

Ground State Energy of the Beryllium Atom Using Variational Monte Carlo Method

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Abstract

The variational Monte Carlo method is applied to calculate the ground state energy eigenvalues and eigenfunctions of the beryllium atom. In the computations which have been carried out, we used trial wave functions in the form of the Slater determinant multiplied by a correlation function corresponding to the interactions between the electrons. Two different types of correlation functions are used in the calculations. Good results are obtained for the ground state energy eigenvalues in comparison with the exact values and previous findings.

Keywords: Beryllium atom; variational Monte Carlo method; trial wave functions; correlation functions.

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1. Introduction

Recently, there are many approximate methods which are concerned with the solutions of the Schrödinger equation of the many-electron systems, especially for few electron atoms. Among these methods are: the variational method [1], the perturbation method [2], the Hartree–Fock (HF) method [3], the ab initio HF (RHF) method [4], the configuration interaction (CI) method [5], which is a post-HF linear variational method, the diffusion Monte Carlo method [6], and the variational Monte Carlo (VMC) method [7]. The VMC method has proved its proficiency in many calculations of atoms and molecules. The VMC method is based on incorporating the variational principle and the estimation of high-dimensional integrals by sampling the integrands using a set of randomly generated points. The integrals converge faster using the VMC technique than more conventional techniques based on sampling the integrands on a regular grid for problems involving more than a few dimensions. Moreover, the statistical error in the estimate of the integral decreases as the square root of the number of points sampled, irrespective of the dimensionality of the problem. For this reason, many studies are presented to study atomic and molecular properties by using the VMC method. We will shed light on the most important ones as follow:

A. D Sañu-Ginarte et al. [8] calculated the ground and first excited states of beryllium by using the direct variational method and considering the systematic asymmetric nature of the trial wave function. They added a cutoff function to ensure confinement boundary conditions and built up the trial wave function from hydrogenic functions. It is of interest to notice that the authors of [8] ignored the interaction between the electrons because they did not use correlation functions. On the other hand, F. Wu and L. Meng [9] applied the perturbation theory to the ground-state energy of the beryllium atom by incorporating

double parameters in the atom's Hamiltonian. The eigenvalues of the Hamiltonian were then gotten with a double-fold perturbation scheme, where the spin-spin interaction of electrons from different shells of the atom was also considered. Their calculations showed that the obtained ground-state energy was in satisfactory agreement with the experimental result. Also, it was 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 was also notable compared with that of the inner-shell electrons.

S. B. Doma et al. [10] applied the VMC method to investigate the total energies of the excited states of the helium atom. The strong magnetic field effect on the energy is also investigated and illustrated graphically in that paper. Their results were in good agreement with the most recent, accurate, and exact values. C. J. Umrigar, M. P. Nightingale, and K. J. Runge [11] proposed modifications to the simple diffusion Monte Carlo algorithm that greatly reduces the time-step error. The improved algorithm had a time-step error smaller by a factor of 70 to 300 in the energy of Be, Li₂, and Ne. For other observables the improvement was already larger. The possible effective time step with the improved algorithm was typically a factor of a few hundred larger than the time step used in the Green's function Monte Carlo domain. They also presented an optimized 109 parameter trial wave function for Be, which was used in combination with their algorithm. An exceedingly accurate ground state energy was obtained. Also, Doma et al. [12] used the VMC method to calculate the 1¹0⁺ state energies, the derivatives of the total energy and the ionization energies of the helium atom, and hydrogen negative ion in the presence of the magnetic field regime between 0 and 10 a. u. Their calculations were based on using two types of compact and accurate trial wave functions, which are used before to calculate energies in the absence of the magnetic field. The results were in good agreement with the most recent previous accurate values and the exact values. Moreover, S. A. Alexander et al. [13] used the VMC method with the features of 118 trial wave function forms for selected ground and excited states of helium, lithium, and beryllium atoms to determine which characteristics give the most rapid convergence toward the exact nonrelativistic energy. They found that fully antisymmetric functions are more accurate than those which use determinants, that exponential functions are more accurate than linear ones. Furthermore, Doma et al. [14] applied the VMC method to investigate the ground state and some excited states of the lithium atom and its ions up to $Z = 10$ in the existence of an external magnetic field regime with $\gamma = 0 \sim 100$ a. u. The effect of increasing field strength on the ground state energy was studied, and precise values for the crossover field strength were obtained. Their calculations were based on using accurate forms of trial wave functions, which were put forward in calculating energies in the absence of the magnetic field. Furthermore, the value of γ at which the ground-state energy of the lithium atom approaches to zero was calculated. The obtained results were in good agreement with the most recent values and with the exact values. In another application of the VMC method to light molecules, S. B. Doma et al. [15] applied this method to evaluate the ground-state energy of a confined hydrogen molecule H₂. They got results that were in good agreement with the most recent values and with the exact values. Also, S. B. Doma et al. [16] used VMC method to calculate the binding energies of the hydrogen molecule and its molecular ion in the presence of an aligned magnetic field regime between 0 and 10 a. u. Their calculations were based on using two types of compact and accurate trial wave functions,

