

# Application of the Variational Monte Carlo Method to the Three Electron Coulomb and Harmonium Systems

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**Abstract**— The problems of three electron interacting systems are considered in this paper. In the first part of the present paper, we considered the ground state, the lithium - like ions, and the core excited states of the lithium atom. Trial wave functions constructed from multiplication of hydrogenic wave functions and correlation wave functions are used in the calculations carried out in the first part. Furthermore, the compressed lithium atom by a hard wall spherical box is also investigated. In the second part of the present paper, we investigated the three-electron harmonium atom at which harmonic potential is used rather than the effect of Coulomb potential. The obtained results are in good agreement with the results of other works.

**Keywords**— Ground state of the lithium atom, lithium iso electronic ions, excited states of lithium, confined lithium atom , three electron harmonium atoms.

## I. INTRODUCTION

The Variational Monte Carlo (VMC) method [1], [2] is considered one of the methods which are used successfully for evaluating the energy eigen values of few electron-atoms, ions, or molecules. It consists of two parts: the variational method (Ritz method) which depends on the minimization of parameters to evaluate the energy values and the Monte Carlo technique of evaluating integrals based on Metropolis algorithm [3]. The statistical errors of the used integrals decrease by increasing the number of points which are sampled to obtain the required accuracy of calculation. Also, the standard deviation is calculated with the energy eigen values.

Moreover, the Monte Carlo technique consists of a simple, highly repetitive algorithm that takes advantage of the fast arithmetic capabilities of the machines. This method depends mainly on optimization of the variational parameters using appropriate methods in order to give the most accurate results with low standard deviation.

The used trial wave function is resulted from the multiplication of two functions: the first function, which is called (Un-Correlated function), as hydrogenic wave functions, related to the interaction between electrons and nucleus (via the Coulomb potential) and the second function, (Correlated function) [4], as a Jastrow factor [5] related to the interaction between electrons with each other (repulsive potential) while the nucleon-nucleon interaction can be neglected due to (Born–Oppenheimer approximation) where the motion of the nucleus is disregarded.

The Quantum Monte Carlo methods were applied successfully by Doma et al. [6], [7], [8], [9], [10] for atomic and molecular systems whether for a free state, confined system or under impact of external magnetic field using suitable trial wave functions. Also, Doma et al [11] used VMC method for the ground state and some excited states of the lithium atom and its ions in an external magnetic field. Furthermore, S. B. Doma et al. [12], [13] calculated the ground state energy of the lithium atom in plasma states using three trial wave functions compared with the experimental value of free lithium atom and the other published results for dense plasma states.

Other methods were used to study and evaluate the energy eigenvalues of the three electron systems. Der-Ruenn Su [14] calculated its ground state energy of lithium atom and the state  $1s^2 3d$  by applying the variational technique of Drake. Turbiner et al [15] calculated ground state energy of helium-like and lithium-like ions for both infinite and finite nuclear mass effect.

As an experimental work for lithium atom, A. Borovik and A. Kupliauskien'e [16] measured the excitation energies of  $1s n_1 l_1 n_2 l_2$  states of lithium atom.

The uncertainties of energy scales were estimated for incident and ejected electrons, respectively. In addition, S. H. Patil and Y. P. Varshni [17] studied the spectrum of confined hydrogen, helium, and lithium atoms at different radii with using the interaction between the electrons.

T. Sako and G. H. Dieerksen [18] studied the spectrum, potential curves and electron density distribution of

confined low-lying states of helium and lithium atoms by an isotropic harmonic potential using the quantum chemical configuration interaction (CI) method by Cartesian anisotropic Gaussian basis set.

S. Dutta et al. [19] estimated the energy eigenvalues of the three-electron ground and excited states in weakly coupled plasma environment. Also, the ionization potential, diamagnetic susceptibility ( $\chi$ ) and nuclear magnetic shielding constant ( $\sigma$ ) are given with respect to the plasma screening parameter ( $\mu$ ).

For harmonium atom, Jerzy Cioslowski and Krzysztof Strasburger [20] studied the three-electron harmonium atom at different confinement strengths using correlated Gaussian lobe wave function. They calculated the kinetic energy, the potential energy, and the electron-electron repulsion energy of the ground state  $^2P_-$  and the excited state  $^4P_+$ .

