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Application of variational Monte Carlo method to the confined helium atom

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Abstract

A new application of variational Monte Carlo method is presented to study the helium atom under the compression effect of a spherical box with radius (r_c). The ground-state energies of the helium atom were calculated for different values of r_c. Our calculations were extended to include Li^+ and Be^{2+} ions. The calculations were based on the use of a compact accurate trial wave function with five variational parameters. To optimize variational parameters, we used the steepest descent method. The obtained results are in good agreement with previous results.

Keywords: Variational Monte Carlo method, Helium atom, Compression effect

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Background

Confined atoms are excellent examples of how problems in theoretical physics can be rediscovered from time to time and modified in the light of experiment. Confined atoms were initially considered from two rather different perspectives: first is the study of atoms under extremely high pressures; the second, the nature of atoms inside a solid. The confinement of a particle in a potential is of course a problem of quantum mechanics.

Scientists have paid great attention to study the atoms and molecules under different compression regimes. This is due to the existence of several application problems in physics and chemistry such as atoms trapped in cavities, in zeolite channels [1,2], or encapsulated in hollow cages of carbon-based nano-materials such as endohedral fullerenes [3,4]. The models of confined atomic and molecular systems have also found applications in the analysis of the so-called artificial atoms or quantum dots [5,6] due to their relevance in technological applications. The spherically enclosed atoms represent a model that has been applied in the analysis of several confined systems with different methodologies where compression is simulated through hard or soft walls. For the hydrogen atom, which is the simplest atom, Michels et al. [7] presented a simple physical model to study the hydrogen atom in an impenetrable spherical cavity to study the effect of pressure on hydrogen atom and how the dipole static polarizability responds to an applied external pressure. In this model, the boundary condition that the wave function vanishes at $r = r_c$ (where r_c is the radius of impenetrable spherical box) is imposed on the solution of the Schrödinger equation. Various physical properties of the confined hydrogen atom, such as the modification of their atomic orbitals, energy levels, the filling of electronic shells, and linear and nonlinear polarizability, have been studied [8]. Goldman and Joslin [9] computed the spectroscopic properties of the hydrogen atom confined in a spherical impenetrable wall and found strong compression-induced changes in the emission frequencies and intensity shifts.

For many-electron atoms, many researchers studied the effect of confinement by an impenetrable as well as non-impenetrable spherical box [10-12]. Most of the studies have especially considered the case of the helium atom as it is considered the simplest system of the few-body system and is ideal in the study of electronic correlation effects as a function of the cavity dimension into which they are embedded. On the other hand, the confined version of this atom provides a lucid way to study the effect of confinement on electron correlation which arises due to the Coulomb interaction between the two

