

Ground States of Few Electron Atoms in a Strong Magnetic Field Using Diffusion Monte Carlo Method

S. B. Doma^{1*}, N. A. El-Nohy², M.A. Salem²

¹Dept. of Mathematics and Computer Science, Faculty of Science, Alexandria University, Egypt

^{2,3}Dept. of Physics, Faculty of Science, Alexandria University, Egypt

*Corresponding Author: sbdoma@alexu.edu.eg, Tel.: +20-12239-91249

Available online at: www.isroset.org

Received: 23/Jan/2020, Accepted: 07/Feb/2020, Online: 28/Feb/2020

Abstract— We applied the diffusion quantum Monte Carlo method to investigate the effect of a strong magnetic field on the few-electron atoms. Gaussian type orbital basis sets are used in the computations developed by using Post-Hartree-Fock methods. We calculated the ground state energy eigenvalues of the helium, lithium, beryllium, and boron atoms. The advantages of adding the electrons correlations to the wave function in the technique of diffusion Monte Carlo method enabled us to solve the Schrödinger equation for these atoms in the external magnetic field for different strengths. The method showed good agreements with the previous results.

Keywords— Diffusion Monte Carlo method, Few electron atoms, Strong magnetic field

I. INTRODUCTION

Quantum Monte Carlo (QMC) is a computational method that uses Monte Carlo techniques to solve many-body quantum problems. There are several different QMC techniques, which vary from exact to the approximate solution of Schrödinger's equation for different types of Hamiltonians. The first approximation method in this field is the variational Monte Carlo (VMC) method. This method depends on the choice of the trial wave function. If this function is close to the exact wave function, then the rate of convergence is higher, and the approximation will be small. If there is a parameter in physics not contained in the wave function, the approximation will be larger. Simpler ground state wave functions may be preferred over complex ground state wave functions because they are easier to parameterize. There are two main options to optimize the wave function. The first is direct energy optimization, and this approach is difficult to achieve. However, modern energy optimization methods can optimize thousands of parameters in the trial wave function, such as the steepest descent method and gradient descent method. The second is variance optimization, which is an older, but still, effective technique to optimize wave functions. It is directly related to the zero variance principle. The variance optimization technique minimizes the variance of the local energy by varying the parameters of the wave function. The variance optimization is more efficient than the energy optimization [1].

The diffusion QMC (DQMC) method is suitable to describe the ground state of many quantum systems [2]. In this method, Schrödinger's equation is solved by assuming imaginary time τ . The DQMC method based on the

evolution of the wave function in imaginary time can determine both the ground state energy and the ground state wave function of a quantum system, regardless of the initial state in which the system is prepared. The first formulation of the DQMC method depends on the similarity between the imaginary time Schrödinger's equation and a generalized diffusion equation. The potential energy term of the Schrödinger's equation corresponds to the diffusion (source/sink or reaction) term in the generalized diffusion equation. The diffusion-reaction equation is solved by employing stochastic calculus as it first suggested by Fermi around 1945 [3]. The imaginary time Schrödinger's equation was solved by simulating random walks of particles according to (birth/death) processes imposed by the (source/sink) term. The formulation of the DQMC method given for the first time by Anderson [4], who used this method to calculate the ground state energy of small molecules such as H_3^+ . The second formulation of the DQMC method arises from the Feynman path integral solution of the time-dependent Schrödinger's equation. The wave function is expressed as a multi-dimensional integral which is evaluated by employing the Monte Carlo method [5].

DQMC method has become increasingly important to the solution of Schrödinger's equation for atoms, molecules and solids, as described by W. A. Lester et al. [6]. The method showed to exhibit high accuracy that scales better with system size than other methods. J. Kolorenč and L. Mitas [7] represented QMC methods as a powerful and broadly applicable computational tool in condensed systems. They concentrated on the (fixed-node/fixed-phase) DQMC method with an emphasis on its applications to the electronic structure of solids and other extended many-particle systems.

DQMC method was introduced by T. Pang [8] at an elementary level. He highlighted the strengths of the method in addressing important issues associated with quantum many-body systems, such as those associated with the ground-state energy and pair-distribution function. ⁴He clusters trapped on a graphite surface simulated as an example of the method. He provided a sample program and documentation for developing simulation projects.

Foulkes et al. [9] described the variational and fixed-node DQMC methods and how they may be used to calculate the properties of many-electron systems. These stochastic wave-function-based approaches provide very direct treatment of quantum many-body effects.

The most important investigation about atoms in a strong magnetic field is the work done by Schmelcher et al. for helium [10], lithium [11],[12], beryllium [13],[14], and boron [15]. They developed a wave function based on Gaussian one-particle basis set in cylindrical coordinates using the numerical mesh method.

