma^{3/2}\left(1-\frac{r\sigma}{2}\right), \tag{12}$$

is the hydrogen atom eigenfunction in the 2s state. Hence, the first-level approximate ground-state energy of $H_{\rm b}$ is given by

$$E_{H_{\rm b}} = E_{H_{\rm b}}^{(0)} + E_{H_{\rm b}}^{(1)}, \tag{13}$$

with

$$E_{H_{\rm b}}^{(0)} = -2\frac{{\sigma_{\rm b}}^2}{2\times 2^2} = -\frac{{\sigma_{\rm b}}^2}{4}, \tag{14}$$

$$\begin{aligned} E_{H_{\rm b}}^{(1)} &= \iint \psi_{H_{\rm b}}^{*}\frac{1}{r_{34}}\psi_{H_{\rm b}}{\rm d}\boldsymbol{r}_3{\rm d}\boldsymbol{r}_4 \\ &= \iint \phi_{2,0,0}(\boldsymbol{r}_3,\sigma_{\rm b})^2\frac{1}{r_{34}}\phi_{2,0,0}(\boldsymbol{r}_4,\sigma_{\rm b})^2{\rm d}\boldsymbol{r}_3{\rm d}\boldsymbol{r}_4 \\ &= 4\pi\int_0^{\infty}\phi_{2,0,0}(\boldsymbol{r}_3,\sigma_{\rm b})^2 \\ &\quad\times\left[2\pi\int_0^{\infty}\int_0^{\pi}\frac{1}{\sqrt{r_3^2+r_4^2-2r_3r_4\cos\theta_4}} \right. \\ &\quad\left.\times\,\phi_{2,0,0}(\boldsymbol{r}_4,\sigma_{\rm b})^2 r_4^2\sin\theta_4\,{\rm d}r_4\,{\rm d}\theta_4\right]r_3^2\,{\rm d}r_3 \\ &= \frac{77\sigma_{\rm b}}{512}. \end{aligned} \tag{15}$$

From Eqs. (8) and (13), the zero-level approximate ground-state energy of H can be determined as

$$E_H^{(0)} = \frac{5\sigma_{\rm a}}{8} - \sigma_{\rm a}^2 + \frac{77\sigma_{\rm b}}{512} - \frac{\sigma_{\rm b}^2}{4}, \tag{16}$$

and the corresponding eigenfunction

$$\psi_H = \psi_{H_{\rm a}}\psi_{H_{\rm b}}. \tag{17}$$

The first-order correction to the ground-state energy of H can now be expressed as

$$E_H^{(1)} = \langle\psi_H|H'|\psi_H\rangle = \left\langle\psi_H\right|-(Z-\sigma_{\rm a})\frac{2}{r_1} - (Z-\sigma_{\rm b})\frac{2}{r_3}+\frac{2}{r_{13}}+\frac{2}{r_{23}}\left|\psi_H\right\rangle, \tag{18}$$

where the exchange symmetry between r_1 and r_2 and that between r_3 and r_4 are utilized in the integration. The integration

of the right-hand side of Eq. (18) is expanded into four terms and calculated as follows:

$$\begin{aligned} I_1 &= -(Z-\sigma_a)\left\langle \psi_H \left| \frac{2}{r_1} \right| \psi_H \right\rangle \\ &= -(Z-\sigma_a)\times 4\pi \int_0^\infty \phi_{1,0,0}(\boldsymbol{r}_1,\sigma_a)^2 \frac{2}{r_1} r_1^2 \mathrm{d}r_1 \\ &= 2\sigma_a(-Z+\sigma_a), \end{aligned} \tag{19}$$

$$\begin{aligned} I_3 &= -(Z-\sigma_b)\left\langle \psi_H \left| \frac{2}{r_3} \right| \psi_H \right\rangle \\ &= -(Z-\sigma_b)\times 4\pi \int_0^\infty \phi_{2,0,0}(\boldsymbol{r}_3,\sigma_a)^2 \frac{2}{r_3} r_3^2 \mathrm{d}r_3 \\ &= \frac{1}{2}\sigma_b(-Z+\sigma_b), \end{aligned} \tag{20}$$

$$\begin{aligned} I_{13} &= \left\langle \psi_H \left| \frac{2}{r_{13}} \right| \psi_H \right\rangle \\ &= \iint \phi_{1,0,0}(\boldsymbol{r}_1,\sigma_a)^2 \frac{2}{r_{13}} \phi_{2,0,0}(\boldsymbol{r}_3,\sigma_b)^2 \mathrm{d}\boldsymbol{r}_1 \mathrm{d}\boldsymbol{r}_3 \\ &= 4\pi \int_0^\infty \phi_{1,0,0}(\boldsymbol{r}_1,\sigma_a)^2 \\ &\quad \times \left[2\pi \int_0^\infty \int_0^\pi \frac{2}{\sqrt{r_1^2+r_3^2-2r_1r_3\cos\theta_3}} \right. \\ &\quad \left. \times \phi_{2,0,0}(\boldsymbol{r}_3,\sigma_b)^2 r_3^2 \sin\theta_3 \mathrm{d}r_3 \mathrm{d}\theta_3 \right] r_1^2 \mathrm{d}r_1 \\ &= 2\sigma_a\sigma_b\left(8\sigma_a^4+20\sigma_a^3\sigma_b+12{\sigma_a}^2\sigma_b^2\right. \\ &\quad \left. +10\sigma_a\sigma_b^3+\sigma_b^4\right)(2\sigma_a+\sigma_b)^{-5}, \end{aligned} \tag{21}$$

