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CONFINEMENT IMPACTS OF MAGNETIC FIELD ON GROUND AND LOW-LYING EXCITED DOUBLET STATES OF PLASMA-EMBEDDED LITHIUM ATOM

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Abstract. A first-time study is made for the ground and excited states of plasma-embedded lithium atom in the presence of a homogeneous magnetic field by using the variational Monte Carlo method. The low-lying excited doublet states considered are $1s^2ns$, $1s^2np$, and $1s^2nd$ states, whereas the used plasma potentials are the screened Coulomb (SCP) and exponential cosine screened Coulomb (ECSCP) potentials. The energy eigenvalues are assessed by choosing suitable trial wave functions, including the correlated (electron-electron repulsion) and spin parts, in addition to an effective plasma factor regarding the wave function of the ECSCP model. Using the two plasma models, an interesting relative ordering for the lithium atom reports the results.

Key words: Variational Monte Carlo method, lithium atom, magnetic field, plasma potentials.

1. INTRODUCTION

The Coulombic correlated many-body systems are described mainly by Schrödinger equation and cannot be solved analytically. The problem arises for the complexity of the involved multi-dimensional integrals in the calculation of the expectation values of the energy. Hereby, the choice of an appropriate approximation method must be finely considered to evaluate the complicated integrals of those many-body systems.

For the three-electron system, the Drake's variational technique was applied for calculating the excited state $1s^23d$ and the ground state energy of the lithium atom [1] without taking the correlation part of the wave function into account. Moreover, the Cartesian anisotropic Gaussian basis set approach was employed for the quantum chemical configuration (CI) method [2]. Besides, the electron density distribution and spectrum potential curves of helium and lithium atoms were examined in confined low floating states, using an isotropic harmonic potential for both on and off-center position. Also, the excitation energies relevant

to the core states of the lithium atom were determined experimentally [3], and the uncertainties of the energy scales for incident and ejected electrons were estimated. In addition, the ground state energy of isoelectronic ions of lithium and helium atoms was investigated for the infinite and finite nuclear mass effect [4]. Furthermore, the ground and excited states of the lithium atom were investigated in the presence of external homogenous magnetic field [5, 6], and also isoelectronic ions up to Z=10 using the variational Monte Carlo method as an approximation method [7].

Another crucial factor that needs to be considered for a variety of physical systems is the plasma screening effect on atomic processes, whereby two characteristics of plasmas, particle density n and temperature T, determine whether they are classical or quantum plasmas in the collisional or collisionless regime [8-10].The exponential-cosine-screened Coulomb potential model [11] was developed to describe dense plasmas in which electrons are regarded as Fermi gas and the electron quantum force resulting from the quantum Bohm potential is considered instead of Fermi pressure. Electron collisions [12] and charge capture processes [13], on the basis of applying the screening effects of this model, have been studied in the plasma environment. In addition, the lithium atom was studied in a weakly coupled plasma environment, where the wave functions were expanded in a correlated Hylleraas type basis set utilizing the electron-electron correlation effect [14]. Also, the nuclear magnetic shielding constant (σ), ionization potential, and diamagnetic susceptibility (χ) were given in relation to the plasma screening parameter (μ). Moreover, the ground state of lithium atom was studied in both free and dense plasma sates was [15], whereas the low-lying and core excited doublet states including also the Hulthén potential plasma model [16] were investigated.

In general, a precise approximation technique for these intricate systems, like quantum Monte Carlo (QMC) methods, is required when solving the Schrödinger equation of many-body quantum systems involved in different external potentials [17-20]. The main concept of the Monte Carlo numerical techniques is to only evaluate the integrand at a representative random sampling of abscissae, rather than at each of the many quadrature points. By analyzing integrals of high dimension, the Monte Carlo method proves to be highly suitable for a wide range of statistical and quantum mechanical problems. Two basic actions comprise the Monte Carlo quadrature: first, generating abscissa randomly dispersed around the integration volume with a certain distribution $w(x)$ and, second, calculating the average value of the function f/w, where f is the function to be integrated, at these abscissae. It is necessary to use an alternate method because, despite the potential for great efficiency, methods for producing random numbers in accordance with a given distribution cannot be generalized to sample a complex weight function in multiple dimensions. One very general way

to produce random variables with a given probability distribution of arbitrary form is known as the Metropolis algorithm [21]. As one of the QMC numerical techniques, the variational Monte Carlo method (VMC) is based on two concepts: the variational principle and the Monte Carlo evaluation of integrals using significance sampling based on the Metropolis algorithm, wherein, regardless of the problem's dimensionality, the statistical error in the estimate of the integral decreases as the square root of the number of points is sampled.

It is important to note that lithium atoms are essential to space science and plasma physics. In order to comprehend and control plasmas in a variety of contexts, including developing and perfecting plasma confinement for potential future fusion energy applications, it serves as a diagnostic tool to measure temperatures and densities in fusion experiments. Furthermore, lithium abundances provide information about the Big Bang nucleosynthesis and aid in our understanding of cosmic-ray interactions and stellar evolution.