Yu. P. Kravchenko and M. A. Liberman [16] showed that systematically constructed Gaussian-type basis sets applied to the simplest one-electron systems in the magnetic field varying from 0 to 2×10^8 (T) can reliably provide accuracy of 10^{-6} Hartrees and better.

M. D. Jones, G. Ortiz and D. M. Ceperley, [17] presented comprehensive calculations of the electronic structure of selected first-row atoms in uniform magnetic fields of strength $\leq 10^6$ (T), within a flexible implementation of the Hartree-Fock formalism. In [17] the ground-state and low-lying excited state properties are presented for first-row atoms He, Li, C, and ion H⁻. The authors predicted and described a series of ground-state quantum transitions as a function of magnetic field strength. Due to its astrophysical importance, highly excited states of neutral helium computed.

Accurate theoretical and experimental methods used to investigate the behavior of atoms in a strong magnetic field. W. Zhu and S. B. Trickey [18] used anisotropic Gaussian type orbital basis functions to calculate H through C ($1 \leq Z \leq 6$) and ions Li⁺, Be⁺ and B⁺ in a wide range of magnetic field (B) ($0 \leq B \leq 2000$ (a.u.)) which showed an accuracy better than single-electron basis sets. Abdullah Zafar et al. [19] used active laser spectroscopy to make high-resolution magnetic field measurements in hydrogen and helium plasmas.

S. B. Doma et al. [20],[21],[22] tested a variety number of wave functions using variational QMC technique in the presence of a magnetic field of strength in the range ($0 \leq B \leq 100$ (a.u.)). Their results showed good accuracy, using in consideration the effect of correlation wave functions, especially the Jastrow wave function.

The present paper aims to apply the DQMC method to calculate the energy eigenvalues of the He, Li, Be and B

atoms in a strong magnetic field. The Born-Oppenheimer approximation and the Hamiltonian operator described in section II. The method of calculations discussed in section III. The used trial wave function illustrated in section IV. The results and discussions showed in section V and the overall conclusion given in section VI.

II. THE HAMILTONIAN OPERATOR

In this section, we assume, as usual, that the nuclear mass is infinite and the magnetic field is oriented along the z-axis. Hence, the non-relativistic Hamiltonian H_M for an atom consisting of N electrons presented in a homogeneous magnetic field can be written, in a. u. as [20]:

$$H_M = -\frac{1}{2} \sum_{i=1}^N \nabla_i^2 - \sum_{i=1}^N \frac{Z}{r_i} + \sum_{i=1}^N \sum_{(i<j)} \frac{1}{r_{ij}} + \frac{1}{8} B^2 \rho^2 + \frac{B(L_z + 2S_z)}{2} \quad (1)$$

where B is the strength of the magnetic field in atomic units and N is the number of electrons, $\rho^2 = \sum_{i=1}^N (x_i^2 + y_i^2)$, S_z is the z-component of the total spin, L_z is the z-component of the total orbital angular momentum, $\frac{B^2 \rho^2}{8}$ is the diamagnetic term, $\frac{B}{2} L_z$ is the Zeeman term and $B S_z$ represents the spin Zeeman term.

III. THE METHOD OF CALCULATIONS

The strategy of the DQMC method is to map the time-dependent Schrödinger's equation into an imaginary-time diffusion equation. The time-dependent Schrödinger's equation is given by

$$i\hbar \frac{\partial \Psi(\mathbf{R}, t)}{\partial t} = H \Psi(\mathbf{R}, t) \quad (2)$$

Performing a trivial, but methodologically crucial shift of the energy scale by introducing the replacements $V(R) \rightarrow V(R) - E_R$ and $E_n \rightarrow E_n - E_R$, the time-dependent Schrödinger's equation can be interpreted as the diffusion equation with imaginary-time, as illustrated in ref. [23]. This leads to the Schrödinger equation

$$\frac{\partial \Psi(\mathbf{R}, \tau)}{\partial \tau} = -(H - E_R) \Psi(\mathbf{R}, \tau) \quad (3)$$

where E_R is a reference energy that interpreted as the zero point of the system's energy at the given moment and the imaginary time $\tau = i t / \hbar$, with t being the real time from the original Schrödinger's equation. Here E_R is adjusted at each time step in the actual simulation so that the simulation will converge faster. The solution of the diffusion equation (3) can symbolically rewrite as

$$\Psi(\mathbf{R}, \tau) = e^{-(H - E_R)\tau} \Psi(\mathbf{R}, 0) \quad (4)$$

provided that we started from an initial state $\Psi(\mathbf{R}, 0)$.