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electrons. Ten Seldam and de Groot [13] studied variationally box size effects on ground-state energy and polarizability of the compressed helium atom by means of Hylleraas-type wave functions where a cutoff factor is added. Rivelino and Vianna [14] utilized a spatially confined linear combination of configuration interaction functions to calculate the compressed helium atom ground state, whereas Marin and Cruz [15,16] computed it under conditions of impenetrable and penetrable confinement by means of products of uncorrelated exponential functions and a cutoff factor. Furthermore, calculations are carried out using the Rayleigh-Ritz variational method together with the modified Hylleraas-type wave function (Hylleraas-type wave functions multiplied with appropriate cutoff factor) to study helium ground-state energies and some averages, and their evolution with the size of the spherical box [11]. Besides the variational method, self-consistent Hartree-Fock [17] configuration interaction [18] and quantum Monte Carlo [10] methods have also been used to study the properties of helium atom and several isoelectronic ions confined in an impenetrable spherical box. An important study has been presented to calculate the compression effects in helium-like atoms (Z = 1,. . ., 5) constrained by hard spherical walls [19]. In the work of Banerjee et al. [20], the three low-lying excited states of confined helium atom centered in an impenetrable spherical box have been calculated by employing the variational method with two-parameter variational forms for the correlated two-particle wave function. Wen-Fang [21] presented a description of the helium atom under spherical parabolic confinement potential using the adiabatic hyperspherical method. The obtained results proved that the energies of a spherical parabolic well are in good agreement with those of an impenetrable spherical box for the larger confined potential radius. The conclusion of this study states that the confinement may cause accidental degeneracies between levels with different low excited states and the inversion of the energy values. As an extension to this study, and in order to obtain a better understanding of the features of the ground and low excited states of confined helium, Wen-Fang introduced calculations of the energy spectrum of the ground and low-lying excited states in a non-impenetrable spherical box (i.e., a spherical Gaussian potential well) using the exact diagonalization method [22]. Recently, Laughlin et. al. [23] used Hylleraas-type basis functions, which include the interelectronic distance or r_{12}, to perform accurate calculations for the ground-state energies of a helium atom confined at the center of a spherical cavity, in both cases, penetrable and impenetrable cavities. The presented calculations and results for the ground-state energies of the atom confined by Gaussian and harmonic penetrable potentials can be considered to be the most reliable that has been obtained so far. The strong confinement case of the helium atom which is embedded in a spherical box with impenetrable walls was studied in the work of Montgomery et al. [24]. In this study, the time-independent Schrödinger equation was solved using the first-order Rayleigh-Schrödinger perturbation theory, and then calculations were extended using the fifth-order variational perturbation theory. The results show that these approaches provide good alternative approaches for the calculation of ground-state energy for a strongly confined helium atom. In the study of Wilson et al. [25], radial, angular, and total correlation energies are calculated for four two-electron systems with atomic numbers Z = 0, 1, 2, and 3 confined within an impenetrable sphere of radius (R). It was proven that for small R, the correlation energies approach limiting values that are independent of Z, while at intermediate R, systems with $Z \geq 1$ exhibit a characteristic maximum in the correlation energy that resulted from an increase in the angular correlation energy which is offset by a decrease in the radial correlation energy.

In our previous work, we used variational Monte Carlo (VMC) method to calculate both ground and excited states of the helium atom [26] as well as lithium atom and its isoelectronic ions up to Z = 10 [27]. Our results proved that VMC method can successfully describe helium and lithium atoms. From this point, the present paper aims to study the helium atom under compression effects using VMC method which has not been employed before to describe this case. Also, we will extend our calculations to include some helium-like atoms, namely Li^+ and Be^{2+}.

Trial wave function

Our calculations for the ground state of the confined helium atom and its isoelectronic ions are based on the use of a highly compact wave function that has a clear physical meaning and satisfies all the boundary conditions; this wave function was proposed firstly in a previous study [28] and is given by the following:

$$\psi(r_1, r_2, r_{12}) = \left(1 + \hat{\boldsymbol{P}}\right) \exp\left(\frac{a_1 r_1 + b_1 r_1^2}{1 + r_1}\right) \times \exp\left(\frac{a_2 r_2 + b_2 r_2^2}{1 + r_2}\right) \exp\left(\frac{d r_{12}}{1 + e r_{12}}\right) \tag{1}$$

Where a_1,a_2,b_1,b_2,d and e are variational parameters. A revision in this wave function is the following functional form: $\exp\left(\frac{ar+br^2}{1+2}\right)$ which helps in satisfying Kato's cusp conditions, which have been stressed in the construction of an accurate wave function in the past. This wave function was used to calculate the ground-state energy for the He atom and He-like isoelectronic ions for Z = 1 – 10, and the results obtained were better than those of previous works for compact wave functions for

two-electron systems. Here, we discuss the validity of using this compact wave function to study the compression effects in helium-like atoms constrained in hard spherical walls. In this way, we can introduce the wave function Ψ combining with the boundary condition imposed by the confining potential in the following form:

$$\psi(r_1, r_2, r_{12}) = \left(1 + \hat{\boldsymbol{P}}\right) \exp\left(\frac{a_1 r_1 + b_1 r_1^2}{1 + r_1}\right) \times \exp\left(\frac{a_2 r_2 + b_2 r_2^2}{1 + r_2}\right) \exp\left(\frac{d r_{12}}{1 + e r_{12}}\right) \times \left(1 - \frac{r^2{}_1}{r^2{}_c}\right)\left(1 - \frac{r_2{}^2}{r_c{}^2}\right) \quad (2)$$

The presence of the cutoff factor $\left(1 - \frac{r_1{}^2}{r_c{}^2}\right)\left(1 - \frac{r^2{}_2}{r^2{}_c}\right)$ is to guarantee that the boundary condition Ψ=0 where $r_1 = r_c$ or $r_2 = r_c$ is satisfied [20]. Here, r_c refers to the spherical box radius. The variational parameters appearing in the wave function are optimized using the steepest descent (SD) method.

