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Ground State, Isoelectronic Ions and Low-Lying Excited States of Lithium Atom in Strong Magnetic Field

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Abstract

In the framework of the variational Monte Carlo method, the ground states of the lithium atom and lithium like ions up to $Z = 10$ in an external strong magnetic field are evaluated. Furthermore, the two low-lying excited states $1s^2 2s$, $1s^2 2p_{-1}$ and $1s2p_{-1}3d_{-2}$ of the lithium atom in strong magnetic field are also investigated. Simple trial wave functions for lithium are used.

Keywords

Variational Monte Carlo Method, Atoms in Magnetic Field, Ground States of Li, Binding Energy, Total Energy

1. Introduction

The properties of atoms in strong magnetic fields are relevant to several domains such as astrophysics, condensed matter physics, and plasma physics [1]. In the past, only hydrogen and helium atoms have been studied for magnetic fields of arbitrary strength [2]. The influence of a magnetic field on the properties of atoms and molecules is of great interest. The study of strongly magnetized atoms was first treated in a solid-state context. In semiconductors, the absorption of photons can promote electrons from the valence to the conduction band, forming an electron-hole pair. The absorption spectra of these excitons, when subjected to a magnetic field, display Zeeman effects [3]. The methods of treating the resulting problems arising from these topics have resulted in few studies of many-body effects in strong magnetic fields, *i.e.*, in the field regime where perturbation theory is no longer applicable.

The motivation in this area arises from several sources. On the one hand, this is due to the astrophysical discovery of strong magnetic fields on the surfaces of

white dwarfs (10^2 - 10^5 T) and neutron stars (10^7 - 10^9 T) [4] [5]. Also, the complex properties of atoms under these extreme conditions are of immediate interest from a purely theoretical point of view. In addition, the observations of excitons with small effective masses and large dielectric constants in semiconductors, which result in very large effective magnetic fields, give additional impetus for this subject [6].

It is well-known that the study of the electronic structure of atoms in the external magnetic field is a quite complicated subject, especially for the strong magnetic field. In a weak magnetic field, which can be treated as a perturbation, the wave function can be expanded in terms of spherical harmonic functions. In a very strong magnetic field, where the Lorentz forces dominate, the wave function can be expanded in terms of Landau-like orbitals. But in the strong magnetic field, where the Lorentz and Coulomb forces are of nearly equal importance, neither of them can be treated as a perturbation [7]. Hence, it is necessary to develop non-perturbative techniques to solve this problem. The parameter β_z can be used to characterize three different regimes of strength: the low (weak, $\beta_z < 10^{-3}$), the intermediate (strong, $10^{-3} \le \beta_z \le 1$), and the high (very strong, $\beta_z > 1$), regimes where $\beta_z = B/2B_0Z^2$, $B_0 = 2.35\times10^5$ T, and Z is the charge of the atomic nucleus. So far, considerable effort has been devoted to the theoretical investigations of atoms in magnetic fields with arbitrary strength. Rösner *et al.* [8] have done detailed work on the spectrum of the hydrogen atom in magnetic fields up to 4.7×10^8 T, which has been successfully applied to the identification of the observed spectra from many magnetic white dwarfs [9] [10]. For the hydrogen atom in magnetic fields up to 9.4×10^8 T, Kravchenko *et al.* [11] [12] presented accurate results with an accuracy of 10^{-12}. In view of this, the issue of the hydrogen atom over a wide range of magnetic fields can be completely solved. Despite this great success, there were also many magnetic white dwarfs whose spectra remain unexplained or could not be completely accounted for with hydrogen atom. It is thus essential to acquire extensive and accurate data of energy levels and resulting transition wavelengths of multi-electron atoms subjected to strong magnetic fields. Hence, the research emphasis of atoms under these extreme conditions focused on the next lightest element, neutral helium. In contrast to the hydrogen atom, the problem of the helium atom is much more intricate because of the occurrence of the electron-electron repulsion. Even so, there exist many investigations on helium atoms in the literature. Thurner *et al.* [13] gave the energies of several triplets excited states of helium atoms for magnetic field strengths in the range 4.7×10^1 to 4.7×10^8 T. Furthermore, they presented a consistent correspondence diagram between the low field and high field domains for the first time.

Many studies have been recently presented by Doma *et al.* using the Variational Monte Carlo (VMC) method for the helium, lithium, and beryllium atoms [14] [15] [16] [17] [18]. The success of the VMC method extended also to the light molecules, where similar investigations have been carried out for the hydrogen molecule and its molecular ion by Doma *et al.* [19] [20] [21].

In fact, the problem of highly accurate calculations of the bound states in the three-electron atomic systems has attracted continuing attention. For lithium atom and its ions up to $Z = 10$, in the strong magnetic field and using the VMC method, Doma *et al.* calculated the energies of these systems [16].