A good choice for the initial configuration is $\Psi(\mathbf{R}, 0) = \Phi(\mathbf{R})$, the trial wave function that we have already found from the variational QMC simulation. We can multiply the imaginary-time Schrödinger's equation by $\Phi(\mathbf{R})$ and

rewrite it as a diffusion equation for $f(\mathbf{R}, \tau) = \Phi(\mathbf{R})\Psi(\mathbf{R}, \tau)$, as follows:

$$\frac{\partial f(\mathbf{R}, \tau)}{\partial \tau} = \frac{\hbar^2}{2m} \nabla^2 f(\mathbf{R}, \tau) - \nabla \cdot [\mathbf{v}(\mathbf{R})f(\mathbf{R}, \tau)] - [E_L(\mathbf{R}) - E_R]f(\mathbf{R}, \tau) \quad (5)$$

where the local energy $E_L(\mathbf{R})$ and $f(\mathbf{R}, \tau)$ interpreted as a distribution function of the system with configuration \mathbf{R} at time τ if $f(\mathbf{R}, \tau)$ is always positive. The vector

$$\mathbf{v}(\mathbf{R}) = \frac{\hbar^2}{m} \nabla \ln |\Phi(\mathbf{R})| \quad (6)$$

interpreted as a drift velocity of the distribution in configuration space.

It is clear from the form of equation (5) that the time evolution of $f(\mathbf{R}, \tau)$ influenced by three contributions, a pure diffusion term involving ∇^2 , a drift term involving \mathbf{v} , and a source/sink term involving $E_L - E_R$.

The short-time evolution of $f(\mathbf{R}, \tau)$ is given by

$$f(\mathbf{R}', \tau + \Delta\tau) = \int G(\mathbf{R}', \mathbf{R}; \Delta\tau) f(\mathbf{R}, \tau) d\mathbf{R} \quad (7)$$

where the propagator

$$G(\mathbf{R}', \mathbf{R}; \Delta\tau) = \left[\frac{1}{2\pi\mu^2} \right]^{\frac{3N}{2}} e^{-[\mathbf{R}' - \mathbf{R} - \Delta\tau\mathbf{v}(\mathbf{R})]^2 / 2\mu^2 - \Delta\tau[E_L(\mathbf{R}) - E_R]} \quad (8)$$

carries the system from configuration \mathbf{R} at time τ to the new configuration \mathbf{R}' at time $\tau + \Delta\tau$. Where $\mu^2 = \hbar^2 \Delta\tau / m$ is variance of Gaussian distribution.

What is left in the propagator is a contribution which either lowers or raises the population of configurations in the ensemble according to the birth/death rate

$$W_B(\mathbf{R}) = e^{-\Delta\tau[E_L(\mathbf{R}) - E_R]} \quad (9)$$

The lower the value of the local energy $E_L(\mathbf{R})$, the higher the rate. This part of the contributions in the propagator sampled by a branching process: copies of the configuration \mathbf{R} created to be part of the new ensemble and a mechanism, which does not influence the relative weight of each configuration, needs to control the overall number of configurations in the ensemble. Usually, this control did by adjusting the reference energy. For a boson system, the function $f(\mathbf{R}, \tau)$ behaves as a true distribution, which is real and positive. But for a fermion system, the wave function has a nodal structure that is usually unknown, and further approximations have to make because of the fermion-sign problem.

The ground-state energy obtained from the time-dependent variational energy interpreted as an average sampled over the distribution function $f(\mathbf{R}, \tau)$. For example, if we have an ensemble of N_E configurations $\mathbf{R}_1, \mathbf{R}_2, \dots, \mathbf{R}_{N_E}$, distributed according to $f(\mathbf{R}, \tau)$, the average energy is given by

$$E(\tau) = \frac{\langle \Phi | H | \Psi \rangle}{\langle \Phi | \Psi \rangle} = \frac{\int E_L(\mathbf{R}) f(\mathbf{R}, \tau) d\mathbf{R}}{\int f(\mathbf{R}, \tau) d\mathbf{R}} = \frac{\sum_{i=1}^{N_E} E(\mathbf{R}_i) W_B(\mathbf{R}_i)}{\sum_{i=1}^{N_E} W_B(\mathbf{R}_i)} \quad (10)$$

which becomes the exact ground-state energy E_0 at infinite time as $f(\mathbf{R}, \tau)$ approaches its limiting value.