Accordingly, the purpose of this work is to apply the VMC method using suitable trial wave functions to investigate the influence of homogenous magnetic field on the ground and low-lying excited doublet states of the lithium atom embedded in two different plasma potentials, the Screened Coulomb Potential (SCP) and exponential cosine screened Coulomb Potential models (ECSCP).

2. THE CALCULATIONS METHOD

In the VMC method, the evaluation of the expectation value of the Hamiltonian operator is obtained by multiplying and dividing the integrand by the trial wave function, as follows

$$E_{VMC} = \frac{\int \psi^*(R)\frac{\hat{H}\psi(R)}{\psi(R)}\psi(R)d\boldsymbol{R}}{\int \psi^*(R)\,\psi(R)d\boldsymbol{R}}, \quad (1)$$

where $\psi(R)$ is a trial wave function depending on variational parameters, which are optimized to obtain the minimum energy eigenvalue using importance sampling based on the Metropolis algorithm. We rewrite Eq. (1) as follows:

$$E_{VMC} = \int P(R)E_L(R)d(\boldsymbol{R}), \quad (2)$$

where $P(R) = \frac{|\psi(R)|^2}{\int|\psi(R)|^2 dR}$ is interpreted as a probability distribution function and $E_L(R) = \frac{\hat{H}\psi(R)}{\psi(R)}$ is the local energy function, which was evaluated using a series of points R_{ij} proportional to $P(R)$ according to the Metropolis algorithm. The trial

wave function for a given state must produce an energy which is above the exact value of that state; $E_{VMC} \geq E_{exact}$.

After enough evaluations, E_{VMC} can be written in the form:

$$E_{VMC} = < E_L >= \lim_{N\to\infty} \lim_{M\to\infty} \frac{1}{N}\frac{1}{M} \sum_{j=1}^{N} \sum_{i=1}^{M} E_L(R_{ij}), \quad (3)$$

where M is the ensemble size of generated random points $\{\boldsymbol{R_1}, \boldsymbol{R_2}, \dots, \boldsymbol{R_M}\}$ and N is the number of ensembles.

With this numerical method, random numbers with a frequency probability distribution like $\psi^2(\boldsymbol{R})$ are subjected to an acceptance-rejection procedure. Using this approach, one takes a random number from the probability distribution $P(\boldsymbol{R})$ and tests its value to see if it can be used as an approximation of the local energy. After an ensemble of random numbers is generated, the acceptance criterion is such that the probability of moving from an initial random number of the ensemble, $\boldsymbol{R_i}$ to a new random number, $\boldsymbol{R_k}$ is defined according to the ratio:

$$A = \frac{\psi^2(\boldsymbol{R_k})}{\psi^2(\boldsymbol{R_i})}. \quad (4)$$

This trial step is approved if A is more than one (that is, we put $\boldsymbol{R_{i+1}} = \boldsymbol{R_k}$), and the new $\boldsymbol{R_k}$ is a point of the following ensemble. The step is accepted with probability A if A is smaller than 1. The latter can be easily achieved by accepting the step if $\epsilon < A$ and comparing it with a uniformly distributed random number (ϵ) in the interval [0, 1]. In the event that the trial step is refused, we set $\boldsymbol{R_{i+1}} = \boldsymbol{R_k}$. To expand later ensembles for a larger sampling range, this procedure is repeated for every point in the ensemble where any arbitrary point $\boldsymbol{R_0}$ can be used as the starting point for the random walk.

Eventually, the consideration of the standard deviation of the energy is very important in the calculations and given by

$$\sigma = \sqrt{\frac{\langle E_L^2\rangle - \langle E_L\rangle^2}{M(N-1)}}. \quad (5)$$

3. THE HAMILTONIAN OF THE SYSTEM

The Hamiltonian operator for free lithium atom within the infinite nuclear mass approximation in atomic units (a. u.), $e = \hbar = m = 4\pi\varepsilon_0 = 1$, is given by

$$H = -\frac{1}{2}\sum_{i=1}^{3}(\nabla_i^2 + \frac{2Z}{r_i}) + \sum_{i<j}\frac{1}{r_{ij}}, \quad (6)$$

where $Z = 3$ is the nuclear charge, r_i is the distance between the *i*th electron and the nucleus, and r_{ij} are the inter-electron distances.