Method and calculations

In this paper, we shall use the well-known variational Monte Carlo method which is based on a combination of two ideas, namely the variational principal and the Monte Carlo evaluation of integrals, using importance sampling based on the Metropolis algorithm [29]. According to the VMC method, the expectation value of any operator $\hat{A}$ is calculated as follows [30]:

$$\left\langle \hat{A} \right\rangle = \frac{\int \psi_T^*(\boldsymbol{R}) \hat{A}\, \psi_T(\boldsymbol{R}) d\boldsymbol{R}}{\int \psi_T^*(\boldsymbol{R}) \psi_T(\boldsymbol{R}) d\boldsymbol{R}}, \quad (3)$$

Where Ψ_T is a trial wave function and R is the 3N-dimensional vector of the electron coordinates. In particular, if the operator $\hat{A}$ is the Hamiltonian $\hat{H}$, then its expectation value will be the variational energy E_{VMC}. According to the variational principle, a trial wave function for a given state must produce an energy which is above the exact value of that state, that is, $E_{\mathrm{VMC}} \geq E_{\mathrm{exact}}$. Variational Monte Carlo calculations determine E_{VMC} by writing it as follows:

$$\left\langle \hat{H} \right\rangle = E_{VMC} = \int P(\boldsymbol{R}) E_L(\boldsymbol{R}) d(\boldsymbol{R}),$$

where

$$P(\boldsymbol{R}) = \frac{|\psi_T(\boldsymbol{R})|^2}{\int |\psi_T(\boldsymbol{R})|^2 d\boldsymbol{R}}$$

is positive everywhere and interpreted as a probability distribution, and $E_L = \frac{\hat{H}\psi_T}{\psi_T}$ is the local energy function. The value of E_L is evaluated using a series of points, $\mathbf{R}_{ij}$, which is proportional to $P(\boldsymbol{R})$. After a sufficient number of evaluations, the VMC estimate of E_{VMC} will be as follows:

$$E_{VMC} = \langle E_L \rangle = \lim_{N\to\infty} \lim_{M\to\infty} \frac{1}{N}\frac{1}{M} \sum_{j=1}^{N} \sum_{i=1}^{M} E_L(\boldsymbol{R}_{ij}), \quad (4)$$

where M is the ensemble size of random numbers {R_1, R_1,....., R_M} and N is the number of ensembles. With a chosen trial wave function, an explicit expression can be worked out for the local energy $E_L(\mathbf{R})$ E in terms of the values and derivatives of Ψ.

The non-relativistic Schrödinger equation for confined two-electron helium-like systems with nuclear charge Z can be written as (in atomic units) the following form [20]:

$$H = -\frac{1}{2}\sum_{l=1}^{2} \nabla_i^2 + \nu_N(r_1, r_2) + \nu_C(r_1, r_2) + \nu_{conf}(r_1, r_2), \quad (5)$$

Where ν_N is the following nuclear potential:

$$\nu_N(r_1, r_2) = -\frac{z}{r_1} - \frac{z}{r_2},$$

And ν_C represents the Coulomb repulsion between the electrons:

$$\nu_C(r_1, r_2) = \frac{1}{r_{12}},$$

and the confining potential $\nu_{conf}(r_1, r_2)$ due to an impenetrable spherical box of radius r_c is given by the following:

$$\nu_{conf}(r_1, r_2) = \begin{cases} 0, & r_1, r_1 < r_c \\ \infty, & r_1, r_1 \geq r_c. \end{cases} \quad (6)$$