In the present paper, we applied the VMC method and constructed three trial wave functions, which take into consideration the correlation functions due to the interactions between the electrons in the atom, to calculate the ground state of the lithium atom and its ions up to $Z = 10$ in the presence of an external magnetic field regime with $\gamma = 0 \sim 100$ a.u. Furthermore, the two low-lying excited states $1s^2 2s$, $1s^2 2p_{-1}$ and $1s2p_{-1}3d_{-2}$ of the lithium atom in the strong magnetic field are also investigated.

2. Method of the Calculations

In the present paper, we solved the Schrödinger equation for the lithium atom and the lithium like ions up to $Z = 10$ in an external magnetic field to find the energy eigenvalues as functions of the field parameter. Furthermore, the case of the low-lying excited states $1s^2 2s$, $1s^2 2p_{-1}$ and $1s2p_{-1}3d_{-2}$ of the lithium atom in an external magnetic field is also solved. For this purpose, simple trial wave functions with low number of variational parameters for lithium are used. To find the minimum energy eigenvalues we applied the VMC method. We first constructed the Hamiltonian operator for the three-electron system in the absence of the external field. We made use of the assumption of an infinitely heavy nucleus in the unrestricted Hrtree-Fock (HF) approximation. Hence, the non-relativistic Hamiltonian for the lithium atom, in the absence of the field, under the Born-Oppenheimer approximation of zero order, that is, with the Li nucleus assumed to be of infinite mass, is (in Hartree atomic units) [22] given by:

$$H = -\frac{1}{2}\sum_{i=1}^{3}\nabla_i^2 + \sum_{i=1}^{3}\frac{-Z}{r_i} + \sum_{i<j}^{3}\frac{1}{r_{ij}}, \tag{2.1}$$

where ∇_i is the 3-vector of the momentum of the ith electron, Z is the nuclear charge (here, $Z = 3$), r_i is the distance between the ith electron and the Li nucleus, and r_{ij} are the interelectron distances. In our calculations we used the form of H in Hylleraas Coordinates [22] [23] as follows:

$$\begin{aligned} H = -\frac{1}{2}\Bigg(& \sum_{i=1}^{3}\frac{\partial^2}{\partial r_i^2} + \sum_{i=1}^{3}\frac{2}{r_i}\frac{\partial}{\partial r_i} + \sum_{i<j}^{3}2\frac{\partial^2}{\partial r_{ij}^2} + \sum_{i<j}^{3}\frac{4}{r_{ij}}\frac{\partial}{\partial r_{ij}} \\ & + \sum_{i\neq j}^{3}\frac{r_i^2 + r_{ij}^2 - r_j^2}{r_i r_{ij}}\frac{\partial^2}{\partial r_i \partial r_{ij}} + \sum_{i\neq j}^{3}\sum_{k>j}^{3}\frac{r_{ij}^2 + r_{ik}^2 - r_{jk}^2}{r_{ij} r_{ik}}\frac{\partial^2}{\partial r_{ij}\partial r_{ik}} \\ & + \sum_{i=1}^{3}\frac{1}{r_i^2}\frac{\partial^2}{\partial \theta_i^2} + \sum_{i=1}^{3}\frac{1}{r_i^2 \sin_{\theta_i}^2}\frac{\partial^2}{\partial \varphi_i^2} + \sum_{i=1}^{3}\frac{\cot\theta_i}{r_i^2}\frac{\partial}{\partial \theta_i} \\ & + \sum_{j\neq 1}^{3}\left(\frac{2r_j}{r_i r_{ij}}\frac{\cos\theta_j}{\sin\theta_i} + \cot\theta_i\frac{r_{ij}^2 - r_i^2 - r_j^2}{r_i^2 r_{ij}}\right)\frac{\partial^2}{\partial\theta_i \partial r_{ij}} \\ & + \sum_{j\neq 1}^{3}2\frac{r_j}{r_i r_{ij}}\frac{\sin\theta_j}{\sin\theta_i}\sin\left(\varphi_i - \varphi_j\right)\frac{\partial^2}{\partial\varphi_i \partial r_{ij}}\Bigg) + \sum_{i=1}^{3}\frac{-Z}{r_i} + \sum_{1=i<j}^{3}\frac{1}{r_{ij}} \end{aligned} \tag{2.2}$$

According to the assumption that the nuclear mass is infinite, and the magnetic field is oriented along the *z*-axis, the non-relativistic Hamiltonian $\mathcal{H}$ for the Li atom in the presence of the magnetic field (in atomic units (a.u.)) takes the form [7]:

$$\mathcal{H} = H + \left[\frac{\gamma^2\rho^2}{8} + \frac{\gamma\left(L_z + 2S_Z\right)}{2}\right]. \tag{2.3}$$

where $\rho^2 = \rho_1^2 + \rho_2^2 + \rho_3^2 = \left(x_1^2 + y_1^2\right) + \left(x_2^2 + y_2^2\right) + \left(x_3^2 + y_3^2\right)$, γ is the magnetic field parameter, $L_z = \sum_{i=1}^{3} l_{iz}$ and $S_z = \sum_{i=1}^{3} s_{iz}$ are the *z*-components of the total angular momentum and spin respectively, $\frac{\gamma^2\rho^2}{8}$ is the diamagnetic term, $\frac{\gamma}{2}L_z$ is the Zeeman term, $-\frac{Z}{r_1} - \frac{Z}{r_2} - \frac{Z}{r_3}$ are the attractive Coulomb interactions with the nucleus and γS_z represents the spin Zeeman term. For weak field, the magnetic field parameter falls in the interval $0 < \gamma \le 0.18$ a.u. For intermediate field, γ takes values in the interval $0.18 < \gamma < 2.071814$ a.u., and for strong field $\gamma > 2.071814$ a.u.