Accordingly, the aim of the present paper is to apply the VMC method to evaluate the energy of three Coulomb and Harmonium systems. The Hamiltonian and trial wave functions of ground state of the lithium atom, its isoelectronic ions and the energies of the core excited states are described in section II. The Hamiltonian and trial wave of confined ground state of the lithium atom are illustrated in section III. The three- electron harmonium atom at different ranges of confinement strengths is shown in section IV. The results and discussions are shown in section V and the conclusion is given in section VI.

**II. THE GROUND, THE ISO-ELECTRONIC IONS AND THE CORE EXCITED STATES OF THE LITHIUM ATOM**

On using Born–Oppenheimer approximation, the Hamiltonian of the three-electron Coulomb system in atomic units, ( $e = \hbar = m = 1$ ), is given by

$$\hat{H} = -\frac{1}{2}\sum_{i=1}^3(\nabla_i^2 + \frac{Z}{r_i}) + \sum_{i<j} \frac{1}{r_{ij}} \tag{1}$$

where  $Z$  is the nuclear charge (here  $Z = 3$  for the ground and the core excited states of the lithium atom and  $Z = 4$  up to  $Z = 10$  for Li-like ions),  $r_i$  is the distance between electron and the nucleus, and  $r_{ij}$  is The distance between the electrons. In Hylleraas Coordinates [21], this Hamiltonian is given by

$$\begin{aligned} \hat{H} = & -\frac{1}{2}\left(\sum_{i=1}^3 \frac{\partial^2}{\partial r_i^2} + \sum_{i=1}^3 \frac{2}{r_i} \frac{\partial}{\partial r_i} + \sum_{i<j}^3 2 \frac{\partial^2}{\partial r_{ij}^2} + \sum_{i<j}^3 \frac{4}{r_{ij}} \frac{\partial}{\partial r_{ij}}\right. \\ & + \sum_{i \neq j}^3 \frac{r_i^2 + r_{ij}^2 - r_j^2}{r_i r_{ij}} \frac{\partial^2}{\partial r_i \partial r_{ij}} + \sum_{i \neq j}^3 \sum_{k > j}^3 \frac{r_{ij}^2 + r_{ik}^2 - r_{jk}^2}{r_{ij} r_{ik}} \frac{\partial^2}{\partial r_{ij} \partial r_{ik}} \\ & + \sum_{i=1}^3 \frac{1}{r_i} \frac{\partial^2}{\partial \theta_i^2} + \\ & \left. \sum_{i=1}^3 \frac{1}{r_i^2 \sin^2 \theta_i} \frac{\partial^2}{\partial \varphi_i^2} + \sum_{i=1}^3 \frac{\cot \theta_i}{r_i^2} \frac{\partial}{\partial \theta_i} + \sum_{i \neq j}^3 \left( \frac{r_j \cos \theta_j}{r_i r_{ij} \sin \theta_i} + \right. \right. \end{aligned}$$

$$\left. \cot \theta_i \frac{r_{ij}^2 - r_i^2 - r_j^2}{r_i^2 r_{ij}} \right) \frac{\partial^2}{\partial \theta_i \partial r_{ij}} + \sum_{i \neq j}^3 2 \frac{r_j \sin \theta_j}{r_i r_{ij} \sin \theta_i} \sin(\varphi_i - \varphi_j) \frac{\partial^2}{\partial \varphi_i \partial r_{ij}} + \sum_{i=1}^3 \frac{-Z}{r_i} + \sum_{i<j}^3 \frac{1}{r_{ij}}, \tag{2}$$

to solve the Schrödinger wave equation

$$\hat{H}\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = E \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \tag{3}$$

for this system, we applied the VMC method by choosing a suitable trial wave function for each state.

Der-Ruenn Su [14] calculated the ground state energy of the lithium atom by applying the variational technique of Drake and using the following product of hydrogenic wave functions

$$\begin{aligned} \psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = & \psi_{Z'}(r_1) \psi_{Z'}(r_2) R_{nl}(Z'', r_3) Y_{lm}(\theta_3, \varphi_3) \\ = & \frac{z'^3 z''^{l+2}}{2\pi\sqrt{2\pi}} e^{-z'(r_1+r_2)-z''(\frac{r_3}{2})} \left(1 - \frac{z''r_3}{2}\right) \end{aligned} \tag{4}$$

where  $R_{nl}(Z'', r_3) Y_{lm}(\theta_3, \varphi_3)$  is the hydrogen-like wave function in the  $nl$  state and  $Z'$  and  $z''$  are variational parameters.