In our calculations, we use the form of H in Hylleraas coordinates [31]:

$$H = -\frac{1}{2}\left(\frac{\partial^2}{\partial r_1^2} + \frac{2}{r_1}\frac{\partial}{\partial r_1} + \frac{\partial^2}{\partial r_{12}^2} \quad \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}} + 2\hat{r}_1.\hat{r}_{12}\frac{\partial^2}{\partial r_1 \partial r_{12}} + \frac{\partial^2}{\partial r_2^2} + \frac{2}{r_2}\frac{\partial}{\partial r_2} + \frac{\partial^2}{\partial r_{12}^2} + \frac{2}{r_{12}}\frac{\partial}{\partial r_{12}} - 2\hat{r}_2.\hat{r}_{12}\frac{\partial^2}{\partial r_2 \partial r_{12}}\right) + \nu_N(r_1, r_2) + \nu_C(r_1, r_2) + \nu_{conf}(r_1, r_2). \quad (7)$$

The electronic eigenvalue is determined from the following Schrödinger equation:

Table 1 Energies for the ground state of confined helium atom as functions of the spherical box radius

r_c	Present work	Flores-Riveros and Rodríguez-Contreras [19]	Ludeña and Gregori [18]	Montgomery et al. [24]
0.5	22.70203	22.7413	22.7437	22.741303
0.6	13.31194	13.3182	13.3204	13.318127
0.8	4.640665	4.6104	4.6125	4.610408
1.2	−0.708609	−0.7088	−0.7070	−0.708802
1.4	−1.616875	−1.6173	−1.6156	−1.617330
1.8	−2.4223	−2.4245	−2.4230	-
2.5	−2.820202	−2.8078	-	-
3.5	−2.890474	−2.8936	-	-
4	−2.894997	−2.9004	−2.8988	−2.900534
5	−2.903886	−2.9034	−2.9020	−2.903408
6	−2.903460	−2.9037	−2.9024	−2.903650

All values are in atomic units.

$$H\psi(r_1, r_2, r_{12}) = E\psi(r_1, r_2, r_{12}) \tag{8}$$

Our goal now is to solve the six-dimensional partial differential eigenvalues (Equation 8) for the lowest eigenvalue.

In order to get accurate values for the five variational parameters a_1, a_2, b_1, b_2, and e, we will use the SD method [32], which is considered as one of the most popular methods to optimize the wave function for Monte Carlo methods. On the other hand, the variational parameter d will be determined using cusp conditions [33] which ensure that the local energy E_L is finite. When the two electrons become closer to the nucleus, then it can be easily verified that $d = \frac{1}{2}$.

The main merit of the SD method is its simplicity which can turn it into an efficient method at least for simple atoms. This method was presented recently, and it was shown that the implementation of the SD method in the direct approach of energy minimization yields good results. In this work, we shall use the SD method to optimize the variational parameters using energy minimization scheme.

To use the SD method, we start by choosing initial values for the five parameters a_1, b_1, a_2, b_2, and d and then iteratively update the values of the parameters according to the following relation:

$$\boldsymbol{c}^{k+1} = \boldsymbol{c}^k - a\boldsymbol{g}^k, \tag{9}$$

where the vector $c = (c_1, c_1 \ldots c_m)$ denotes the parameters in the wave function; k is the iteration step, and α denotes the constant of the SD method. In Equation 9, $\mathbf{g}^k$, is defined as the gradient vector of energy with respect to the parameters, and it is given as follows:

$$\boldsymbol{g} = \left(\frac{\partial E}{\partial C_1}, \frac{\partial E}{\partial C_1}, \ldots, \frac{\partial E}{\partial C_m}\right) \tag{10}$$

The energy gradient vector is computed according to the following relation [34]:

$$\frac{\partial E}{\partial C_m} = \lim_{N\to\infty} \frac{2}{N} \sum_{s=1}^{N} \left\{ \left(E_L \times \frac{\partial \psi}{\partial C_m}\right)_s - E \times \left(\frac{\partial \psi}{\partial C_m}\right)_s \right\} \tag{11}$$

We then proceed with some iterations of Equation 9 until we obtain the optimum values of the parameters and the variational energy approach to the desired value. Normally taking five to six iterations, the variational parameters should have reached the vicinity of their ultimate values. Using the obtained values of variational parameters, the energy will be calculated with a large number of Monte Carlo points.