To reduce the branching fluctuations, we can replace the local energy $E_L(\mathbf{R})$ in $W_B(\mathbf{R})$ by the average energy of the old and new configurations, $[E_L(\mathbf{R}) + E_L(\mathbf{R}')]/2$, resulting in a smoother propagator. Also, a Metropolis [24] move can be inserted between the configuration update and branching with the acceptance probability

$$p = \min \left\{ 1, \frac{|\Phi(\mathbf{R}')|^2 G(\mathbf{R}, \mathbf{R}'; \Delta\tau)}{|\Phi(\mathbf{R})|^2 G(\mathbf{R}', \mathbf{R}; \Delta\tau)} \right\} > \eta [0, 1] \quad (11)$$

for the new configuration \mathbf{R}' . This additional step ensures detailed balance between \mathbf{R} and \mathbf{R}' in configuration space. For a fermion system, the fixed-node approximation [25] can introduce to reject any attempt that would cross a node in the trial wave function. Several methods introduced to relax the nodes of the guide wave function with only limited success due in part to the intrinsic complexity of the fermion-sign problem [26].

VI. THE TRIAL WAVEFUNCTION

In the DQMC technique, we use the trial wave function as a guide wave function. It consists of basis functions to represent the electronic wave function. Several types of atomic orbitals are using: Gaussian-type orbitals, Slater-type orbitals, or numerical atomic orbitals. Gaussian-type orbitals [27] are the most using functions, as they allow efficient implementations of Post-Hartree-Fock methods.

In computational physics, Post-Hartree-Fock methods are the set of methods developed to improve on the Hartree-Fock (HF), or self-consistent field (SCF) method. They add electron correlation in a more accurate way of including the repulsions between electrons than in the HF method, where repulsions only averaged.

One of the most widely used basis sets is those developed by Dunning and coworkers [28],[29] from hydrogen to neon since they designed for converging Post-HF calculations systematically to the complete basis set limit using empirical extrapolation techniques.

For first and second-row atoms, the basis sets are cc-pVNZ where $N = D, T, Q, 5, 6, \dots$ ($D =$ double, $T =$ triples, etc.). The 'cc-p', stands for 'correlation-consistent polarized' and the 'V' indicates they are valence-only basis sets. They include successively larger shells of polarization (correlating) functions (d, f, g, etc.). More recently, these 'correlation-consistent polarized' basis sets have become widely used and are the current state of the art for correlated or post-HF calculations.

For fermionic systems, the many-body wave function is antisymmetric under particle exchange. The simplest antisymmetric function one can choose is the Slater determinant, often referred to as the HF approximation. This determinant constructed from products of orbitals and spins functions in the form

$$\Psi(\mathbf{r}_1, \mathbf{r}_2, \dots, \mathbf{r}_N) = \frac{1}{\sqrt{N!}} \begin{vmatrix} \phi_1(\mathbf{r}_1) & \phi_1(\mathbf{r}_2) & \dots & \phi_1(\mathbf{r}_N) \\ \phi_2(\mathbf{r}_1) & \phi_2(\mathbf{r}_2) & \dots & \phi_2(\mathbf{r}_N) \\ \vdots & \vdots & \ddots & \vdots \\ \phi_N(\mathbf{r}_1) & \phi_N(\mathbf{r}_2) & \dots & \phi_N(\mathbf{r}_N) \end{vmatrix} \quad (12)$$

where \mathbf{r}_i denotes the position and spin of the i^{th} electron. Our used form of the functions ϕ_j is simply in the form of Cartesian primitive Gaussian functions

$$\phi_j = \sum_{i=1}^n c_i x^{l_x} y^{l_y} z^{l_z} e^{-\zeta r^2} \quad (13)$$

The atomic orbitals is in Cartesian Gaussian atomic function where n is the number of basis, ζ is exponent and c_i is contraction coefficient, l_x , l_y and l_z are the angular momenta in x -axis, y -axis and z -axis respectively.

The effect of adding a correlation function to the wave function is important in this field of quantum mechanics [30]. T. H. Dunning [29] used the HF technique to describe the electrons' correlation effects. He showed that the compact sets of primitive Gaussian functions obtained to describe the correlation effects for the first-row of atoms. The calculations of the correlated atomic orbitals yielded functions taken to be simple primitive Gaussian functions in exponent ζ .

V. RESULTS AND DISCUSSION

In the present paper, we applied the DMC method to calculate the ground-state energy eigenvalues of the helium, lithium, beryllium, and boron atoms in the magnetic field regime between 0 to 100 (a. u.). All energies are in atomic units ($m_e = e = \hbar = 1$). Also, the magnetic field strength is in atomic units ($1 \text{ a.u.} = 2.35 \times 10^5 \text{ T}$). Since the wave functions and energies of the atomic states are strongly dependent on the magnetic field strength (weak, intermediate, and strong), the configurations are also affected by the magnetic field. So, the state of a given atom may undergo another transition involving different electronic configurations. Although the values of S_z and L_z for the ground state of a given atom must be negative for $B \rightarrow \infty$ [11], we fixed the configuration states of the four atoms for the same values of S_z and L_z to get the lowest energy eigenvalues of these atoms.