For the ground states of the lithium atom and it's like ions, we used a modified trial wave function as follows

$$\Psi_1(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = A[\psi(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \chi(1,2,3) \prod_{i<j} f(r_{ij})] \tag{5a}$$

where  $A$  is antisymmetrizer

$$A = I - \hat{P}_{12} - \hat{P}_{13} - \hat{P}_{23} + \hat{P}_{123} + \hat{P}_{132} \tag{5b}$$

and the spin function  $\chi(1,2,3)$  is given by

$$\chi(1,2,3) = \alpha(1)\beta(2)\alpha(3) - \beta(1)\alpha(2)\alpha(3) \tag{5c}$$

The function  $f(r_{ij})$  is the Jastrow correlation function [5] given by

$$f(r_{ij}) = \exp\left[\frac{r_{ij}}{n(1+\mu r_{ij})}\right] \tag{6}$$

For core excited states of the lithium atom  $1s n_1 l_1 n_2 l_2$ , the trial wave function is

$$\begin{aligned} \Psi_2(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = & A[\psi_{Z'}(r_1) R_{nl}(Z'', r_2) Y_{lm}(\theta_2, \varphi_2) R_{nl}(Z'', r_3) Y_{lm}(\theta_3, \varphi_3) \\ & \times \chi(1,2,3) \prod_{i<j} f(r_{ij})] \end{aligned} \tag{7a}$$

But for  $1s n_1 l_1 n_2 l_2$  core excited states, we used the following trial wave function

$$\begin{aligned} \Psi_3(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) = & A[\psi_{Z'}(r_1) R_{nl}(Z'', r_2) Y_{lm}(\theta_2, \varphi_2) R_{nl}(Z''', r_3) Y_{lm}(\theta_3, \varphi_3) \\ & \times \chi(1,2,3) \prod_{i<j} f(r_{ij})] \end{aligned} \tag{7b}$$

Here,  $z', z''$  and  $z'''$  are the variational parameters of the orbital part while  $\mu$  is the variational parameter of the correlation part.

In (7a) and (7b),  $n = \begin{cases} 2 & \text{for unlike spins} \\ 4 & \text{for like spins} \end{cases}$  which makes the function  $f(r_{ij})$  satisfies the cusp conditions and the spin functions are shown in Table 3. The four variational parameters  $z', z'', z'''$  and  $\mu$  are varied in order to obtain the best fit to the energy eigenvalues of the lithium atom and its isoelectronic ions, by using the VMC method.

### III. THE CONFINED GROUND STATE OF THE LITHIUM ATOM

We now consider a compressed lithium atom placed in hard walls spherical box which is a repulsive cavity to avoid eccentricity of the atom to be an orbit within the cavity. The Schrödinger equation for this confined system is given by

$$\hat{H}_C \psi_C = E_C \psi_C \quad (8)$$

Here,  $\hat{H}_C = \hat{H} + V_C(r_1, r_2, r_3)$  where  $V_C(r_1, r_2, r_3)$  is the confined potential due to the box, of radius  $r_C$ , and is given by

$$V_C(r_1, r_2, r_3) = \begin{cases} 0, & r_1, r_2, r_3 < r_C \\ \infty, & r_1, r_2, r_3 \geq r_C \end{cases} \quad (9)$$

The used trial wave function is

$$\psi_C = \Psi_1(\mathbf{r}_1, \mathbf{r}_2, \mathbf{r}_3) \prod_i \left(1 - \frac{r_i}{r_C}\right), \quad (10)$$

where the cut-off factor  $\prod_i \left(1 - \frac{r_i}{r_C}\right)$  satisfies Dirichlet boundary conditions at which  $\psi_C = 0$  at  $r_i = r_C$ .