Using the Hylleraas Coordinates [22], the Hamiltonian is introduced as

$$H = -\frac{1}{2}\left(\sum_{i=1}^{3}\frac{\partial^2}{\partial r_i^2} + \sum_{i=1}^{3}\frac{2}{r_i}\frac{\partial}{\partial r_i} + \sum_{i<j}^{3} 2\frac{\partial^2}{\partial r_{ij}^2} + \sum_{i<j}^{3}\frac{4}{r_{ij}}\frac{\partial}{\partial r_{ij}} + \sum_{i\neq j}^{3}\frac{r_i^2+r_{ij}^2-r_j^2}{r_i r_{ij}}\frac{\partial^2}{\partial r_i \partial r_{ij}} + \sum_{i\neq j}^{3}\sum_{k>j}^{3}\frac{r_{ij}^2+r_{ik}^2-r_{jk}^2}{r_{ij}r_{ik}}\frac{\partial^2}{\partial r_{ij}\partial r_{ik}} + + \sum_{i=1}^{3}\frac{1}{r_i{}^2}\frac{\partial^2}{\partial \theta_i^2} + \sum_{i=1}^{3}\frac{1}{r_i^2 sin^2\theta_i}\frac{\partial^2}{\partial \varphi_i^2} + \sum_{i=1}^{3}\frac{cot\theta_i}{r_i^2}\frac{\partial}{\partial \theta_i} + \sum_{i\neq j}^{3}\left(2\frac{r_j cos\theta_j}{r_i r_{ij} sin\theta_i} + cot\theta_i\frac{r_{ij}^2-r_i^2-r_j^2}{r_i^2 r_{ij}}\right)\frac{\partial^2}{\partial \theta_i \partial r_{ij}} + + \sum_{i\neq j}^{3} 2\frac{r_j sin\theta_j}{r_i r_{ij} sin\theta_i}\sin(\varphi_i-\varphi_j)\frac{\partial^2}{\partial \varphi_i \partial r_{ij}}\right) + \sum_{i=1}^{3}\frac{-Z}{r_i} + \sum_{i<j}^{3}\frac{1}{r_{ij}}. \quad (7)$$

For plasma models, the collective impacts due to the correlated many-particle interactions lead to screened Coulomb interactions in hot dense plasma conditions, which are commonly represented by the SCP and given by

$$V_{SCP}(r) = -\frac{Ze^2}{r}exp(-\mu r), \quad (8)$$

where $\mu = \frac{1}{\lambda_D}$ is the Debye screening parameter and it determines the interaction between electron–electron in Debye plasma. It depends on the temperature and the density of the plasma as follows [23]

$$\mu = \frac{1}{\lambda_D} = \sqrt{4\pi e^2 N_e/KT_e}\,, \quad (9)$$

where λ_D is called the Debye screening length, *K* is the Boltzmann constant, T_e is the electron temperature, *e* is the electronic charge, and N_e is the plasma-electron density.

The study of effective screened potential in dense quantum plasmas or the ECSCP [24] is introduced as

$$V_{ECSCP}(r) = -\frac{Ze^2}{r}ex\,p(-\mu r)\,cos(\mu r). \quad (10)$$

Accordingly, the Hamiltonian for the lithium atom according to the SCP model is given by:

$$H_1 = -\frac{1}{2}\sum_{i=1}^{3}\nabla_i^2 - 3\sum_{i=1}^{3}\frac{exp(-\mu r_i)}{r_i} + \sum_{i<j}^{3}\frac{exp(-\mu r_{ij})}{r_{ij}}. \quad (11)$$

But for the ECSCP model, it is given by:

$$H_2 = -\frac{1}{2}\sum_{i=1}^{3}\nabla_i^2 - 3\sum_{i=1}^{3}\frac{exp(-\mu r_i)cos(\mu r_i)}{r_i} + \sum_{i<j}^{3}\frac{exp(-\mu r_{ij})\,cos(\mu r_{ij})}{r_{ij}}. \quad (12)$$

Here, the kinetic term in Eqs. (11) and (12) is introduced in the form of Hylleraas coordinates, as in Eq. (7). Also, μ is treated as a parameter in our work so that the physical difference of μ between these plasma models is not discussed and is out of our reach.

In the presence of external magnetic field, the total Hamiltonian is introduced as

$$H_{Mag} = H_p + \frac{1}{8}\gamma^2\rho^2 + \frac{\gamma(L_z+2S_z)}{2}, \quad (13)$$

where H_p = (H_1, H_2) is the Hamiltonian of the used plasma model. Also, γ is the strength of the magnetic field in a. u., $\rho^2 = \sum_{i=1}^{n}\rho_i^2 = \sum_{i=1}^{n} x_i^2 + y_i^2$, S_z is the *z*-component of the total spin, L_z is the *z*-component of the total angular momentum, $\frac{\gamma L_z}{2}$ is the diamagnetic term, and γS_z represents the Zeeman term. It ought to be noticed that the diamagnetic term ($\frac{\gamma L_z}{2}$) has not any effective role only for the $1s^2ns$ states and was excluded from the calculations, as $L_z = 0$.