which were put forward for consideration in calculating energies in the absence of a magnetic field. Finally, Alexei M. Frolov et al. [17] developed a variational method, which allows one to construct very compact and relatively accurate wave functions for the four-electron atomic systems. Moreover, in contrast with other methods their procedure is relatively simple in applications and can be used for an arbitrary four-electron atomic system. Their obtained results were in good agreement with the most recent values and with the exact values.

In the present paper, we applied the VMC method to compute the ground-state energy of the beryllium atom. Accordingly, we constructed the trial wave functions using the Slater determinant (SLD) with two different correlation functions.

2. The Hamiltonian of the System

The nonrelativistic Hamiltonian in the infinite nuclear mass approximation for four electrons in the field of a nucleus of charge Z (in Hartree atomic units) is given by:

$$H = -\frac{1}{2}\sum_{i=1}^4 \nabla_i^2 - \sum_{i=1}^4 \frac{Z}{r_i} + \sum_{i<j}^4 \frac{1}{r_{ij}}, \quad (2.1)$$

where ∇_i is the 3-vector of the momentum of the i^{th} electron, Z is the nuclear charge ($Z = 4$), r_i is the distance between the i^{th} electron and the Be nucleus, and r_{ij} is the distance between the i^{th} and the j^{th} electrons. It is convenient to transform the kinetic energy part of Eq. (2.1) into mutually independent distance coordinates, r_i, r_{ij} , and the functions of the polar angles of the electrons of the nucleus, θ_i and ϕ_i . The general Hamiltonian in Hylleraas coordinates is [18]:

$$\begin{aligned} H = & \frac{-1}{2} \sum_{i=1}^4 \frac{\partial^2}{\partial r_i^2} - \sum_{i=1}^4 \frac{1}{r_i} \frac{\partial}{\partial r_i} - \sum_{i=1}^4 \frac{Z}{r_i} + \sum_{i<j}^4 \frac{1}{r_{ij}} - \sum_{i<j}^4 \frac{\partial^2}{\partial r_{ij}^2} \\ & - \sum_{i<j}^4 \frac{2}{r_{ij}} \frac{\partial}{\partial r_{ij}} - \frac{1}{2} \sum_{i \neq j}^4 \frac{r_i^2 + r_{ij}^2 - r_j^2}{r_i r_{ij}} \frac{\partial^2}{\partial r_i \partial r_{ij}} - \frac{1}{2} \sum_{i \neq j}^4 \sum_{k>j}^4 \frac{r_{ij}^2 + r_{ik}^2 - r_{jk}^2}{r_{ij} r_{ik}} \frac{\partial^2}{\partial r_{ij} \partial r_{ik}} \\ & - \frac{1}{2} \sum_{i=1}^4 \frac{1}{r_i^2} \frac{\partial^2}{\partial \theta_i^2} - \frac{1}{2} \sum_{i=1}^4 \frac{1}{r_i^2 \sin^2(\theta_i)} \frac{\partial^2}{\partial \phi_i^2} - \frac{1}{2} \sum_{i=1}^4 \frac{\cot(\theta_i)}{r_i^2} \frac{\partial}{\partial \theta_i} \\ & - \sum_{1 \neq j}^4 \left(\frac{r_j \cos(\theta_j)}{r_i r_{ij} \sin(\theta_i)} + \frac{1}{2} \cot(\theta_i) \frac{r_{ij}^2 - r_i^2 - r_j^2}{r_i^2 r_{ij}} \right) \frac{\partial^2}{\partial \theta_i \partial r_{ij}} \\ & - \sum_{i \neq j}^4 \frac{r_j \sin(\theta_j)}{r_i r_{ij} \sin(\theta_i)} \sin(\phi_i - \phi_j) \frac{\partial^2}{\partial \phi_i \partial r_{ij}} \end{aligned} \quad (2.2)$$