In addition, the pressure exerted on an atom by the system boundaries was evaluated, at different values of the box radius, as follows [22]

$$p(r_C) = - \frac{1}{4\pi r_C^2} \frac{dE}{dr_C} = \frac{1}{4\pi r_C^3} (2E - \langle V \rangle) \quad (11)$$

Here,  $E = E(r_C)$  is the total energy and  $\langle V \rangle$  is the expectation value of the potential at various radii of the spherical box. Beside this, the kinetic energy [23] of the system is estimated as

$$K(r_C) = 4\pi r_C^3 p(r_C) - E(r_C). \quad (12)$$

### IV. THE THREE- ELECTRON HARMONIUM ATOM

In this section, the VMC was applied to a different type of system which is called harmonium atom at which the electrons are trapped by harmonic potential. The Hamiltonian of this system, in a. u., could be described by

$$\mathcal{H} = -\frac{1}{2} \sum_{i=1}^3 (\nabla_i^2 - \omega^2 r_i^2) + \sum_{i<j} \frac{1}{r_{ij}}, \quad (13)$$

where  $\frac{1}{2} \omega^2 r_i^2$  is the isotropic harmonic oscillator potential of frequency  $\omega$ . The trial wave function of such system is produced from the electron-harmonic interacting term multiplied by electron-electron repulsion term and is introduced as follows

$$\Psi = \exp\left(-\xi \frac{\omega}{2} (r_1^2 + r_2^2 + r_3^2)\right) \times \exp(\alpha(r_{12} + r_{13} + r_{23})), \quad (14)$$

where  $\xi$  and  $\alpha$  are the variational parameters of the interacting and correlation terms, respectively. Also, the components of the total energy [24] can be evaluated, namely: the kinetic energy term

$$T(\omega) = \frac{3}{2} \omega E'(\omega) - E(\omega), \quad (15)$$

the harmonic potential energy term

$$V(\omega) = \frac{1}{2} \omega E'(\omega), \quad (16)$$

and the repulsion term

$$W(\omega) = 2E(\omega) - 2\omega E'(\omega). \quad (17)$$

## V. RESULTS AND DISCUSSION

### A. The ground state of the lithium atom and its isoelectronic ions

The energy eigenvalues of the ground states of the lithium atom and its isoelectronic ions up to  $Z = 10$  are obtained by applying the VMC method with number of integration points equals  $10^6$  and using the trial wave function  $\Psi_1$  of (5). This wave function contains three variational parameters, namely:  $z', z''$ , and  $\mu$ . Our computational program enables us to vary the parameters successively in loops until the minimum energy eigenvalue is obtained. The variations of the ground state and iso-electronic ions energies with respect to  $z'$  and  $z''$  are given in Figs. (1-8). Their values which produced the best energy eigenvalues from ( $Z=3$ ) up to ( $Z = 10$ ) are given in Table 1.

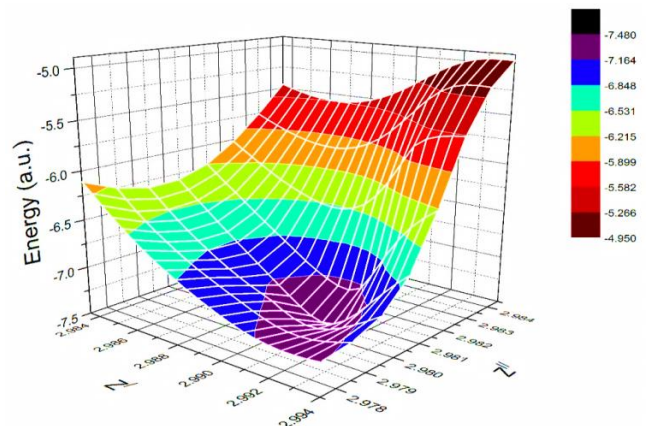


Figure 1. The variation of the ground state energy of the lithium atom with  $z'$  and  $z''$  for  $\mu = 0.4$ .

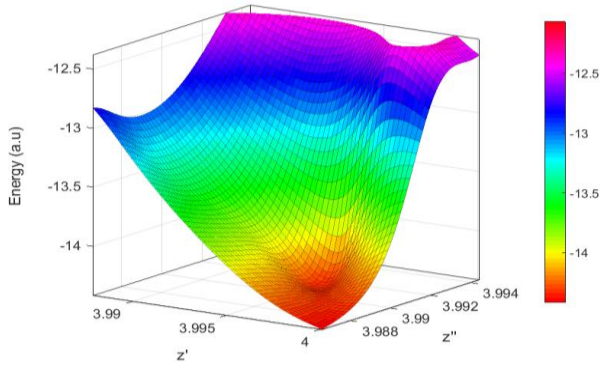


Figure 2. The variation of the iso-electronic ion ( $Z = 4$ ) at  $\mu = 0.7$ .