A. Ground State of Helium Atom in a Strong Magnetic Field

In Table 1, we present the ground state of the helium atom with electronic configuration $1s^2$ in a magnetic field strength from $B = 0$ (a.u.) up to $B = 100$ (a.u.). The numerical results of energies for the singlet state gave for $L_z = 0$ and $S_z = 0$. The DMC technique shows the most accurate calculated energy for the ground state of the helium atom in the absence of an external magnetic field ($E_{\text{exact}} = -2.903724377$ (a.u.)) [31].

Table 1 Calculated energies of the helium atom in a strong magnetic field.

B (a. u.)	[32]	[33]	Our Work
0	-2.9037155	-2.903473	-2.903724
0.01	-2.9036898	-2.903451	-2.903708
0.02	-2.9036275	-2.903386	-2.903419
0.05	-2.9032106	-2.902966	-2.902333
0.1	-2.9017263	-2.901479	-2.902067
0.2	-2.8958159	-2.895499	-2.896806
0.5	-2.8562141	-2.855906	-2.856697
1	-2.7302745	-2.730015	-2.731095
2	-2.3305260	-2.330270	-2.329547
5	-0.5757384	-0.575411	-0.575997
10	3.0636900	3.064202	3.065334
20	11.2660889	11.266617	11.269696
50	38.0754859	38.07607	38.086737
100	84.9176979	84.918049	84.978872

B. Ground State of Lithium Atom in a Strong Magnetic Field

For the ground state of lithium atom with electronic configuration $1s^2 2s$, we calculate the lithium atom in a strong magnetic field from $B = 0$ (a. u.) up to $B = 100$ (a. u.). For energies in [11], 2D mesh HF method applied using Gaussian basis sets as wave function. In. [23] variational Monte Carlo applied using three different wave functions for weak, intermediate and strong magnetic field strength regions. Table 2 contains the total energies obtained for the Li atom within our calculations in comparison with the data obtained from pervious results. The numerical results of energies for Li is given for $L_z = 0$ and for $S_z = -\frac{1}{2}$. The DMC technique shows approximately coincide with the exact energy for the ground state of lithium atom in the absence of a magnetic field ($E_{\text{exact}} = -7.4780603$ (a. u.)) [34]. Although the ground state of the lithium atom in free space has $S_z = \frac{1}{2}$, its free energy eigenvalue does not affected by the sign of S_z since the Hamiltonian is independent of the spin in this case.

Table 2 Calculated energies of lithium atom in a strong magnetic field.

B (a.u.)	[11]	[23]	Our Work
0	-7.43275	-7.432748	-7.478060
0.01	-7.43760	-7.437693	-7.483708
0.02	-7.44214	-7.442008	-7.488281
0.05	-7.45398	-7.455361	-7.499798
0.1	-7.46857	-7.468596	-7.514892
0.2	-7.48400	-7.484008	-7.531183
0.5	-7.47741	-7.47740	-7.521804
1	-7.40879	-7.408674	-7.447062
2	-7.19621	-7.195953	-7.227530

5	-6.08811	-6.088033	-6.100468
10	-3.35777	-3.357665	-3.355567
20	3.49120	3.491142	3.537065
50	27.6916	27.690166	27.878768
100	71.807	71.806551	71.788331

C. Ground State of Beryllium Atom in a Strong Magnetic Field

The ground state of the beryllium atom in external uniform magnetic fields calculated by means of 2D mesh Hartree-Fock [13] method for field strengths ranging from zero up to 100 (a.u.). The ground state configuration arises from the $1s^2 2s^2$, $L_z = 0$ and $S_z = 0$ electronic configuration. Table 3 presents the energies for each magnetic field strength, and our method shows more accurate ground state energy for $B = 0$, ($E = -14.667388$ (a.u.)), relative to ($E_{exact} = -14.66741$ (a.u.)) [35].

Table 3 Calculated energies of beryllium atom in a strong magnetic field.