3. Method of the Calculations and the Trial Wave Functions

Our calculations are based on using the VMC method, which is regarded as one of the most important tools in studying atoms and molecules. It is built on a combination of two ideas; namely: the variational principle and the Monte Carlo evaluation of integrals using importance sampling based on the Metropolis algorithm. The VMC method is utilized to compute the quantum expectation values of an operator with a given trial wave function.

Given a Hamiltonian operator and a trial wave function, it is then possible to calculate the least energy eigenvalues of a given state of an atom with respect to the parameters of the used trial wave function, as explained briefly in Doma et al. previous works [10], [12], [14], [15], [16].

The ground state trial wave function for the Be atom may be symbolically written in the form

$$\psi(\text{Be}) = \psi_0 f(r_{12}, r_{13}, r_{14}, r_{23}, r_{24}, r_{34}) \quad (3.1)$$

where ψ_0 is the SLD function, and f is the correlation function due to the interactions between the electrons. If we neglect the interactions between the electrons, then the ground-state trial wave function of beryllium, with total spin $S = 0$ and its z-component $S_z = 0$ may be symbolically denoted by

$$\psi_0 = \frac{1}{\sqrt{4!}} \begin{vmatrix} 1s(1)\alpha(1) & 1s(1)\beta(1) & 2s(1)\alpha(1) & 2s(1)\beta(1) \\ 1s(2)\alpha(2) & 1s(2)\beta(2) & 2s(2)\alpha(2) & 2s(2)\beta(2) \\ 1s(3)\alpha(3) & 1s(3)\beta(3) & 2s(3)\alpha(3) & 2s(3)\beta(3) \\ 1s(4)\alpha(4) & 1s(4)\beta(4) & 2s(4)\alpha(4) & 2s(4)\beta(4) \end{vmatrix} \quad (3.2)$$

where $\alpha(i)$ represent spin-up functions and $\beta(i)$ represent spin down-functions of the i^{th} -electron. The functions $1s(i)$ and $2s(i)$ stand for the orbital functions of the states $(n, \ell) = (1, 0)$ and $(2, 0)$ of the i^{th} -electron, respectively. In the calculations we used two types of orbital functions: the first is the hydrogenic function, and the second is a modified hydrogenic function. As is well-known, the hydrogenic function constitutes an enough basis for energy calculation.

By some simple algebra and substituting for the hydrogen wave functions $1s(i)$ and $2s(i)$ in atomic units we get