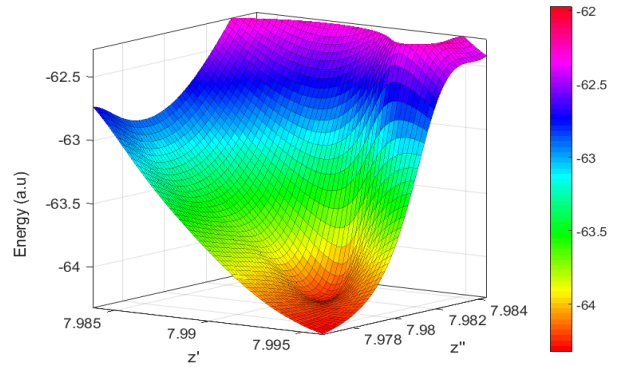


Figure 6. The variation of the iso-electronic ion ( $Z = 8$ ) at  $\mu = 0.9$ .

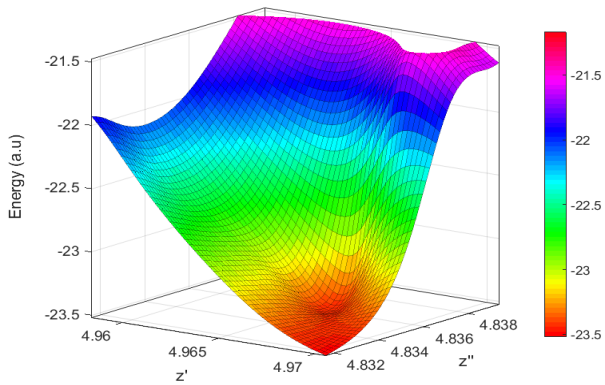


Figure 3. The variation of the iso-electronic ion ( $Z = 5$ ) at  $\mu = 0.503$ .

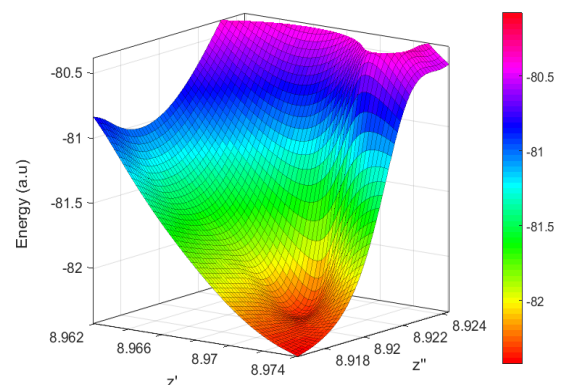


Figure 7. The variation of the iso-electronic ion ( $Z = 9$ ) at  $\mu = 0.2$ .

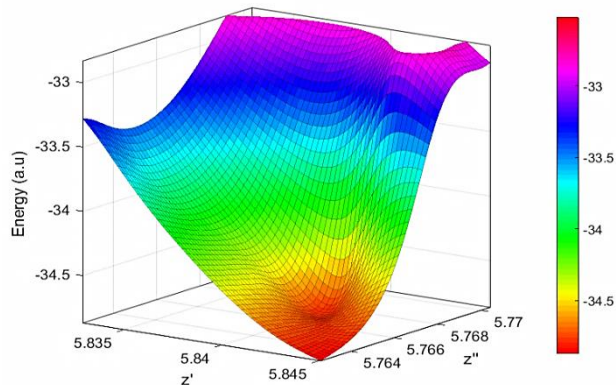


Figure 4. The variation of the iso-electronic ion ( $Z = 6$ ) at  $\mu = 0.55$ .