$$\begin{aligned} I_{23} &= \left\langle \psi_H \left| \frac{2}{r_{23}} \right| \psi_H \right\rangle \\ &= \iint \phi_{1,0,0}(\boldsymbol{r}_2,\sigma_a)^2 \frac{2}{r_{23}} \phi_{2,0,0}(\boldsymbol{r}_3,\sigma_b)^2 \mathrm{d}\boldsymbol{r}_2 \mathrm{d}\boldsymbol{r}_3 \\ &= I_{13}. \end{aligned} \tag{22}$$

Here the orthogonality and normalization properties of the hydrogen atom eigenfunctions are utilized to simplify the integrations in I_1, I_3, I_{13}, and I_{23}. In addition, the exchange symmetry between r_1 and r_2 is applied to obtain the result of I_{23}.

Employing the results of Eqs. (19)–(22), the sum of Eqs. (16) and (18) gives the first-level approximate ground-state energy of H as

$$\begin{aligned} E_H &= \frac{5\sigma_a}{8} - \sigma_a^2 + 2\sigma_a(-Z+\sigma_a) \\ &\quad + \frac{77\sigma_b}{512} - \frac{\sigma_b^2}{4} + \frac{1}{2}\sigma_b(-Z+\sigma_b) \\ &\quad + 4\sigma_a\sigma_b(8\sigma_a^4+20\sigma_a^3\sigma_b+12\sigma_a^2\sigma_b^2 \\ &\quad + 10\sigma_a\sigma_b^3+\sigma_b^4)(2\sigma_a+\sigma_b)^{-5}. \end{aligned} \tag{23}$$

2.3. Spin–spin interaction correction of electrons to the ground-state energy

As is known, the electron spin–spin interaction would lead to direct integration and exchange integration. The direct integration is included in the above calculation, but the exchange integration is not. Obviously, providing an analytic expression for the exchange integration is a key for incorporating the spin–spin interaction correction. According to the Pauli exclusion principle, the electrons in the same orbital state must have opposite spins. So, for the Be atom, the two 1s electrons have opposite spins, and the two 2s electrons also have opposite spins. Due to the exchange symmetry of identical particles, the exchange of the 1s electron and 2s electron with the same spin direction would not change the quantum state. Without loss of generality, we let the spins of electrons 1 and 3 in the Be atom be up, and the other electrons be down, then we can write the exchange integration correction to the ground-state energy as follows:

$$\begin{aligned} E_J &= -\left[\left\langle \phi_{1,0,0}(\boldsymbol{r}_1,\sigma_a)\phi_{2,0,0}(\boldsymbol{r}_3,\sigma_b) \right| \right. \\ &\quad \left. \frac{1}{r_{13}} \left| \phi_{1,0,0}(\boldsymbol{r}_3,\sigma_a)\phi_{2,0,0}(\boldsymbol{r}_1,\sigma_b) \right\rangle \right. \\ &\quad + \left\langle \phi_{1,0,0}(\boldsymbol{r}_2,\sigma_a)\phi_{2,0,0}(\boldsymbol{r}_4,\sigma_b) \right| \\ &\quad \left. \frac{1}{r_{24}} \left| \phi_{1,0,0}(\boldsymbol{r}_4,\sigma_a)\phi_{2,0,0}(\boldsymbol{r}_2,\sigma_b) \right\rangle \right] \\ &= -2\left\langle \phi_{1,0,0}(\boldsymbol{r}_1,\sigma_a)\phi_{2,0,0}(\boldsymbol{r}_3,\sigma_b) \right| \\ &\quad \frac{1}{r_{13}} \left| \phi_{1,0,0}(\boldsymbol{r}_3,\sigma_a)\phi_{2,0,0}(\boldsymbol{r}_1,\sigma_b) \right\rangle \\ &= -32\sigma_a^3\sigma_b^3\left(20\sigma_a^2-30\sigma_a\sigma_b+13\sigma_b^2\right) \\ &\quad (2\sigma_a+\sigma_b)^{-7}. \end{aligned} \tag{24}$$

2.4. The final ground-state energy expression

Combining Eqs. (23) and (24), the ground state energy of the Be atom with perturbation parameters reads

$$\begin{aligned} E_{gs} &= E_H + E_J = \frac{5\sigma_a}{8} - \sigma_a^2 + 2\sigma_a(-Z+\sigma_a) \\ &\quad + \frac{77\sigma_b}{512} - \frac{\sigma_b^2}{4} + \frac{1}{2}\sigma_b(-Z+\sigma_b) \\ &\quad + 4\left(8\sigma_a^5\sigma_b+20\sigma_a^4\sigma_b^2+12\sigma_a^3\sigma_b^3+10\sigma_a^2\sigma_b^4+\sigma_a\sigma_b^5\right) \\ &\quad \times (2\sigma_a+\sigma_b)^{-5} - 32\sigma_a^3\sigma_b^3 \\ &\quad \times \left(20\sigma_a^2-30\sigma_a\sigma_b+13\sigma_b^2\right)(2\sigma_a+\sigma_b)^{-7}. \end{aligned} \tag{25}$$

3. Results and discussion

The ground-state energy of the Be atom is obtained by minimizing Eq. (25) with respect to perturbation parameters σ_a and σ_b using the Broyden–Fletcher–Goldfarb–Shanno algorithm written in Fortran,[11] where the starter parameter values of σ_a and σ_b are selected around the bottom of the function of E_{gs} (see Fig. 1).