The VMC method is used to compute quantum expectation values of an operator with a given trial wave function. This method is a combination of the will-known variational principle and the Monte Carlo technique of evaluating multi-dimensional integrals. The variational principle states that the expectation value of the Hamiltonian H with respect to the trial wave function ψ_T is the varitional energy [24]:

$$E_{VMC} = \frac{\int \psi_T^*(\boldsymbol{R}) H \psi_T(\boldsymbol{R}) \mathrm{d}\boldsymbol{R}}{\int \psi_T^*(\boldsymbol{R}) \psi_T(\boldsymbol{R}) \mathrm{d}\boldsymbol{R}} \ge E_{exact}, \tag{2.4}$$

where $\boldsymbol{R}$ is the $3N$-dimensional vector of the electron coordinates and E_{exact} is the exact value of the energy of a given state. To evaluate E_{VMC}, Equation (2.4), we rewrite it as:

$$E_{VMC} = \int \frac{\left|\Psi_T(\boldsymbol{\mathcal{R}})\right|^2}{\left\langle \Psi_T \middle| \Psi_T \right\rangle} \frac{\left[\hat{H}\Psi_T(\boldsymbol{\mathcal{R}})\right]\mathrm{d}\boldsymbol{R}}{\Psi_T(\boldsymbol{\mathcal{R}})} = \int P(\boldsymbol{R}) E_L(\boldsymbol{R}) \mathrm{d}(\boldsymbol{R}), \tag{2.5}$$

where $P(\boldsymbol{R}) = \frac{\left|\Psi_T(\boldsymbol{R})\right|^2}{\int \left|\Psi_T(\boldsymbol{R})\right|^2 \mathrm{d}\boldsymbol{R}}$ is positive everywhere and interpreted as a probability distribution function and $E_L(\boldsymbol{\mathcal{R}}) = \frac{\left[\hat{H}\Psi_T(\boldsymbol{\mathcal{R}})\right]}{\Psi_T(\boldsymbol{\mathcal{R}})}$ is the local energy. Also, it is important to calculate the standard deviation of the energy [17] [18]:

$$\sigma = \sqrt{\frac{\left\langle E_L^2 \right\rangle - \left\langle E_L \right\rangle^2}{L(N-1)}} \tag{2.6}$$

where L is the ensemble size of random numbers $\left\{\boldsymbol{R}_1, \boldsymbol{R}_1, \cdots, \boldsymbol{R}_L\right\}$, which may be generated using a variety of methods and N is the number of ensembles. These ensembles so generated must reflect the distribution function itself.

At each of the points $\{\mathcal{R}_i\}$, the weighted average $E_L(\mathcal{R})$ is evaluated. After enough evaluations, the VMC estimate of E_{VMC} will be:

$$E_{VMC} = \langle E_L \rangle = \lim_{N\to\infty}\lim_{L\to\infty}\frac{1}{N}\frac{1}{L}\sum_{j=1}^{N}\sum_{i=1}^{L}E_L(\boldsymbol{R}_{ij}). \tag{2.7}$$

3. The Trial Wave Functions

In the VMC method, a good trial wave function, $\Psi_T(R)$, should exhibit much of the same features as does the exact wave function. One possible guideline in choosing the trial wave function is the use of the constraints about the behavior of the wave function when the distance between one electron and the nucleus or two electrons approaches zero. These constraints are called "cusp conditions" and are related to the derivative of the wave function. More details about the trial wave function can be found in [20] [24].

For the ground state of the lithium atom, $1s^2 2s$ and its isoelectronic ions, in the presence of weak magnetic field, we used the following trial wave function [14]:

$$\psi_1 = \psi_0 f \tag{3.1}$$

where

$$\begin{aligned}\psi_0 = \Big\{ &\alpha(1)\beta(2)\alpha(3)\left[e^{-\frac{(2r_1+2r_2+r_3)Z'}{2}}\left(1-\frac{r_3Z'}{2}\right)-\left(1-\frac{r_1Z'}{2}\right)e^{-\frac{(r_1+2r_2+2r_3)Z'}{2}}\right]\\ &+\alpha(1)\alpha(2)\beta(3)\left[\left(1-\frac{r_1Z'}{2}\right)e^{-\frac{(r_1+2r_2+2r_3)Z'}{2}}-\left(1-\frac{r_2Z'}{2}\right)e^{-\frac{(2r_1+r_2+2r_3)Z'}{2}}\right]\\ &+\beta(1)\alpha(2)\alpha(3)\left[\left(1-\frac{r_2Z'}{2}\right)e^{-\frac{(2r_1+r_2+2r_3)Z'}{2}}-\left(1-\frac{r_3Z'}{2}\right)e^{-\frac{(2r_1+2r_2+r_3)Z'}{2}}\right]\Big\}\end{aligned} \tag{3.2}$$