$$\begin{aligned} \psi_0 = & \frac{1}{\sqrt{4!}} \left(\frac{Z'^6}{8\pi^2} \right) \left\{ \alpha(1)\beta(2)\alpha(3)\beta(4) \left[e^{-\frac{(2r_1+2r_2+r_3+r_4)Z'}{2}} \left(1 - \frac{r_3Z'}{2} \right) \left(1 - \frac{r_4Z'}{2} \right) - \right. \right. \\ & e^{-\frac{(2r_1+r_2+2r_3+2r_4)Z'}{2}} \left(1 - \frac{r_3Z'}{2} \right) \left(1 - \frac{r_2Z'}{2} \right) - e^{-\frac{(r_1+2r_2+2r_3+r_4)Z'}{2}} \left(1 - \frac{r_1Z'}{2} \right) \left(1 - \frac{r_4Z'}{2} \right) + \\ & \left. e^{-\frac{(r_1+r_2+2r_3+2r_4)Z'}{2}} \left(1 - \frac{r_1Z'}{2} \right) \left(1 - \frac{r_2Z'}{2} \right) \right] + \alpha(1)\beta(2)\beta(3)\alpha(4) \left[e^{-\frac{(2r_1+r_2+2r_3+r_4)Z'}{2}} \left(1 - \right. \right. \\ & \left. \frac{r_2Z'}{2} \right) \left(1 - \frac{r_4Z'}{2} \right) - e^{-\frac{(2r_1+2r_2+r_3+r_4)Z'}{2}} \left(1 - \frac{r_4Z'}{2} \right) \left(1 - \frac{r_3Z'}{2} \right) + e^{-\frac{(r_1+2r_2+r_3+2r_4)Z'}{2}} \left(1 - \frac{r_1Z'}{2} \right) \left(1 - \right. \\ & \left. \frac{r_3Z'}{2} \right) - e^{-\frac{(r_1+r_2+2r_3+2r_4)Z'}{2}} \left(1 - \frac{r_1Z'}{2} \right) \left(1 - \frac{r_2Z'}{2} \right) \right] + \alpha(1)\alpha(2)\beta(3)\beta(4) \left[e^{-\frac{(2r_1+r_2+2r_3+r_4)Z'}{2}} \left(1 - \right. \right. \\ & \left. \frac{r_3Z'}{2} \right) \left(1 - \frac{r_2Z'}{2} \right) - e^{-\frac{(2r_1+r_2+2r_3+r_4)Z'}{2}} \left(1 - \frac{r_4Z'}{2} \right) \left(1 - \frac{r_2Z'}{2} \right) + e^{-\frac{(r_1+2r_2+2r_3+r_4)Z'}{2}} \left(1 - \frac{r_1Z'}{2} \right) \left(1 - \right. \\ & \left. \frac{r_4Z'}{2} \right) - e^{-\frac{(r_1+2r_2+r_3+2r_4)Z'}{2}} \left(1 - \frac{r_1Z'}{2} \right) \left(1 - \frac{r_3Z'}{2} \right) \right] + \beta(1)\alpha(2)\beta(3)\alpha(4) \left[e^{-\frac{(2r_1+2r_2+r_3+r_4)Z'}{2}} \left(1 - \right. \right. \\ & \left. \frac{r_3Z'}{2} \right) \left(1 - \frac{r_4Z'}{2} \right) - e^{-\frac{(2r_1+r_2+r_3+2r_4)Z'}{2}} \left(1 - \frac{r_3Z'}{2} \right) \left(1 - \frac{r_2Z'}{2} \right) - e^{-\frac{(r_1+2r_2+2r_3+r_4)Z'}{2}} \left(1 - \frac{r_1Z'}{2} \right) \left(1 - \right. \\ & \left. \frac{r_4Z'}{2} \right) + e^{-\frac{(r_1+r_2+2r_3+2r_4)Z'}{2}} \left(1 - \frac{r_1Z'}{2} \right) \left(1 - \frac{r_2Z'}{2} \right) \right] + \beta(1)\alpha(2)\alpha(3)\beta(4) \left[e^{-\frac{(2r_1+r_2+2r_3+r_4)Z'}{2}} \left(1 - \right. \right. \\ & \left. \frac{r_2Z'}{2} \right) \left(1 - \frac{r_4Z'}{2} \right) - e^{-\frac{(2r_1+2r_2+r_3+r_4)Z'}{2}} \left(1 - \frac{r_4Z'}{2} \right) \left(1 - \frac{r_3Z'}{2} \right) + e^{-\frac{(r_1+2r_2+r_3+2r_4)Z'}{2}} \left(1 - \frac{r_1Z'}{2} \right) \left(1 - \right. \end{aligned}$$

$$\frac{r_3 Z'}{2} - e^{-\frac{(r_1+r_2+2r_3+2r_4)Z'}{2}} \left(1 - \frac{r_1 Z'}{2}\right) \left(1 - \frac{r_2 Z'}{2}\right) \left] + \beta(1)\beta(2)\alpha(3)\alpha(4) \left[e^{-\frac{(2r_1+r_2+2r_3+r_4)Z'}{2}} \left(1 - \frac{r_3 Z'}{2}\right) \left(1 - \frac{r_2 Z'}{2}\right) - e^{-\frac{(2r_1+r_2+2r_3+r_4)Z'}{2}} \left(1 - \frac{r_4 Z'}{2}\right) \left(1 - \frac{r_2 Z'}{2}\right) + e^{-\frac{(r_1+2r_2+2r_3+r_4)Z'}{2}} \left(1 - \frac{r_1 Z'}{2}\right) \left(1 - \frac{r_3 Z'}{2}\right) - e^{-\frac{(r_1+2r_2+2r_3+r_4)Z'}{2}} \left(1 - \frac{r_1 Z'}{2}\right) \left(1 - \frac{r_3 Z'}{2}\right) \right] \right\}, \quad (3.3)$$

where Z' , here, is an effective charge, which is treated as a variational parameter, to minimize the energy. Hence, ψ_0 is a linear combination of terms constructed from the single-particle hydrogenic wave functions in such a way that the total spin of the system is $S = 0$ and its z-component is $M_S = 0$.