B (a.u.)	[13]	Our Work
0	-14.57336	-14.667388
0.01	-14.57322	-14.666840
0.02	-14.57279	-14.666773
0.05	-14.56986	-14.664083
0.15	-14.54367	-14.639779
0.3	-14.46861	-14.562269
0.5	-14.32860	-14.407258
1	-13.89120	-13.926043
2	-12.88908	-12.747120
5	-9.40602	-8.996774
10	-2.5988	-1.994677
20	12.8201	13.640027
50	64.186	65.334582
100	155.286	156.465700

D. Ground State of Boron Atom in a Strong Magnetic Field

The ground state of the boron atom in external uniform magnetic fields calculated by means of 2D mesh Hartree-Fock [15] method for field strengths ranging from zero up to 100 (a.u.). The ground state configuration arises from the $1s^2 2s^2 2p$, $L_z = -1$ and $S_z = -\frac{1}{2}$ electronic configuration. Table 4 presents the energies for each magnetic field strength, and our method shows more accurate ground state energy for $B = 0$, ($E = -24.652550$ (a.u.)), relative to ($E_{exact} = -24.65391$ (a.u.)) [36].

Table 4 Calculated energies of boron atom in a strong magnetic field.

B (a. u.)	[15]	Our Work
0	-24.53029	-24.652550
0.01	-24.54018	-24.662494
0.02	-24.54976	-24.670772
0.05	-24.57679	-24.704070
0.1	-24.61631	-24.746664
0.2	-24.67634	-24.822167
0.5	-24.73975	-24.867051
1	-24.63172	-24.749681
2	-23.57727	-24.075196
5	-21.81614	-21.312714
10	-16.68963	-15.855869
20	-3.92689	-2.837486
50	—	44.224268
100	—	136.750344

VI. CONCLUSION

In the present paper, we applied the DMC method to investigate the effect of an external uniform magnetic field on the ground states of the helium, lithium, beryllium, and boron atoms, covering a broad regime of field strengths from $B = 0$ up to $B = 100$ a.u. Using the trial wave functions developed by Dunning and coworkers [28],[29], we determined the ground states of helium ($E = -2.903724$ (a.u.)), lithium ($E = -7.478060$ (a.u.)), beryllium ($E = -14.667388$ (a.u.)), and boron ($E = -24.652550$ (a.u.)) atoms with energies approximately close to the exact ones. We considered the advantage of adding the electron correlation to the wave function and the advantage of imaginary time in the guide wave function, as shown in the technique of the method, to solve Schrödinger's equation for these atoms in the external magnetic field with different strengths. We used 12000 initial configurations, which are distributed in space to make up some initial wave functions for each atom and begin the diffusion for each magnetic field strength. The results showed that for each atom configuration, there is a magnetic field strength in which the atom transforms into a higher electronic excited state. The magnetic field strength transitions from the ground state configuration to the higher configurations are: for helium at $B = 0.08$ (a.u.) [10], for lithium at $B = 0.17633$ (a.u.) [11], for beryllium at $B = 0.0412$ (a.u.) [13] and for boron at $B = 0.0778$ (a.u.) [15]. The best results achieved in this work are obtained by taking $\Delta\tau$ between 0.002 (HA^{-1}) and 0.005 (HA^{-1}). The method showed good agreement with the previous results.

REFERENCES

- [1] L. K. Wagner, "First-Principles Quantum Monte Carlo," in *Encyclopedia of Nanotechnology*, Springer, **Dordrecht**, pp. **1217 - 1223**, **2016**.
- [2] Xiaojun Zhou and Fan Wang, "Singlet-triplet gaps in diradicals