In the last equation, Z' is an effective charge, which is treated as a variational parameter, to minimize the energy. It is seen that 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 $S=\frac{1}{2}$ and its z-component is $M_S=\frac{1}{2}$. In Equation (3.2), α is a spin up function and β is a spin down function.

For the correlation function f, we considered the Jastrow correlation function which is a product of functions of the form [15]:

$$f = \prod_{i<j} f_{ij},\quad f_{ij} = \exp\left[\frac{r_{ij}}{l(1+kr_{ij})}\right]. \tag{3.3}$$

It seems very reasonable to enforce the cusp conditions on trial wave functions because they are obeyed by the exact wave function. These constraints lead to smoother behavior in the local energy, $E_L(\boldsymbol{R}) = \frac{\left[H\Psi_T(\boldsymbol{R})\right]}{\Psi_T(\boldsymbol{R})}$. When two particles interacting via the Coulomb potential approach one another, the potential ener-

gy diverges, and therefore the exact wave function must have a cusp so that the local kinetic energy, $\left[-(1/2)\Psi_T^{-1}(\boldsymbol{R})\nabla^2\Psi_T(\boldsymbol{R})\right]$, supplies an equal and opposite divergences. For the electron-nuclear cusp this condition is $\frac{1}{\Psi_T}\frac{\partial\Psi_T}{\partial r_i}\Big|_{r_i=0} = -Z$, where Z is the nuclear charge and r_i is any single electron-nucleus coordinate. Imposition of the cusp conditions is in fact very important in VMC calculations because divergences in the local energy led to poor statistical behavior and even instabilities in the calculations. In order that the function f satisfies the cusp conditions we must have:

$$l = \begin{cases} 4 & \text{for like spins} \\ 2 & \text{for unlike spins} \end{cases} \tag{3.4}$$

Hence, the ground state trial wave ψ_1 has two variational parameters, namely k and Z'. Since the wave functions and energies of the states are strongly dependent on the magnetic field strength, the configurations are also affected by the magnetic field. With increasing field strength, the ground state undergoes two transitions involving three different electronic configurations [25]. In fact, the configuration $1s^2 2s$ describes the ground state of lithium atom only for relatively weak fields.

For intermediate field regime, the ground state configuration changes to $1s^2 2p_{-1}$ configuration. To represent the atomic configuration of all the electrons in intermediate field, for ground state as well as for the low-lying excited states, another type of trial wave function is employed to obtain our results. This trial wave function is constructed from the hydrogen-like wave function as follows:

$$\psi_2(\boldsymbol{r}_1,\boldsymbol{r}_2,\boldsymbol{r}_3) = A\left[\varphi(\boldsymbol{r}_1)\varphi(\boldsymbol{r}_2)\varphi(\boldsymbol{r}_3)\prod_{i<j} f(r_{ij})\chi(s)\right] \tag{3.5}$$

where $\varphi(\boldsymbol{r}) = R_{nl}(r)Y_{lm}(\theta,\phi)$ is the usual hydrogen like function in nl state. The factor $f(r_{ij})$ is the correlation function given by Equation (3.3). In the above equation, $\chi(s)$ is the spin function, which is given by [26] [27]:

$$\chi(s) = \alpha(1)\beta(2)\alpha(3) - \beta(1)\alpha(2)\alpha(3). \tag{3.6}$$

In Equation (3.5), A is the three-particle anti symmetrizer $A = I - P_{12} - P_{13} - P_{23} + P_{231} + P_{312}$. Here, P_{ij} represents the permutation $i \leftrightarrow j$ and P_{ijk} stands for the permutation of 123 into ijk.

For the strong field, the ground state is constituted by $1s2p_{-1}3d_{-2}$. According to the azimuthal symmetry with respect to the magnetic field axis, cylindrical coordinates are suitable for representing the one-particle basis functions for strong field. Hence, in the case of strong field, the following Hylleraas-Gaussian basis set-trial wave function with cylindrical symmetry is a good candidate for highly precise calculations, for the ground as well as the low-lying excited states of lithium [28]:

$$\psi_3(\rho,\varphi,z,s) = A\left[\rho^{n_{\rho i}} z^{n_{zi}} \mathrm{e}^{-\alpha_i^2\rho^2-\beta_i^2 z^2} \mathrm{e}^{im_l\varphi}\chi(s) f\right], \tag{3.7}$$