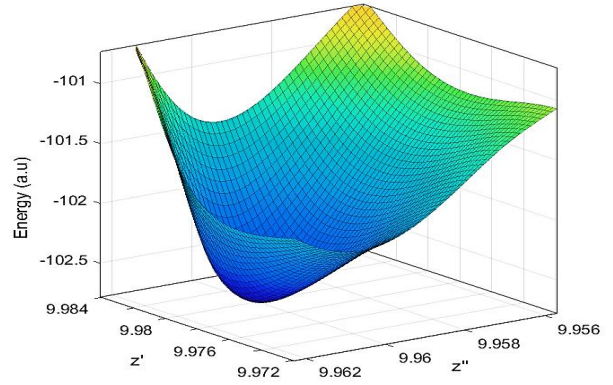


Figure 8. The variation of the iso-electronic ion ( $Z = 10$ ) at  $\mu = 2.2$ .

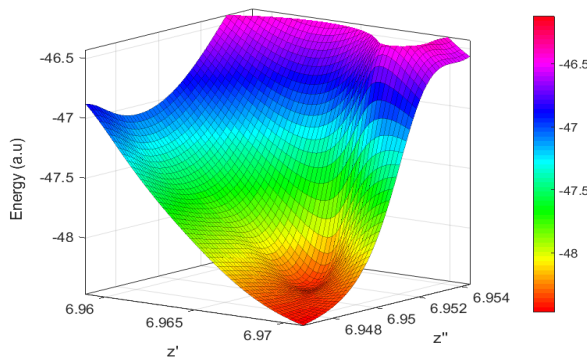


Figure 5. The variation of the iso-electronic ion ( $Z = 7$ ) at  $\mu = 0.65$ .

Table 1. The best values of the variational parameters of the trial wave function (5) from ( $Z=3$ ) to ( $Z = 10$ ).

$Z$	$z'$	$z''$	$\mu$
3	2.9905	2.9805	0.4
4	3.996	3.990	0.7
5	4.9665	4.835	0.503
6	5.841	5.766	0.55
7	6.967	6.950	0.65
8	7.992	7.980	0.9
9	8.970	8.920	2
10	9.980	9.960	2.2

The obtained results of the energy eigenvalues of the ground state of the lithium atom and its isoelectronic ions are given in Table 2. The calculated values of the standard deviations are also given. Furthermore, the exact values of [15] are also given in Table 2. It is seen from Table 2 that our results showed good agreement with the exact values.

Table 2. The ground state energy of the lithium atom and its isoelectronic ions, in a. u., compared to [15] with the standard deviations.

S. D.	[15]	This work	Z
$3 \times 10^{-5}$	-7.478060	-7.478020	3
$1.2 \times 10^{-3}$	-14.324763	-14.324520	4
$1 \times 10^{-3}$	-23.424605	-23.424400	5
$2 \times 10^{-3}$	-34.775511	-34.775600	6
$1 \times 10^{-3}$	-48.376898	-48.376690	7
$1.6 \times 10^{-3}$	-64.228542	-64.228590	8
$3 \times 10^{-4}$	-82.330338	-82.330300	9
$2 \times 10^{-4}$	-102.682231	-102.682200	10

**B. The core excited states of the lithium atom**

Table 3 shows the obtained results of the energies of the core excited states of the lithium atom ( $1s n_1 l_1 n_2 l_2$  and  $1s n_1 l_1 n_2 l_2$ ) using the functions  $\Psi_2$  and  $\Psi_3$ , respectively, with a set of  $10^6$  Monte Carlo integration points by using the VMC method. Here, these energies were calculated by adding the ground state energy of the lithium atom [15] to the required excitation energy for each state [16] to obtain nine different excited state energies as given in the last column of Table 3. Also, three variational parameters were used for the un-correlated part of the wave function to optimize the energy eigenvalues of the last two states. As seen, our results agree with the exact values and the required excitation energy for each state was converted here to a. u., which was previously given in (eV) in [16].

Table 3. The core excited state energies of the lithium atom with the spin functions in comparison with the previous work ([15] and [16]) in a. u.