For the correlation function f we used two different types of correlations. The first one is the Jastrow correlation function which is a product of exponential functions of the form [19]

$$f_1 = \prod_{1=i<j}^4 \exp \left[\frac{r_{ij}}{l(1+k r_{ij})} \right], \quad (3.4)$$

to satisfy the cusp conditions [20], we must have:

$$l = \begin{cases} 4 & \text{for like spins} \\ 2 & \text{for unlike spins} \end{cases}, \quad (3.5)$$

in Eq. (3.4), k is a variational parameter, which is denoted by k_1 for like spins and k_2 for the unlike spins. Hence, our first trial wave function is given by

$$\psi_1 = \psi_0 f_1, \quad (3.6)$$

and it contains three variational parameters, namely: k_1 , k_2 and Z' .

The second correlation function is a product of functions of the form [21]

$$f_2 = \prod_{1=i<j}^4 (1 + A r_{ij} \exp[-B r_{ij}]). \quad (3.7)$$

To satisfy the cusp conditions, we must have:

$$A = \begin{cases} \frac{1}{4} & \text{for like spins} \\ \frac{1}{2} & \text{for unlike spins} \end{cases} \quad (3.8)$$

in Eq. (3.7), B is a variational parameter, which is denoted by B_1 for like spins and B_2 for the unlike spins. Hence, our second trial wave function is given by

$$\psi_2 = \psi_0 f_2, \quad (3.9)$$

and it contains three variational parameters, namely: B_1 , B_2 and Z' .

4. Results and Discussions

Our investigations in the present paper are based on applying the VMC method to find the least energy eigenvalue of the ground-state of the beryllium atom. To achieve this goal, we used three trial wave functions of the form of SLD functions multiplied by correlation

functions. Two types of correlation functions are used. Also, the SLD with modified hydrogenic radial functions multiplied by our second correlation function is also used in our calculations. All energies are obtained in atomic units with a set of 4×10^7 Monte Carlo points to make the statistical error as low as possible. Since the principle of the VMC method depends on finding the minimum energy by using the appropriate trial wave function, therefore, our goal in the present study is to find a simple trial wave function which can produce a minimum energy eigenvalue for the ground-state of beryllium in good agreement with the corresponding exact value, with the least possible standard deviation.

In Table-1, we present the values of the parameters of our used three trial wave functions which produced the best values of the calculated ground state energy and standard deviation of the beryllium atom.

Table-1. The values of the parameters which produced the best values of the ground state energy eigenvalue of Beryllium.

	ψ_1	ψ_2
Z'	3.965	3.2885
k_1	2.2	-
k_2	0.135	-
B_1	-	0.001
B_2	-	0.88

The corresponding values of the ground state energy eigenvalues of the beryllium atom by using the best three trial wave functions are given in Table-2. The corresponding values of the standard deviations are also given. The exact value and previous value are also given in Table-2.

Table-2. Ground state energy eigenvalue of beryllium (E) in a. u. by using the three trial wave functions. The values of the standard deviations are also given. The exact value and previous value are also given.

	E (a. u.)	σ
ψ_1	-14.6557	0.0013
ψ_2	-14.664401	0.0013
Previous [22]	-14.66735	--
Exact value [23]	- 14.667 356	--

In Figure-1, we present the variation of the ground state energy of the beryllium atom with respect to the two parameters Z' and k_1 by using the first trial wave function ψ_1 . The variation of the standard deviation associated with the ground-state energy of beryllium with respect to the number of VMC points by using ψ_1 is provided in Figure-2.