where α_i, β_i are positive nonlinear variational parameters. The exponents $n_{\rho i}$ and n_{zi} obey the following restrictions: $n_{\rho i} = |m_i| + 2k_i$; $k_i = 0,1,2,\cdots$ with $m_i = \cdots,-2,-1,0,1,2,\cdots$. $n_{zi} = \pi_{zi} + 2l_i$; $l_i = 0,1,2,\cdots$ with $\pi_{zi} = 0,1$. In Equation (3.7), $\chi(s)$ is the spin function given by (3.6) and f is the correlation function given by (3.3). The function (3.7) is an eigenfunction of the z-component of the orbital angular momentum with an eigenvalue of m_i and is an eigenfunction of the z-parity with eigenvalue $(-1)^{\pi_{zi}}$. The Gaussian like expression $\rho^{|m_i|}\mathrm{e}^{-\alpha_i^2\rho^2}$ is identical to the ρ dependence of the lowest Landau state in the field B if we choose α_i to be $B/4$ and thus represents an adjustment to the existence of the magnetic field. Also, the monomials ρ^{2k_i} and $z^{n_{zi}}$ are suitable for describing excitations. At high field strengths, however, where the magnetic field destroys the spherical symmetry of the problem, an isotropic basis set method would be inefficient. The distribution of the α_i is chosen to be peaked around $B/4$, whereas the β_i are well tempered in a large regime [29].

4. Results and Discussions

In the present paper, we solved the Schrödinger equation for the lithium atom in a magnetic field under the assumption of an infinitely heavy nucleus. Accordingly, we applied the VMC method to calculate the ground state energies of the lithium atom in the magnetic field regime between 0 a.u. and 100 a.u. as well as the lithium like ions up to $Z = 10$. All energies are obtained in atomic units ($m_e = e = \hbar = 1$), with a set of 1×10^7 Monte Carlo integration points to make the statistical error as low as possible. Our calculations for the ground-state and the two-low lying excited states of the lithium atom in an external magnetic field are based on using three accurate trial wave functions ψ_1, ψ_2 and ψ_3. In Table 1, we present the best values of the calculated ground state energy and standard deviation of the lithium atom by using the three trial wave functions. The exact value of the ground state energy of Li is taken from [26].

In the presence of a magnetic field an atom and its physics is subject to a variety of changes. For instance, the conserved quantum numbers are reduced to the total angular momentum z-projection M, the total z-parity Π_z, the total spin z-projection S_Z and the total spin S^2. For weak fields up to $\gamma = 0.18$, the ground state arises from the field-free $1s^2 2s$ configuration. For intermediate fields ($0.18 < \gamma < 2.071814$), the ground state is constituted by the $1s^2 2p_{-1}$ configuration and for $\gamma > 2.071814$ the ground state configuration is $1s2p_{-1}3d_{-2}$.

In Table 2, we present our results for the behavior of the total energy at different

Table 1. Ground-state energy of Li, E, (in a.u.) and standard deviation (σ).

	E	σ
ψ_1	−7.47803	0.00006
ψ_2	−7.47801	0.00031
ψ_3	−7.47804	0.00004
Exact	−7.47806 [26]	---

Table 2. Ground and first excited states of the lithium atom (in a.u.) as functions of the magnetic field strength. Previous results are also given. Weak field: $0 < \gamma \le 0.18$, intermediate field: $0.18 < \gamma < 2.071814$, and strong field: $\gamma > 2.071814$. ψ_1 is used for weak field, ψ_2 for intermediate field, and ψ_3 for strong field.