4. THE TRIAL WAVE FUNCTIONS

For the ground and low-lying excited doublet states of the lithium atom, the used trial wave functions using SCP and ECSCP models are introduced as

$$\Psi_{SCP}(\boldsymbol{r}_1, \boldsymbol{r}_2, \boldsymbol{r}_3) = \mathcal{A}\big[\psi(\boldsymbol{r_1}, \boldsymbol{r_2}, \boldsymbol{r_3})\,\chi\,(1,2,3)\prod_{i<j} f\big(r_{ij}\big)\big] \quad (15)$$

and

$$\Psi_{ECSCP}(r_1, r_2, r_3) = \mathcal{A}\big[\psi(r_1, r_2, r_3)\,\chi\,(1,2,3)\prod_{i<j} f\big(r_{ij}\big)\big]\prod_i(1-\mu r_i), \quad (16)$$

where $\mathcal{A}$ is the antisymmetrizer

$$\mathcal{A} = I - \hat{P}_{12} - \hat{P}_{23} - \hat{P}_{31} + \hat{P}_{123} + \hat{P}_{132}. \quad (17)$$

Here I is the identity permutation, while $\hat{P}_{ij}$ and $\hat{P}_{ijk}$ are the permutation operators of two and three electrons, respectively.

Also, the spatial wave function $\psi\,(\boldsymbol{r_1}, \boldsymbol{r_2}, \boldsymbol{r_3})$ is the hydrogen-like wave function in the $n\ell$ state, including the radial wave functions of 4ℓ and 5ℓ states [24]. Then, it is given by:

$$\psi\,(\boldsymbol{r_1}, \boldsymbol{r_2}, \boldsymbol{r_3}) = \psi_{Z'}(r_1)\,\psi_{Z'}(r_2)\,R_{nl}(Z'', r_3)\,Y_{lm}(\theta_3, \varphi_3), \tag{18}$$

and the spin function for $1s^2ns$ and $1s^2nd$ states is:

$$\chi\,(1,2,3) = \alpha(1)\beta(2)\alpha(3) - \beta(1)\,\alpha(2)\alpha(3). \tag{19a}$$

But for $1s^2\,np$ states,

$$\chi\,(1,2,3) = \alpha(1)\beta(2)\alpha(3) + \beta(1)\,\alpha(2)\alpha(3), \tag{19b}$$

where α and β are the spinor indices so that the introduced spin functions could satisfy the Pauli-Exclusion principle . Also, $f(r_{ij})$ is the Jastrow correlation function [25] and is introduced as

$$f(r_{ij}) = exp\left[\frac{r_{ij}}{\varepsilon\,(1+\sigma\,r_{ij})}\right]. \tag{20}$$

Here, the variational parameters z', z'', and σ are finely varied in order to obtain the best fit to the energy eigenvalues, while ε makes $f(r_{ij})$ satisfy the cusp conditions , as $\varepsilon = \begin{cases} 2 & for\ unlike\ spins \\ 4 & for\ like\ spins \end{cases}$.

In addition, the effective-plasma factor $\prod_i(1-\mu r_i)$ of Eq. (16) was considered in this work for dense quantum plasma environment, ECSCP model, provided that $r_i < \frac{1}{\mu}$ and $\Psi_{ECSCP} = 0$ at $r_i = \frac{1}{\mu}$, where the simultaneous interactions between plasma particles occur.

5. RESULTS AND DISCUSSION

The VMC numerical method was utilized in this work, using 10^7 Monte Carlo integration points, to obtain the minimum energy eigenvalues with lower statistical errors for the ground and low-lying excited doublet sates of lithium atom, as well as a standard deviation of order 10^{-5}. Our computational program enables us to finely vary the variational parameters in loops, whereby the computational code for each system was implemented by considering the Metropolis algorithm within the variational Monte Carlo method.

There are two different mechanisms are used to describe the electronic structure and energy levels of the lithium atom when it is subjected to external potentials of varying intensities.

Depending on the strength of the magnetic field, four distinct regimes exist in which an excited electron can interact with an atom. The electron moves into an area where the Coulomb potential predominates, after exiting through the core of the atom, and the diamagnetic potential is minimal. Then, by passing through a zone where the strengths of the two fields are equivalent, the magnetic field finally reaches the asymptotic region where the cylindrical symmetry magnetic field potential predominates.

On the other hand, depending on densities and temperatures, an atom under the influence of plasmas can be in the collisional or collisionless domain, where it can exist in one of two plasma regimes: classical or quantum plasmas. The first is weakly connected plasmas, where the predominance of thermal motion makes the collective or collisionless effects more noticeable. Then, the screened Coulomb potential (SCP) describes the potential of an atom in such plasmas. The other regime is the strongly coupled (collisional) plasma, where the quantum effect becomes more prominent because of the substantial overlap of bound state wave functions with neighboring plasma particles, and where there is an increase in plasma density at low temperature and the potential energy is more significant than the kinetic energy. In this case, the electrons are regarded as Fermi gas and the electron quantum force resulting from the quantum Bohm potential is involved, whereas the quantum statistical Fermi-pressure has been disregarded. Thus, the dense quantum plasmas have been proposed to be characterized by the exponential-cosine-screened Coulomb potential (ECSCP).