Calculations show that when $\sigma_a = 3.681$ and $\sigma_b = 2.140$, the Be atom has a ground-state energy of -14.698 Hartree. This value is very close to the experimental value[12] of

-14.668 Hartree within a relative error of $E_r = 0.2\%$, indicating that our theoretical scheme is feasible and satisfactory.

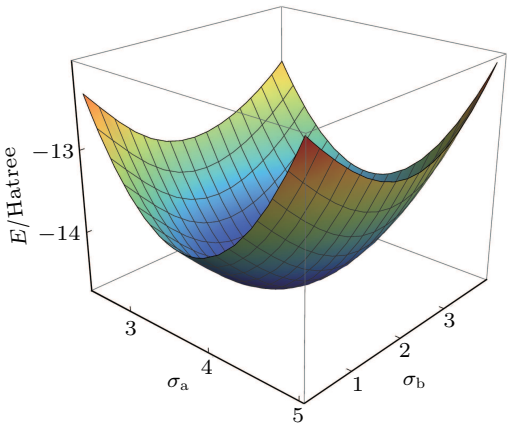


Fig. 1. (color online) Three-dimensional plot of the ground-state energy of the Be atom with perturbation parameters.

To further reveal the role of the double-parameter perturbation and spin–spin interaction correction, we also perform three kinds of calculations to obtain the ground-state energy of the Be atom: (i) with double-parameter perturbation but without incorporating the spin–spin interaction correction; (ii) with non-parameter perturbation ($\sigma_a = \sigma_b = Z$) and incorporating the spin–spin interaction correction; (iii) with non-parameter perturbation ($\sigma_a = \sigma_b = Z$) but without incorporating the spin–spin interaction correction. The corresponding ground-state energies are evaluated to be -14.488 Hartree, -13.716 Hartree, and -13.540 Hartree, and their relative errors with experiment are 1.2%, 6.5%, and 7.7%, respectively.

We can see that for the double-parameter perturbation calculation without the spin–spin interaction correction, the error is six times that of E_r, implying that including the spin–spin interaction correction can significantly improve the accuracy of the calculated energy. In addition, for the non-parameter perturbation calculation, whether considering the spin–spin interaction correction or not, the error is about an order of magnitude larger than E_r. By comparison, we can find that the double-parameter perturbation scheme is essential for us to obtain a relatively accurate ground-state energy for the Be atom.

In the following, we further discuss the shielding effect of electrons in atoms to the nucleus. According to the double-parameter perturbation calculation with spin–spin interaction correction, $\sigma_a = 3.681$, which indicates that the 1s electron in the Be atom feels an effective nuclear charge that is smaller than the nuclear charge of 4 by about 0.319. Obviously, the shielding effect of the 1s electrons is similar to that shown in the Helium atom.[1] Therefore, it is natural to think that the 2s electron in the Be atom would feel an effective charge smaller than 2 due to the net effect of the 1s electrons and the nucleus. However, calculations show that σ_b has a value of 2.140 that is larger than 2. This can be explained as follows, though unexpected at first glance. Although the electron cloud in the same shell can shield the nucleus charge, the Coulomb repulsion of the electrons would lift the effective charge seen by the outer-shell electrons. To rule out the influence of the interaction between the 2s electrons, we also perform similar calculations for the ground-state Be^+. The obtained $\sigma_b = 2.412$ is indeed larger than 2.

Moreover, the numerical difference of σ_bs for Be and Be^+ atoms also implies that, due to the shielding effect of the 2s electron to the nucleus in the Be atom, the effective nuclear charge that the 2s electron feels decreases by 0.272. This decrease is close to the corresponding value of 0.319 for the 1s electron. Therefore, the shielding effect of the 2s electrons to the nucleus in the Be atom remains as noticeable as that of the 1s electrons.

4. Conclusion

We have performed a parameter perturbation investigation of the ground-state energy in the beryllium atom by a double-parameter double-fold perturbation scheme. The calculated ground-state energy is in good agreement with experiment within a relative error of 0.2%. We find that the Coulomb repulsion of the inner-shell electrons enhances the effective nuclear charge seen by the outer-shell electrons and the shielding effect of the outer-shell electrons to the nucleus is also notable compared with that of the inner-shell electrons. The present work not only shows the advantage of the parameter perturbation method in studying many-electron atoms, but also deepens our understanding of the influence of the electron to the electron and the nucleus in atoms.

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