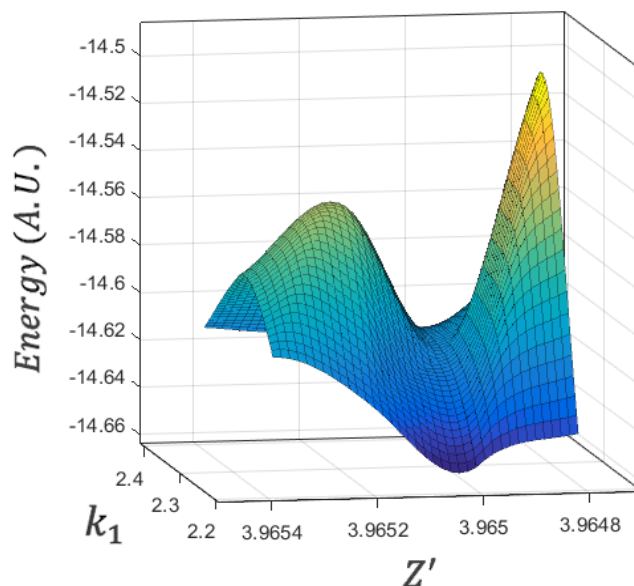


Fig.1 The variation of the ground-state energy of beryllium, calculated by using the trial wave function ψ_1 with respect to the parameters Z' and k_1 . The value of k_2 is 0.135.

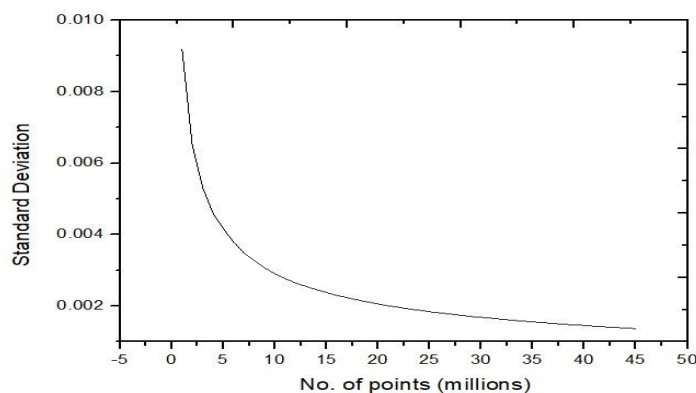


Fig.2 The variation of the standard deviation associated with the ground-state energy of beryllium with respect to the number of VMC points by using ψ_1 .

In Figure-3, we present the variations of the ground-state energy of beryllium, calculated by using the trial wave function ψ_2 with respect to the two parameters Z' and B_1 . We also present the variations of the ground-state energy of beryllium, calculated by using the trial wave function ψ_2 with respect to the two parameters Z' and B_2 in Figure-4. Besides, the variation of the standard deviation associated with the ground-state energy of the beryllium atom with respect to the number of VMC points by using ψ_2 is shown in Figure-5.

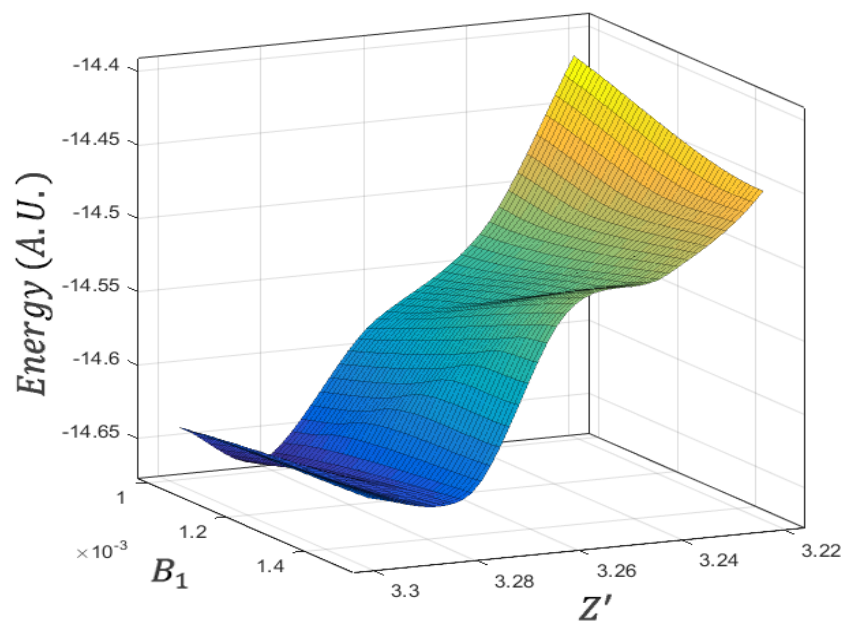


Fig.3 The variations of the ground-state energy of beryllium, calculated by using the trial wave function ψ_2 with respect to the parameters Z' and B_1 . The value of B_2 is 0.88.