Consequently, we have employed the ECSCP model to treat the lithium atom in our work as a confined atom by plasma particles, including the proposed effective-plasma component $\prod_i(1-\mu r_i)$ in the wave function. It should be noted that the confined model in this action caused by the plasma particles is completely distinct from the confined atom inside a spherical box of an impermeable wall. To interpret the situation, the confined model in this work has definite effective plasma potential and exerts a rapid decreasing in the correlation part, whereas the latter always has a permanent zero confined potential inside the box in addition to an increasing in the correlation part (electron-electron repulsion) by decreasing the box radii.

Considering our first case, in the presence of a magnetic field and without the plasma potentials, the calculations were performed for the ground and low-lying

excited doublet states of the lithium atom using the Hamiltonian of Eq. (13), where $H_p = 0$. Besides, the used trial wave function is Eq. (15), including Eq. (19a) as a spin function for $1s^2ns$ and $1s^2nd$ states, while Eq. (19b) is for $1s^2np$ states. The obtained results are shown in Table 1 compared to the other previous results [6] at different magnetic field strengths.

Table 1

Energies of the ground and low-lying excited doublet states of lithium atom as a function of the magnetic field strength (γ) compared to the other published results, in a. u.

γ	$1s^2\,2s$	$1s^2\,3s$	$1s^2\,4s$	$1s^2\,2p$	$1s^2\,3p$	$1s^2\,4p$	$1s^2\,3d$	$1s^2\,4d$	$1s^2\,5d$
0	-7.478020 -7.477766*	-7.354073 -7.350744*	-7.318347 -7.280117*	-7.410154 -7.407126*	-7.337198 -7.334196*	-7.311926 -7.307804*	-7.335522 -7.332617*	-7.311193 -7.308297*	-7.299937 -7.297036*
0.01	-7.483142 -7.482888*	-7.361270 -7.357941*	-7.350061 -7.311831*	-7.420022 -7.416994*	-7.345664 -7.342662*	-7.319277 -7.315155*	-7.349201 -7.346296*	-7.321491 -7.318595*	-7.309648 -7.306747*
0.05	-7.502978 -7.502724*	-7.368833 -7.365504*	-7.360415 -7.322185*	-7.454114 -7.451086*	-7.359353 -7.356351*	-7.333599 -7.329477*	-7.386553 -7.383648*	-7.333375 -7.330479*	-7.317412 -7.314511*
0.1	-7.517408 -7.517154*	-7.370893 -7.367564*	-7.339150 -7.300920*	-7.487801 -7.484773*	-7.363816 -7.360814*	-7.332484 -7.328362*	-7.417112 -7.414207*	-7.342367 -7.339471*	-7.315228 -7.312327*
0.5	-7.528309 -7.528055*	-7.365320 -7.361991*	-7.323378 -7.285148*	-7.637575 -7.634547*	-7.375076 -7.372074*	-7.316606 -7.312484*	-7.527386 -7.524481*	-7.356880 -7.353984*	-7.308826 -7.305925*
1	-7.458804 -7.458550*	-7.304399 -7.301070*	-7.271382 -7.233152*	-7.719707 -7.716679*	-7.338942 -7.335940*	-7.267625 -7.263503*	-7.565797 -7.562892*	-7.319453 -7.316557*	-7.259945 -7.257044*
5	-6.137172 -6.136918*	-5.984248 -5.980919*	-5.957888 -5.919658*	-7.005374 -7.002346*	-6.071383 -6.068381*	-5.965811 -5.961689*	-6.636023 -6.633118*	-6.048670 -6.045774*	-5.958028 -5.955127*

*Ref. [6].

For the other case, the calculations were made for the SCP and ECSCP models influenced by the magnetic field using the Hamiltonian of Eq. (13), including Eqs. (11) and (12). The used trial wave functions are given by Eqs. (15) and (16) for the SCP and ECSCP models, respectively. Also, the spin wave function is Eq. (19a) for the $1s^2ns$ and $1s^2nd$ states, while Eq. (19b) is for the $1s^2np$ states. All the obtained results in the presence of the two plasma models are presented in Tables 2 and 3.

In the region of weak magnetic field strength $0 < \gamma \leq 0.1$ and at small values of μ, μ = 0.01 to μ = 0.05, the electronic charge distribution of the valence shell along the z-axis expands slightly, and the energies of all systems are perturbed slowly, although the attractive pure Coulomb potential dominates the system.

Table 2

Energies of the ground and low-lying excited doublet states of lithium atom using the SCP model at different magnetic field strengths (γ), in a. u.