- obtained with diffusion quantum Monte Carlo using a Slater-Jastrow trial wavefunction with a minimum number of determinants," *Phys. Chem. Chem. Phys.*, Vol. **21**, Issue. **36**, pp. **20422–20431**, **2019**.
- [3] Zakarya Zarezadeh and Giovanni Costantini, "Particle diffusion Monte Carlo (PDMC), *Monte Carlo Methods Appl.*, Vol. **25**, Issue. **2**, pp. **120–130**, **2019**.
- [4] J. B. Anderson, "A random-walk simulation of the Schrödinger equation: H^{3+} ," *J. Chem. Phys.*, Vol. **63**, Issue. **4**, pp. **1499–1503**, **1975**.
- [5] J. E. Lynn, I. Tews, S. Gandolfi and A. Lovato, "Quantum Monte Carlo Methods in Nuclear Physics: Recent Advances," *Annu. Rev. Nucl. Part. Sci.*, Vol. **69**, Issue. **1**, pp. **279–305**, **2019**.
- [6] W. A. Lester, L. Mitas, and B. Hammond, "Quantum Monte Carlo for atoms, molecules and solids," *Chem. Phys. Lett.*, Vol. **478**, Issue. **1–3**, pp. **1–10**, **2009**.
- [7] J. Kolorenč and L. Mitas, "Applications of quantum Monte Carlo methods in condensed systems," *Reports Prog. Phys.*, Vol. **74**, Issue. **2**, pp. **026502-1 – 026502-28**, **2011**.
- [8] T. Pang, "Diffusion Monte Carlo: A powerful tool for studying quantum many-body systems," *Am. J. Phys.*, Vol. **82**, Issue. **10**, pp. **980–988**, **2014**.
- [9] W. M. C. Foulkes *et al.*, "Quantum Monte Carlo Simulations of Real Solids," in *High-Performance Computing*, Springer, Boston, pp. **165–174**, **1999**.
- [10] W. Becken, P. Schmelcher, and F. K. Diakonou, "Helium atom in a strong magnetic field," *J. Phys. B At. Mol. Opt. Phys.*, Vol. **32**, Issue. **6**, pp. **1557–1584**, **1999**.
- [11] M. V. Ivanov and P. Schmelcher, "Ground state of the lithium atom in strong magnetic fields," *Phys. Rev. A*, Vol. **57**, Issue. **5**, pp. **3793–3800**, **1998**.
- [12] O. A. Al-Hujaj and P. Schmelcher, "Lithium in strong magnetic fields," *Phys. Rev. A*, Vol. **70**, Issue. **3**, pp. **033411-1 – 033411-12**, **2004**.
- [13] M. V. Ivanov and P. Schmelcher, "The beryllium atom and beryllium positive ion in strong magnetic fields," *Eur. Phys. J. D*, Vol. **17**, Issue. **3**, pp. **279–288**, **2001**.
- [14] O. A. Al-Hujaj and P. Schmelcher, "Beryllium in strong magnetic fields," *Phys. Rev. A*, Vol. **70**, Issue. **2**, pp. **023411-1 – 023411-11**, **2004**.
- [15] M. V. Ivanov and P. Schmelcher, "The boron atom and boron positive ion in strong magnetic fields," *J. Phys. B At. Mol. Opt. Phys.*, Vol. **34**, Issue. **10**, pp. **2031–2044**, **2001**.
- [16] Y. P. Kravchenko and M. A. Liberman, "Application of gaussian-type basis sets to Ab initio calculations in strong magnetic fields," *Int. J. Quantum Chem.*, Vol. **64**, Issue. **5**, pp. **513–522**, **1997**.
- [17] M. D. Jones, G. Ortiz, and D. M. Ceperley, "Hartree-Fock studies of atoms in strong magnetic fields," *Phys. Rev. A - At. Mol. Opt. Phys.*, Vol. **54**, Issue. **1**, pp. **219–231**, **1996**.
- [18] W. Zhu and S. B. Trickey, "Accurate and balanced anisotropic Gaussian type orbital basis sets for atoms in strong magnetic fields," *J. Chem. Phys.*, Vol. **147**, Issue. **24**, pp. **244108 -1 – 244108 -11**, **2017**.
- [19] A. Zafar, E. Martin, and S. Shannon, "High resolution magnetic field measurements in hydrogen and helium plasmas using active laser spectroscopy," *Rev. Sci. Instrum.*, Vol. **89**, Issue. **10**, pp. **1–5**, **2018**.
- [20] S. B. Doma, M. O. Shaker, A. M. Farag, and F. N. El-Gammal, "Ground states of helium atom and hydrogen negative ion in the presence of magnetic field using variational Monte Carlo technique," *Acta Phys. Pol. A*, Vol. **126**, Issue. **3**, pp. **700–704**, **2014**.
- [21] S. Doma, M. Shaker, A. Farag, and F. El-Gammal, "Excited states of helium atom in a strong magnetic field using variational Monte Carlo technique," *Indian J. Phys.*, Vol. **92**, Issue. **3**, pp. **279–288**, **2018**.
- [22] S. B. Doma, M. O. Shaker, A. M. Farag, and F. N. El-Gammal, "Variational Monte Carlo calculations of lithium atom in strong magnetic field," *J. Exp. Theor. Phys.*, Vol. **124**, Issue. **1**, pp. **1–9**, **2017**.
- [23] T. Pang, "Diffusion Monte Carlo," in *An Introduction to Quantum Monte Carlo Methods*, Morgan & Claypool Publishers, USA, pp. **4-1 – 4-14**, **2016**.