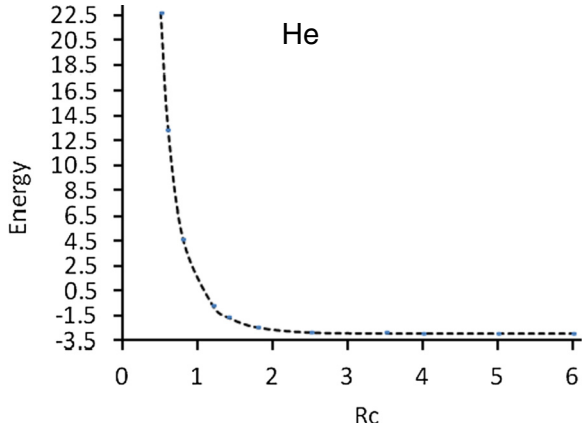

Figure 1 The ground state energy of the helium atom versus the spherical box radius r_c.

Table 2 Energies for the ground state of confined Li^+ as functions of the spherical box radius

r_c	Present work	Flores-Riveros and Rodríguez-Contreras [19]	Ludeña and Gregori [18]
0.5	11.76771	11.7768	11.7790
0.6	3.9934290	3.9262	3.9284
0.8	−2.893898	−2.8632	−2.8612
1.2	−6.407358	−6.4065	−6.4047
1.4	−6.855290	−6.8732	−6.8713
1.8	−7.192726	−7.1906	−7.1880
2.5	−7.258839	−7.2740	-
3.5	−7.279050	−7.2798	-
4	−7.279230	−7.2799	−7.2783
5	−7.279254	−7.2799	−7.2784
6	−7.279253	−7.2799	−7.2784

All values are in atomic units.

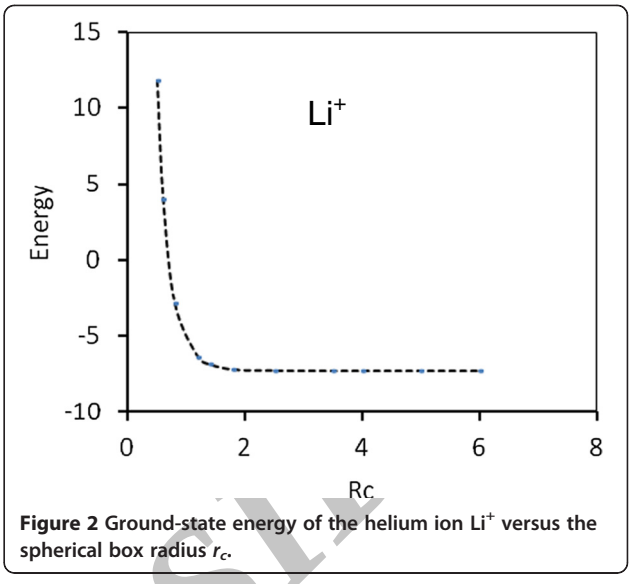

Figure 2 Ground-state energy of the helium ion Li^+ versus the spherical box radius r_c.

Results and discussion

In this paper, we present a new application of the well-known variational Monte Carlo method to study the confined helium atom. The ground states of the confined helium atoms, Li^+ and Be^{2+}, were calculated for different radii r_c. All energies are obtained in atomic units (i.e., $h=e=m_e=1h$) with a set of 10^6 Monte Carlo points to make the statistical error as low as possible. In Table 1, we displayed the results obtained for the ground state of the helium atom ($Z = 2$) together with the corresponding results available in the literature and the most recent results. The obtained energies were calculated for a wide range of values of r_c. The small values of the spherical box radius r_c describe the case of strong confinement where for large values of $r_c \geq 3.5$, the compression effect becomes not noticeable, and the energy is nearly stable and approaches the corresponding exact value. It is clear that our results are in good agreement with previous data. Figure 1 represents the energy of the ground state of helium as a function of the radius r_c. Also, Figure 1 insures the fact that the energy of the low-lying states in a confined quantum charged system is determined by a competition of confinement kinetic energy and Coulomb interaction energy. As the atoms are compressed, they become constrained in a diminishing spherical box such that, according to the quantum mechanical uncertainty principle, the electrons increase their momentum and thereby leading to a net gathering of kinetic energy. In other words, the smaller the confined potential radius r_c is, the higher the confinement kinetic energy. When the increase in the confinement kinetic energy becomes predominant and cannot be compensated by the increase of the Coulomb attractive energy, the energies of the