μ	γ	$1s^2\,2s$	$1s^2\,3s$	$1s^2\,4s$	$1s^2\,2p$	$1s^2\,3p$	$1s^2\,4p$	$1s^2\,3d$	$1s^2\,4d$	$1s^2\,5d$
0.01	0	-7.418064	-7.294390	-7.258660	-7.350466	-7.277510	-7.252238	-7.275834	-7.251505	-7.240249
	0.01	-7.423186	-7.301587	-7.290374	-7.360338	-7.285976	-7.259591	-7.289509	-7.261808	-7.249961
	0.05	-7.443022	-7.309150	-7.300728	-7.394430	-7.299665	-7.273913	-7.326861	-7.273692	-7.257725
	0.1	-7.457452	-7.311210	-7.279463	-7.428117	-7.304128	-7.272798	-7.357420	-7.282684	-7.255541
	0.5	-7.468353	-7.305637	-7.263691	-7.577891	-7.315388	-7.256920	-7.467694	-7.297197	-7.249139
	1	-7.398848	-7.244716	-7.211695	-7.660023	-7.279254	-7.207939	-7.506105	-7.259770	-7.200258
	5	-6.077216	-5.924565	-5.898201	-6.945690	-6.011695	-5.906125	-6.576331	-5.988987	-5.898341
0.05	0	-7.180393	-7.061609	-7.025883	-7.117690	-7.044734	-7.019462	-7.043058	-7.018729	-7.007473
	0.01	-7.185515	-7.068806	-7.057597	-7.127558	-7.053200	-7.026813	-7.056737	-7.029027	-7.017184
	0.05	-7.205351	-7.076369	-7.067951	-7.161650	-7.066889	-7.041135	-7.094089	-7.040911	-7.024948
	0.1	-7.219781	-7.078429	-7.046686	-7.195337	-7.071352	-7.040020	-7.124648	-7.049903	-7.022764
	0.5	-7.230682	-7.072856	-7.030914	-7.345111	-7.082612	-7.024142	-7.234922	-7.064416	-7.016362
	1	-7.161177	-7.011935	-6.978918	-7.427243	-7.046478	-6.975161	-7.273333	-7.026989	-6.967481
	5	-5.839545	-5.691784	-5.665424	-6.712910	-5.778919	-5.673347	-6.343559	-5.756206	-5.665564
0.1	0	-6.893926	-6.783092	-6.747366	-6.839173	-6.766217	-6.740945	-6.764541	-6.740212	-6.728956
	0.01	-6.899048	-6.790289	-6.779080	-6.849041	-6.774683	-6.748296	-6.778220	-6.750510	-6.738667
	0.05	-6.918884	-6.797852	-6.789434	-6.883133	-6.788372	-6.762618	-6.815572	-6.762394	-6.746431
	0.1	-6.933314	-6.799912	-6.768169	-6.916820	-6.792835	-6.761503	-6.846131	-6.771386	-6.744247
	0.5	-6.944215	-6.794339	-6.752397	-7.066594	-6.804095	-6.745625	-6.956405	-6.785899	-6.737845
	1	-6.874710	-6.733418	-6.700401	-7.148726	-6.767961	-6.696644	-6.994816	-6.748472	-6.688964
	5	-5.553078	-5.413267	-5.386907	-6.434393	-5.500402	-5.394830	-6.065042	-5.477689	-5.387047
0.2	0	-6.377529	-6.268180	-6.232454	-6.324261	-6.251305	-6.226033	-6.249629	-6.225300	-6.214044
	0.01	-6.382651	-6.275377	-6.264168	-6.334129	-6.259771	-6.233384	-6.263308	-6.235598	-6.223755
	0.05	-6.402487	-6.282940	-6.274522	-6.368221	-6.273460	-6.247706	-6.300660	-6.247482	-6.231519
	0.1	-6.416917	-6.285000	-6.253257	-6.401908	-6.277923	-6.246591	-6.331219	-6.256474	-6.229335
	0.5	-6.427818	-6.279427	-6.237485	-6.551682	-6.289183	-6.230713	-6.441493	-6.270987	-6.222933
	1	-6.358313	-6.218506	-6.185489	-6.633814	-6.253049	-6.181732	-6.479904	-6.233560	-6.174052
	5	-5.036681	-4.898355	-4.871995	-5.919481	-4.985490	-4.879918	-5.550130	-4.962777	-4.872135
0.5	0	-5.131548	-5.019115	-4.983389	-5.075196	-5.002240	-4.976968	-5.000564	-4.976235	-4.964979
	0.01	-5.136670	-5.015103	-5.085064	-5.010706	-4.984319	-5.014243	-4.986533	-4.974690	-5.026312
	0.05	-5.156506	-5.025457	-5.119156	-5.024395	-4.998641	-5.051595	-4.998417	-4.982454	-5.033875
	0.1	-5.170936	-5.004192	-5.152843	-5.028858	-4.997526	-5.082154	-5.007409	-4.980270	-5.035935
	0.5	-5.181837	-4.988420	-5.302617	-5.040118	-4.981648	-5.192428	-5.021922	-4.973868	-5.030362
	1	-5.112332	-4.936424	-5.384749	-5.003984	-4.932667	-5.230839	-4.984495	-4.924987	-4.969441
	5	-3.790700	-3.622930	-4.670416	-3.736425	-3.630853	-4.301065	-3.713712	-3.623070	-3.649290
1	0	-3.825778	-3.713345	-3.677619	-3.769426	-3.696470	-3.671198	-3.694794	-3.670465	-3.659209
	0.01	-3.830900	-3.720542	-3.709333	-3.779294	-3.704936	-3.678549	-3.708473	-3.680763	-3.668920
	0.05	-3.850736	-3.728105	-3.719687	-3.813386	-3.718625	-3.692871	-3.745825	-3.692647	-3.676684
	0.1	-3.865166	-3.730165	-3.698422	-3.847073	-3.723088	-3.691756	-3.776384	-3.701639	-3.674500
	0.5	-3.876067	-3.724592	-3.682650	-3.996847	-3.734348	-3.675878	-3.886658	-3.716152	-3.668098
	1	-3.806562	-3.663671	-3.630654	-4.078979	-3.698214	-3.626897	-3.925069	-3.678725	-3.619217
	5	-2.484930	-2.343520	-2.317160	-3.364646	-2.430655	-2.325083	-2.995295	-2.407942	-2.317300