State	Spin function $\chi(1, 2, 3)$	This work	work of [15] and [16]
$(1s2s^2)^2S$	$\alpha(1)\alpha(2)\beta(3)$ $-\alpha(1)\beta(2)\alpha(3)$	-5.398004	-5.405660
$(1s2s2p)^4P$	$\alpha(1)\alpha(2)\alpha(3)$	-5.368502	-5.368541
$1s(2s2p^3)^2P$	$2\beta(1)\alpha(2)\alpha(3)$ $+\alpha(1)\beta(2)\alpha(3)$ $+\alpha(1)\alpha(2)\beta(3)$	-5.313376	-5.313047
$1s(2s2p^1P)^2P$	$2\alpha(1)\alpha(2)\beta(3)$ $+\alpha(1)\beta(2)\alpha(3)$ $+\beta(1)\alpha(2)\alpha(3)$	-5.257881	-5.257920
$(1s2p^3)^4P$	$\alpha(1)\alpha(2)\alpha(3)$	-5.245386	-5.245425
$(1s2p^2)^2D$	$\alpha(1)\alpha(2)\beta(3)$ $-\alpha(1)\beta(2)\alpha(3)$	-5.233654	-5.233665
$(1s2p^2)^2P$	$\alpha(1)\alpha(2)\beta(3)$ $-\alpha(1)\beta(2)\alpha(3)$	-5.213412	-5.213451
$1s2s(3S)3s^2S$	$2\alpha(1)\alpha(2)\beta(3)$ $-\alpha(1)\beta(2)\alpha(3)$ $-\beta(1)\alpha(2)\alpha(3)$	-5.199447	-5.199486
$1s2s(3S)3p^2P$	$2\alpha(1)\alpha(2)\beta(3)$ $+\alpha(1)\beta(2)\alpha(3)$ $+\beta(1)\alpha(2)\alpha(3)$	-5.184746	-5.184785

**C. The confined ground state of the lithium atom**

In this section, we present the obtained results of placing the lithium atom at the center of an impenetrable spherical box (hard walls) by using the VMC method with  $10^7$  Monte Carlo points at certain value of the spherical box radius. The obtained results of the confined ground lithium atom correspond to a lithium excited states or ions. In Table 4, we present the results of calculating the energy of the confined lithium atom with the optimized variational parameters of the function  $\psi_c$  of (10). We notice from Table 4 that by decreasing the radius of the box the atom is more compressed and hence the energy of the system increases, where the kinetic energy becomes predominant perturbed by the attractive Coulomb potential. Also, the total energy was plotted as a function of the box radius  $r_c$  in Fig. 10 and the results of calculating the pressure exerted on the lithium atom and the kinetic energy, by using (11) and (12) for the system, are given in Table 5 at different radii. We present in the third column of Table 4 the states for which the calculated energy values of the confined lithium atom correspond. In the last column of the table, the results of the energies of the states in the other previous works are mentioned.

Table 4. The energies of the lithium ground state as functions of the box radius  $R_c$  in a. u.

$R_c$	This work	Corresponding State	Energy of the state
1	9.890	Un bound	9.9180 [17]
2.1	-4.5001	$Li^{++}$	-4.5000 [25]
4.9	-7.2724	$Li^+$	-7.2799 [15]
5.6	-7.3350	$1s^23d$	-7.3355 [18]
5.7	-7.3546	$1s^23s$	-7.3541 [18]
6.7	-7.4154	$1s^22p$	-7.4154 [18]

Table 5. The pressure (P) and kinetic energy (K.E.) of the confined ground lithium atom in a. u. s

$R_c$	P	K. E.
1	2.7642	24.8460
2.1	0.05118	10.4563
4.9	0.00028	7.6864
5.6	0.00013	7.6219
5.7	0.00011	7.6106
6.7	0.00003	7.5288

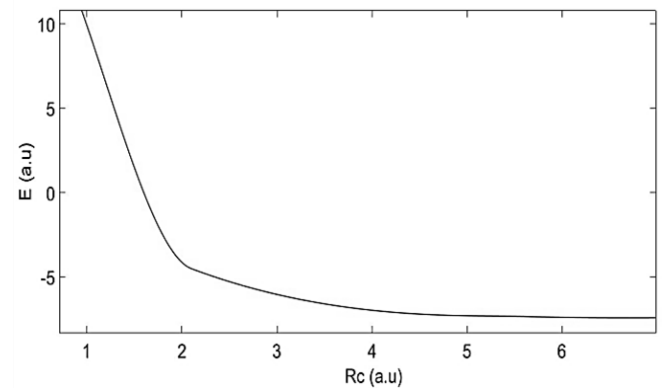


Figure 10. The energy of the lithium atom as function of the box radius ( $R_c$ )

#### D. The three-electron harmonium atom

In Table 6, we present the results of calculating the energies of the  $^2P_-$  ground state of the three-electron harmonium atom at small different values of the frequency  $\omega$  with the optimized variational parameters. The results of Jerzy Cioslowski and Krzysztof Strasburger [20] are also given in Table 6.