- [24] N. Metropolis, A. W. Rosenbluth, M. N. Rosenbluth, A. H. Teller, and E. Teller, "Equation of state calculations by fast computing machines," *J. Chem. Phys.*, Vol. **21**, Issue. **6**, pp. **1087–1092**, **1953**.
- [25] Andrea Zen, Jan Gerit Brandenburg, Angelos Michaelides and Dario Alfè, "A new scheme for fixed node diffusion quantum Monte Carlo with pseudopotentials: Improving reproducibility and reducing the trial-wave-function bias," *J. Chem. Phys.*, Vol. **151**, Issue. **13**, pp. **134105-1 – 134105-15**, **2019**.
- [26] M. Troyer and U. J. Wiese, "Computational complexity and fundamental limitations to fermionic quantum Monte Carlo simulations," *Phys. Rev. Lett.*, Vol. **94**, Issue. **17**, pp. **170201-1 – 170201-4**, **2005**.
- [27] B. P. Prascher, D. E. Woon, K. A. Peterson, T. H. Dunning, and A. K. Wilson, "Gaussian basis sets for use in correlated molecular calculations. VII. Valence, core-valence, and scalar relativistic basis sets for Li, Be, Na, and Mg," *Theor. Chem. Acc.*, Vol. **128**, Issue. **1**, pp. **69–82**, **2011**.
- [28] D. E. Woon and T. H. Dunning, "Gaussian basis sets for use in correlated molecular calculations. IV. Calculation of static electrical response properties," *J. Chem. Phys.*, Vol. **100**, Issue. **4**, pp. **2975–2988**, **1994**.
- [29] T. H. Dunning, "Gaussian basis sets for use in correlated molecular calculations. I. The atoms boron through neon and hydrogen," *J. Chem. Phys.*, Vol. **90**, Issue. **2**, pp. **1007–1023**, **1989**.
- [30] G. Dhinra, "Static Pair Correlation Functions and Static Structure Factors of Unidirectional Quantum Systems," *Int. J. Sci. Res. Phys. Appl. Sci.*, Vol. **7**, Issue. **3**, pp. **1 – 5**, **2019**.
- [31] H. Nakashima and H. Nakatsuji, "Solving the electron-nuclear Schrödinger equation of helium atom and its isoelectronic ions with the free iterative-complement-interaction method," *J. Chem. Phys.*, Vol. **128**, Issue. **15**, pp. **154107-1 – 154107-7**, **2008**.
- [32] X. Wang, J. Zhao, and H. Qiao, "Helium atom in strong magnetic fields: An application of the configuration-interaction method with Hylleraas-Gaussian basis," *Phys. Rev. A*, Vol. **80**, Issue. **5**, pp. **053425-1 – 053425-5**, **2009**.
- [33] X. Wang and H. Qiao, "Configuration-interaction method with Hylleraas-Gaussian-type basis functions in cylindrical coordinates: Helium atom in a strong magnetic field," *Phys. Rev. A*, Vol. **77**, Issue. **4**, pp. **043414-1 – 043414-7**, **2008**.
- [34] Z. C. Yan and G. W. F. Drake, "Eigenvalues and expectation values for the $1s^2 2s^2 S$, $1s^2 2p^2 P$, and $1s^2 3d^2 D$ states of lithium," *Phys. Rev. A*, Vol. **52**, Issue. **5**, pp. **3711–3717**, **1995**.
- [35] A. Kotchoubey and L. H. Thomas, "Numerical Calculation of the Energy and Wavefunction of the Ground State of Beryllium," *J. Chem. Phys.*, Vol. **45**, Issue. **9**, pp. **3342–3349**, **1966**.
- [36] S. J. Chakravorty, S. R. Gwaltney, E. R. Davidson, F. A. Parpia and C. Froese Fisher, "Ground-state correlation energies for atomic ions with 3 to 18 electrons," *Phys. Rev. A*, Vol. **47**, Issue. **5**, pp. **3649–3670**, **1993**.

AUTHORS PROFILE

Dr. Salah Badawi Doma is a professor of applied mathematics and theoretical physics at the Department of Mathematics and Computer Science, Faculty of Science, Alexandria University, Egypt from 1986 until present. He published several books and more than 135 research papers in the fields of theoretical nuclear physics, atomic structure and molecular structure.



Dr. Nazih Abdelhamid El-Nohy is a professor of theoretical nuclear physics, Department of Physics, Faculty of Science, Alexandria University, Egypt. He published several research papers in theoretical nuclear physics and co-authors several research papers with professor S. B. Doma in the fields of nuclear and atomic physics.



Mr. Mahmoud Ahmed Salem pursued Bachelor of Science and Master of Science from University of Alexandria, Egypt in 2006 & 2011. He is currently pursuing Ph.D. and currently working as Lecturer of Physics in Department of Basic and Applied Sciences, Arab Academy for Science, Technology & Maritime Transport, Egypt, since 2012.