Also, the spin Zeeman- effect occurs in this region and leading to a reduction in the total energy since S_z = 1/2. In addition, the diamagnetic term ($\frac{\gamma L_z}{2}$) is considered for $1s^2np$ and $1s^2nd$ states, where the increasing in angular momentum of the valence shell electron increases the electronic separation, except for $1s^2ns$ states, as L_z = 0. Moreover, for μ > 0.05, the effect of a pure plasma environment leads to a gradual increase in the total energy, reflecting that the extent of the screening plasma potential on the nuclear charge is stronger at larger μ.

Table 3

Energies of the ground and low-lying excited doublet states of lithium atom using the ECSCP model at different magnetic field strengths (γ), in a. u.

μ	γ	$1s^2\,2s$	$1s^2\,3s$	$1s^2\,4s$	$1s^2\,2p$	$1s^2\,3p$	$1s^2\,4p$	$1s^2\,3d$	$1s^2\,4d$	$1s^2\,5d$
0.01	0	-6.943650	-6.81967	-6.78394	-6.87575	-6.80279	-6.77752	-6.80112	-6.77679	-6.76553
	0.01	-6.948772	-6.826867	-6.815654	-6.885618	-6.811256	-6.784871	-6.814799	-6.787088	-6.775241
	0.05	-6.968608	-6.834430	-6.826008	-6.919710	-6.824945	-6.799193	-6.852151	-6.798972	-6.783005
	0.1	-6.983038	-6.836490	-6.804743	-6.953397	-6.829408	-6.798078	-6.882710	-6.807964	-6.780821
	0.5	-6.993939	-6.830917	-6.788971	-7.103171	-6.840668	-6.782200	-6.992984	-6.822477	-6.774419
	1	-6.924434	-6.769996	-6.736975	-7.185303	-6.804534	-6.733219	-7.031395	-6.785050	-6.725538
	5	-5.602802	-5.449845	-5.423481	-6.470970	-5.536975	-5.431405	-6.101621	-5.514267	-5.423621
0.05	0	-6.534960	-6.70742	-6.67170	-6.76350	-6.69055	-6.66528	-6.68887	-6.66454	-6.65329
	0.01	-6.540082	-6.714617	-6.703414	-6.773368	-6.699016	-6.672631	-6.702549	-6.674838	-6.663001
	0.05	-6.559918	-6.722180	-6.713768	-6.807460	-6.712705	-6.686953	-6.739901	-6.686722	-6.670765
	0.1	-6.574348	-6.724240	-6.692503	-6.841147	-6.717168	-6.685838	-6.770460	-6.695714	-6.668581
	0.5	-6.585249	-6.718667	-6.676731	-6.990921	-6.728428	-6.669960	-6.880734	-6.710227	-6.662179
	1	-6.515744	-6.657746	-6.624735	-7.073053	-6.692294	-6.620979	-6.919145	-6.672800	-6.613298
	5	-5.194112	-5.337595	-5.311241	-6.358720	-5.424735	-5.319165	-5.989371	-5.402017	-5.311381
0.1	0	-6.1423330	-6.41098	-6.37525	-6.46706	-6.39410	-6.36883	-6.39243	-6.36810	-6.35684
	0.01	-6.147455	-6.418177	-6.406964	-6.476928	-6.402566	-6.376181	-6.406109	-6.378398	-6.366551
	0.05	-6.167291	-6.425740	-6.417318	-6.511020	-6.416255	-6.390503	-6.443461	-6.390282	-6.374315
	0.1	-6.181721	-6.427800	-6.396053	-6.544707	-6.420718	-6.389388	-6.474020	-6.399274	-6.372131
	0.5	-6.192622	-6.422227	-6.380281	-6.694481	-6.431978	-6.373510	-6.584294	-6.413787	-6.365729
	1	-6.123117	-6.361306	-6.328285	-6.776613	-6.395844	-6.324529	-6.622705	-6.376360	-6.316848
	5	-4.801485	-5.041155	-5.014791	-6.062280	-5.128285	-5.022715	-5.692931	-5.105577	-5.014931
0.2	0	-5.889637	-5.52556	-5.48957	-5.58295	-5.50842	-5.48315	-5.50675	-5.48242	-5.47116
	0.01	-5.914595	-5.532757	-5.521284	-5.592818	-5.516886	-5.490501	-5.520429	-5.492718	-5.480871
	0.05	-5.929025	-5.540320	-5.531638	-5.626910	-5.530575	-5.504823	-5.557781	-5.504602	-5.488635
	0.1	-5.939926	-5.542380	-5.510373	-5.660597	-5.535038	-5.503708	-5.588340	-5.513594	-5.486451