Table 3 Energies for the ground state of confined Be^{2+} as functions of the spherical box radius

r_c	Present work	Flores-Riveros and Rodríguez-Contreras [19]	Ludeña and Gregori [18]
0.5	0.10801980	0.1056	0.1078
0.6	−6.288159	−6.2423	−6.2402
0.8	−11.26839	−11.2679	−11.2658
1.2	−13.36396	−13.3733	−13.3701
1.4	−13.556580	−13.5590	−13.5552
1.8	−13.639290	−13.6449	−13.6415
2.5	−13.654130	−13.6553	-
3.5	−13.655678	−13.6555	-
4	−13.65640	−13.6555	−13.6539
5	−13.657630	−13.6555	−13.6519
6	−13.65781	−13.6555	−13.6539

All values are in atomic units.

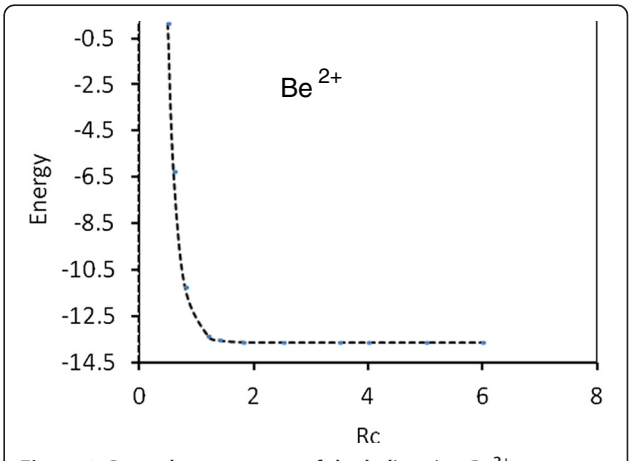

Figure 3 Ground-state energy of the helium ion Be^{2+} versus the spherical box radius r_c.

confined helium atom increase. Tables 2 and 3 display the results concerning the confined Li^+ ($Z = 3$) and Be^{2+} ($Z = 4$), respectively, for various values of r_c as well as the available previous values in order to check the accuracy of our results. It is clear that our results for helium ions ($Z = 3, 4$) are slightly different than the previous data for small radii $r_c \leq 1.8$. This may be attributed to the trial wave functions used in previous works [18,19], which are especially well suited to describe strongly compressed atoms. This is not the case for large values of r_c where our results exhibit good accuracy compared with those data. Figures 2 and 3 show graphically the behavior of the energy of the confined atom versus the spherical box radius r_c. In fact, when the nuclear charge is increased, the Coulomb attraction between the nucleus and the electron becomes stronger which keeps the electrons moving ever closer to the nucleus and then leads to a more compact atom. It is clear that the rate of energy increase speeds up as the nuclear charge of the atom increases, so when the effective confinement regions become narrower for the most compact species, the rate of energy increase speeds up for atoms of higher nuclear charge.

Conclusions

The well-known VMC method was employed to study the helium atom which is compressed by a spherical box. For various values of the spherical box radii, we have calculated the energies for both helium and its isoelectronic ions, Li^+ and Be^{2+}. We considered the case of small values of r_c, which describe the strong compression, as well as the case of large values of r_c. In both cases, our results exhibit good accuracy compared with previous values using different methods and different forms of trial wave functions. We then can conclude that VMC techniques can describe the compression effect for helium and its ions successfully.

Competing interests

The authors declare that they have no competing interests.

Authors' contributions

The two authors - SBD and FNEG - contributed equally in all steps of the present paper. Both authors read and approved the final manuscript.

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