Table 6. Comparison of Total energy of the three-electron harmonium atom, in a. u., as function of the frequency  $\omega$  with [20].

$\omega$	This work	[20]
0.001	0.0347	0.0348
0.002	0.0568	0.0568
0.005	0.1097	0.1096
0.01	0.1819	0.1819
0.02	0.3047	0.3048
0.05	0.6139	0.6138
0.1	1.0594	1.0594
0.2	1.8579	1.8582
0.5	4.0135	4.0132

In Fig. 11, we present the variation of the total energy of the three-electron harmonium atom, in a. u., as function of the frequency  $\omega$ . Furthermore, the energy components are given in Table 7. It is seen from this table that for  $\omega > 0.2$ ,  $E(\omega)$  is dominated by the kinetic and the potential energies

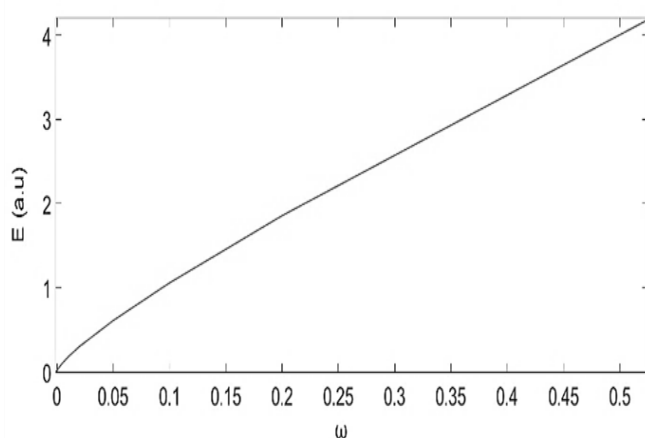


Figure 11. The energy of the three-electron harmonium atom as function of the harmonic strength in a. u.

Table 7. Energy components of the three-electron harmonium atom, in a. u., as function of the frequency  $\omega$ . The results of [20] are also given.

$\omega$	$T(\omega)$	[20]	$V(\omega)$	[20]	$W(\omega)$	[20]
0.001	0.00180	0.00185	0.01220	0.01220	0.02080	0.02080
0.002	0.0041	0.0037	0.02030	0.02020	0.03240	0.03292
0.005	0.0093	0.0094	0.03954	0.03970	0.06045	0.06049
0.01	0.01920	0.01920	0.06702	0.06704	0.09571	0.09568
0.02	0.03889	0.03914	0.11446	0.11465	0.15115	0.15101
0.05	0.10100	0.10120	0.23807	0.23840	0.27433	0.27418
0.1	0.20963	0.20954	0.42314	0.42300	0.42703	0.42691
0.2	0.43596	0.43580	0.76485	0.76470	0.65779	0.65764
0.5	0.93575	1.15070	1.64775	1.72132	1.42400	1.14113

## VI. CONCLUSION

In this work, the VMC method was applied with a number of  $10^7$  Monte Carlo integration points to study several problems concerning the three-electron Coulombic and harmonium systems. To achieve these goals, we used suitable trial wave functions which are based on hydrogenic wave functions multiplied by Jastrow correlation functions which represent the electron-electron interactions. Accordingly, in the first part of the present paper we calculated the ground state energy, the energies of the iso-electronic ions up to  $Z = 10$  and the energies of the core excited states of the lithium atom. Moreover, in the second part of the present paper we applied the VMC method to study the ground state of the lithium atom as a confined system in an impenetrable spherical box at different radii which showed that the kinetic energies increase by reducing the radius of box and the potential energies decrease (the interaction between electrons and nucleus). Also, at certain radii the energies were calculated beside the exerted pressure as well as the kinetic energy as a function of radii. And eventually, we studied the three-electron harmonium atom at different ranges of confinement strengths where the kinetic and potential energies increase by increasing the confinement strength.

In all our calculations, we used trial wave functions which contain small number of variational parameters, so that the calculations are mainly simplified without any loss of the accuracy of the obtained results. Accordingly, we can conclude that the VMC method can be applied successfully to the three electron systems by a suitably chosen trial wave functions.

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