γ	$1s^2 2s$			$1s^2 2p_{-1}$			$1s2p_{-1}3d_{-2}$	
	Our work E, σ	E [30]	E [31]	Our work E, σ	E [30]	E [31]	Our work E, σ	E [31]
0.0000	−7.47803 6×10^{-5}	−7.4327	−7.43272	−7.365092 3×10^{-5}	−7.3651	−7.36509	−5.083789 8×10^{-5}	−5.08379
0.0010	−7.433196 5×10^{-5}		−7.43326	−7.366091 3×10^{-5}		−7.36609	−5.086788 8×10^{-5}	−5.08679
0.0018	−7.433624 4×10^{-5}	−7.4337	−7.43367	−7.366889 3×10^{-5}	−7.3669	−7.36689	−7.089149 6×10^{-5}	−5.08915
0.0020	−7.433893 2×10^{-5}		−7.43375	−7.367089 4×10^{-5}		−7.36709	−7.089759 6×10^{-5}	−5.08976
0.0050	−7.435158 5×10^{-4}		−7.43522	−7.370011 3×10^{-5}		−7.37002	−5.098519 7×10^{-5}	−5.09852
0.0090	−7.437062 3×10^{-4}	−7.4371	−7.43711	−7.373875 3×10^{-5}	−7.3738	−7.37387	−5.109880 7×10^{-5}	−5.10988
0.0100	−7.437693 7×10^{-4}		−7.43760	−7.374806 3×10^{-5}		−7.37481	−5.112679 8×10^{-5}	−5.11268
0.0180	−7.441323 5×10^{-4}	−7.4412	−7.44122	−7.382177 4×10^{-5}	−7.3832	−7.38218	−5.134329 8×10^{-5}	−5.13433
0.0200	−7.442008 4×10^{-4}		−7.44214	−7.383969 7×10^{-5}		−7.38397	−5.139601 7×10^{-5}	−5.13960
0.0500	−7.453947 7×10^{-4}		−7.45398	−7.408443 4×10^{-5}		−7.40844	−5.212809 6×10^{-5}	−5.21281
0.0540	−7.455361 5×10^{-4}	−7.4553	−7.45532	−7.411407 5×10^{-5}	−7.4114	−7.41141	−5.221993 7×10^{-5}	−5.22199
0.1000	−7.468596 6×10^{-4}		−7.46857	−7.441757 5×10^{-5}		−7.44176	−5.321402 6×10^{-5}	−5.32140
0.1260	−7.473900 5×10^{-4}	−7.4739	−7.47401	−7.456497 5×10^{-5}	−7.4565	−7.45650	−5.373698 6×10^{-5}	−5.37371
0.17633	−7.481644 3×10^{-4}		−7.48162	−7.481618 5×10^{-5}		−7.48162	−5.467544 6×10^{-5}	
0.1800	−7.482032 4×10^{-4}	−7.4814	−7.48151	−7.482032 4×10^{-5}	−7.4832	−7.48330	−5.475679 6×10^{-5}	−5.47568
0.2000	−7.484008 3×10^{-4}		−7.48400	−7.492219 4×10^{-5}		−7.49220	−5.511509 6×10^{-5}	−5.51151
0.5000	−7.47740 5×10^{-4}		−7.47741	−7.587890 4×10^{-5}		−7.58790	−5.970519 7×10^{-5}	−5.97052
0.5400	−7.473515 8×10^{-4}	−7.4731	−7.47321	−7.597086 4×10^{-5}	−7.5965	−7.59709	−6.024139 7×10^{-5}	−6.02414
0.9000	−7.424827 5×10^{-4}	−7.4240	−7.42404	−7.656279 4×10^{-5}	−7.6563	−7.65628	−6.460609 7×10^{-5}	−6.46061
1.0000	−7.408674 3×10^{-4}		−7.40879	−7.666529 3×10^{-5}		−7.66653	−6.570809 7×10^{-5}	−6.57081

Continued

1.2600	−7.361833 4×10^{-4}	−7.3609	−7.36113	−7.682878 3×10^{-5}	−7.6820	−7.68288	−6.841219 8×10^{-5}	−6.84122
1.8000	−7.245712 3×10^{-4}	−7.2446	−7.24473	−7.676569 4×10^{-5}	−7.6747	−7.67657	−7.347229 8×10^{-5}	−7.34723
2.0000	−7.195953 2×10^{-4}		−7.19621	−7.662457 4×10^{-5}		−7.66246	−7.520029 8×10^{-5}	−7.52003
2.071814	−7.177415 3×10^{-4}		−7.17745	−7.656002 4×10^{-5}		−7.65600	−7.591011 8×10^{-5}	−7.58047
2.5000	−7.056177 3×10^{-4}		−7.05619	−7.603509 4×10^{-5}		−7.60351	−7.925319 8×10^{-5}	−7.92532
3.0000	−6.895463 4×10^{-4}		−6.89559	−7.515081 4×10^{-5}		−7.51516	−8.299185 8×10^{-5}	−8.29920
3.6000	−6.678665 5×10^{-4}	−6.6640	−6.66521	−7.376351 4×10^{-5}	−7.3627	−7.37638	−8.714639 8×10^{-5}	−8.71464
5.0000	−6.088033 1×10^{-4}		−6.08811	−6.942290 4×10^{-5}		−6.94230	−9.576939 8×10^{-5}	−9.57694
5.4000	−5.901022 4×10^{-4}	−5.8772	−5.88103	−7.795135 4×10^{-5}	−6.7747	−7.79517	−9.801468 7×10^{-5}	−9.80147
7.0000	−5.088876 2×10^{-4}		−5.08909	−6.126681 4×10^{-5}		−6.12670	−10.62577 8×10^{-5}	−10.62578
10.00	−3.357665 4×10^{-4}		−3.35777	−4.617673 4×10^{-5}		−4.61777	−11.939017 8×10^{-5}	−11.93902
20.00	3.491142 4×10^{-4}		3.49120	1.705552 4×10^{-5}		1.70565	−15.162585 7×10^{-5}	−15.16260
50.00	27.690166 5×10^{-4}		27.6916	24.97934 4×10^{-5}		24.97942	−21.050482 6×10^{-5}	−21.0505
100.00	71.806551 5×10^{-4}		71.807	68.17336 4×10^{-5}		68.1735	−27.019189 7×10^{-5}	−27.0192

values of the magnetic field strength γ. The previous values obtained in [30] [31] are also presented for comparison. It is seen from **Table 2** that our energy values are in excellent agreement with the corresponding previous works for all values of $\gamma > 0$. It is clear that the energy values of the ground state of the lithium atom in the presence of magnetic field are closer to the values obtained by Wang and Qiao [30] for the ground as well as the two states $1s^2 2s$ and $1s^2 2p_{-1}$. In the absence of the field, our result is in excellent agreement with the exact value.