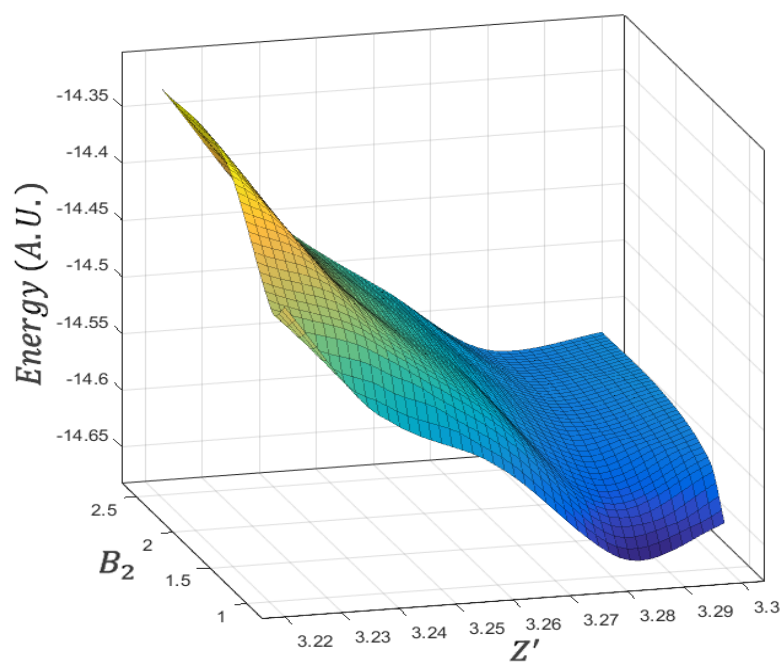


Fig.4 The variations of the ground-state energy of beryllium, calculated by using the trial wave function ψ_2 with respect to the parameters Z' and B_2 . The value of B_1 is 0.001.

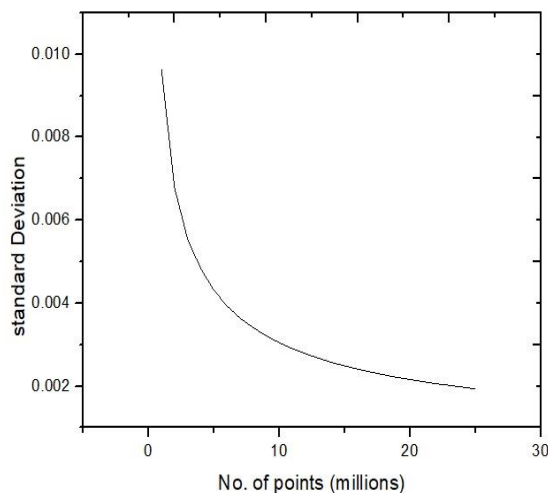


Fig.5. The variation of the standard deviation associated with the ground-state energy of beryllium with respect to the number of VMC points by using ψ_2 .

5. Conclusion

In this paper, we applied the VMC method with two trial wave functions of the form of the SLD multiplied by different correlation functions, due to the interactions between the electrons, to calculate the ground state energy of the beryllium atom. Accordingly, we studied the effect of different correlation functions with the SLD as a trial wave function for the configuration of the ground state of the beryllium atom. In conclusion, we noticed that the obtained result concerning the ground state energy eigenvalue of the beryllium atom by using the second trial wave function ψ_2 is in better agreement with the corresponding exact value rather than the other trial wave function, while the standard deviations by using the functions ψ_1 and ψ_2 are the same. The obtained results showed also that the VMC method can be applied successfully for the investigation of the ground state characteristics of the beryllium atom by a suitably chosen trial wave function which takes into account the correlation part, due to the interactions between the electrons, and the cusp condition.

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