Also, we calculated the total energies of the lithium like ions up to $Z = 10$ as functions of the magnetic field. In **Table 3**, we present the total energies of the lithium like ions by using the trial wave function ψ_3. In most cases of **Table 3**, the obtained results are in good agreement with the exact values. The associated standard deviations have very small values, which vary between 10^{-5} and 10^{-4}. This is due to the large number of VMC points. It is clear from **Table 3** that our result for the ground state of the lithium atom ($Z = 3$) is −7.69085 (a.u.), which is very close to the value of [32].

Table 3. The energy values E (a.u.) and the magnetic field strengths γ as the ground state configuration changes for lithium-like ions. The standard deviations, σ, of our results are also given.

Z	γ	E (a.u.) σ Our work	E [32] (a.u.)
3	0.12212	−7.69085 1×10^{-4}	−7.6905
4	0.14229	−15.0576 4×10^{-5}	−15.0670
5	0.15510	−24.9326 4×10^{-5}	−24.9386
6	0.16404	−37.3084 3×10^{-5}	−37.309
7	0.17059	−52.1764 6×10^{-5}	−52.184
8	0.17556	−69.545 4×10^{-5}	−69.551
9	0.17947	−89.114 7×10^{-6}	−89.418
10	0.18266	−111.653 6×10^{-6}	−111.783

To demonstrate the behavior of the total energies of the lithium like ions against the change in the magnetic field strength, the energies are calculated at a fixed value of $\gamma = 0.12212$ by using the trial wave function ψ_2 with the corresponding standard deviation σ. The obtained results are listed in **Table 4**. **Figure 1** shows the variation of the ground state total energy versus the magnetic field strength γ (a.u.) for the three states $1s^2 2s, 1s^2 2p_{-1}$ and $1s2p_{-1}3d_{-2}$. In weak, field $0 < \gamma \le 0.18$, the state $1s^2 2s$ represents the ground state of lithium atom. It is a doubly tightly bound state, *i.e.*, it involves two tightly bound orbitals of $1s$ character. The $2s$ electronic charge distribution along the z axis expands slightly in weak magnetic fields. Also, we remark that the total energy decreases because of the spin Zeeman-effect. On the other hand, as the field gets larger, the system tends to shrink, and by raising the angular momentum of the most exterior electron, the atom can increase the electronic separation. In the intermediate field regime, the crossover from configuration $1s^2 2s$ to $1s^2 2p_{-1}$ is found to occur at $\gamma \approx 0.18$. For $\gamma > 2.071814$, the ground state configuration will be $1s2p_{-1}3d_{-2}$ which represents the ground state of the lithium atom for high field strengths. For this configuration, in which all single-electron binding energies increase unlimited for $\gamma \to \infty$, a shrinking process of this distribution in z direction is also visible. In general, one can see that for each separate configuration, the effect of the increasing field strength consists in compressing the electronic distribution towards the z axis and the spherical symmetry of the atom is clearly broken.

Moreover, we remark that the total energy decreases because of the spin Zeeman-effect. On the other hand, as the field gets larger, the system tends to shrink,

Table 4. Total energies of the lithium like ions versus Z, up to $Z = 10$, for a fixed value of $\gamma = 0.12212$ a.u. by using the trial wave function ψ_2 with the corresponding standard deviation σ.

Z	E(a.u.)	σ
4	−15.0563	7×10^{-4}
5	−24.8867	6×10^{-4}
6	−37.256	6×10^{-4}
7	−52.1563	8×10^{-4}
8	−69.487	6×10^{-4}
9	−89.106	5×10^{-4}
10	−111.617	8×10^{-4}

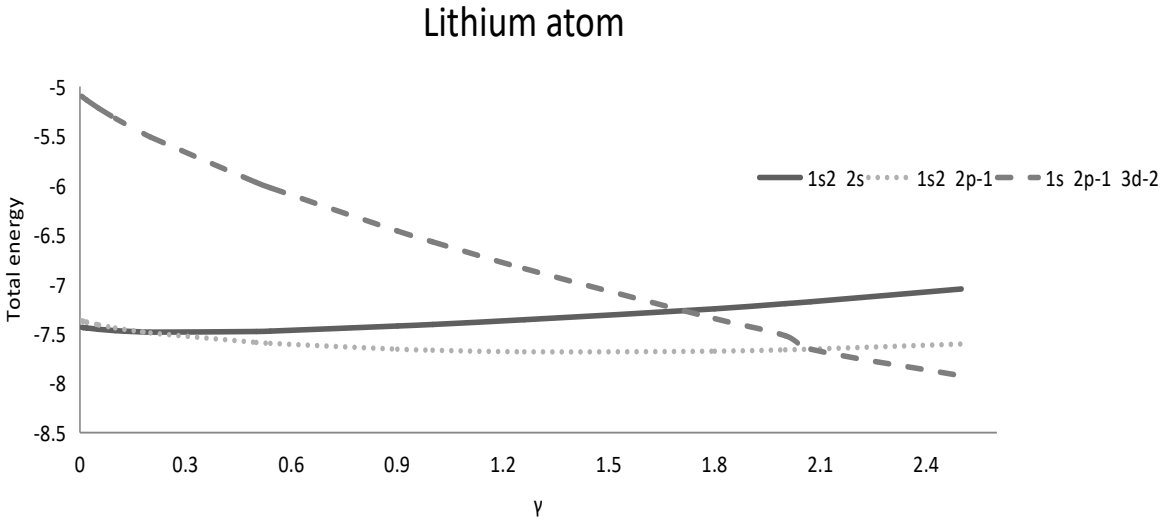

Figure 1. The total energy versus the magnetic field strength γ (a.u.) for the states $1s^2 2s$, $1s^2 2p_{-1}$ and $1s2p_{-1}3d_{-2}$.

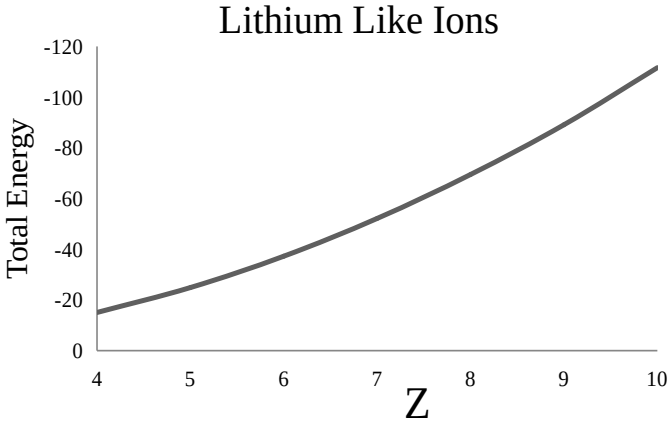

Figure 2. Total energies of the lithium like ions (at $\gamma = 0.12212$) versus Z, up to $Z = 10$.

and by raising the angular momentum of the most exterior electron, the atom can increase the electronic separation. Furthermore, we present in **Figure 2** the

total energies of the lithium like ions (at $\gamma = 0.12212$) versus Z, up to $Z = 10$, by using the trial wave function ψ_2.

5. Conclusions

In the present paper, we used the well-known VMC method, with a set of 1×10^7 Monte Carlo integration points to make the statistical error as low as possible, to study the ground state of the lithium atom and its like ions up to $Z = 10$ in the presence of a magnetic field. Also, we present the results of calculating the energies of the first two excited states of the lithium atom in the external magnetic field. The method is flexible enough to yield precise results for arbitrary field strengths. Our calculations for the ground and first two excited states are performed for magnetic field strengths ranging from zero up to $\gamma = 100$. The effect of increasing the magnetic field on the ground state is studied. With increasing field strength, the ground state undergoes two transitions involving three different electronic configurations. For small values of γ (weak field) the state $1s^2 2s$ represents the ground state where for intermediate and strong fields the ground state configuration arises from the $1s^2 2p_{-1}$ and $1s2p_{-1}3d_{-2}$ configurations, respectively. The transition field strengths are determined and precise values for the field strength parameter γ corresponding to the crossovers of the ground state configurations are obtained. For this purpose, suitable types of trial wave functions are used to gain greater flexibility in representing the different atomic configurations when the magnetic field increases, and the cylindrical symmetry associated with the magnetic field becomes dominant. For the weak field, we used a trial wave function which 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 $S = \frac{1}{2}$ and its z-component is $M_S = \frac{1}{2}$. For the intermediate field, where the ground state configuration changes to $1s^2 2p_{-1}$ configuration, we used for the ground state as well as for the low-lying excited states another type of trial wave function. This trial wave function is constructed from the hydrogen-like wave function as explained in Section 3.

For strong field, our calculations are based on using a compact few-parameter trial wave function which can be considered as the most accurate among several existing few-parameter trial wave functions for the lithium atom and its ions. Our results for the total energies exhibit good accuracy comparing with the existing data in the literature.

The energies were plotted as functions of the magnetic field strengths γ to show graphically the effect of the magnetic field on the behavior of the total energy. We conclude that the presented analysis introduced in this paper ensures that the VMC method can be considered as an efficient tool to study the three-electron system under the effect of the strong magnetic field. Furthermore, our results confirm that the chosen trial wave functions are more efficient in the low and high field regimes.

Conflicts of Interest

The author declares no conflicts of interest regarding the publication of this paper.

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