	0.5	-5.870421	-5.536807	-5.494601	-5.810371	-5.546298	-5.487830	-5.698614	-5.528107	-5.480049
	1	-5.656790	-5.475886	-5.442605	-5.892503	-5.510164	-5.438849	-5.737025	-5.490680	-5.431168
	5	-4.548789	-4.155735	-4.129111	-5.178170	-4.242605	-4.137035	-4.807251	-4.219897	-4.129251
0.5	0	-4.515450	-4.47972	-4.57153	-4.49857	-4.47330	-4.49690	-4.47257	-4.46131	-4.51545
	0.01	-4.522647	-4.511434	-4.581398	-4.507036	-4.480651	-4.510579	-4.482868	-4.471021	-4.522647
	0.05	-4.530210	-4.521788	-4.615490	-4.520725	-4.494973	-4.547931	-4.494752	-4.478785	-4.530210
	0.1	-4.532270	-4.500523	-4.649177	-4.525188	-4.493858	-4.578490	-4.503744	-4.476601	-4.532270
	0.5	-4.526697	-4.484751	-4.798951	-4.536448	-4.477980	-4.688764	-4.518257	-4.470199	-4.526697
	1	-4.465776	-4.432755	-4.881083	-4.500314	-4.428999	-4.727175	-4.480830	-4.421318	-4.465776
	5	-3.145625	-3.119261	-4.166750	-3.232755	-3.127185	-3.797401	-3.210047	-3.119401	-3.145625
1	0	-3.265380	-3.23965	-3.27146	-3.25850	-3.23323	-3.25682	-3.23250	-3.22124	-3.26538
	0.01	-3.272577	-3.271364	-3.281328	-3.266966	-3.240581	-3.270499	-3.242798	-3.230951	-3.272577
	0.05	-3.280140	-3.281718	-3.315420	-3.280655	-3.254903	-3.307851	-3.254682	-3.238715	-3.280140
	0.1	-3.282200	-3.260453	-3.349107	-3.285118	-3.253788	-3.338410	-3.263674	-3.236531	-3.282200
	0.5	-3.276627	-3.244681	-3.498881	-3.296378	-3.237910	-3.448684	-3.278187	-3.230129	-3.276627
	1	-3.215706	-3.192685	-3.581013	-3.260244	-3.188929	-3.487095	-3.240760	-3.181248	-3.215706
	5	-1.895555	-1.879191	-2.866680	-1.992685	-1.887115	-2.557321	-1.969977	-1.879331	-1.895555

For the intermediate filed strength region $0.1 < \gamma \leq 1$, the energy values of the quantum levels increase, where the magnetic field begins to slightly compress the valence shell electronic distribution towards the *z*-axis and hence the system tends to shrink. Besides, as the plasma screening parameter increases, the correlation energy (electron-electron repulsion) starts to decrease and the system tends to be unstable. But for the strong filed strength range $\gamma > 1$, the compression of the electronic distribution increases in the *z*-axis direction, and hence the spherical symmetry of the atom is significantly broken, making the cylindrical

symmetry associated with the magnetic field dominant. Also, as μ increases, $\mu > 1$ the total energy of a bound system reaches the ionization limit and this ultimately leads to an unstable system (an unbound system). To illustrate that, in the absence of a magnetic field, the instability in the system is mainly caused by the increase in screening plasma parameter, as a result of which the pure Coulomb and correlation potentials continuously decrease owing to the increase in the electron-nucleus and inter-electronic distances. Then, the avalanche of the Coulomb system occurs, which ultimately leads to an unstable system (unbound system) and the kinetic energy dominates the entire system. Therefore, increasing in the magnetic field strength plays an important role in quickly reaching the unbound states at large values of the screening plasma parameters.

The energy eigenvalues for all states were plotted versus γ as shown in Figs. (1-3) using the SCP and ECSCP models at $\mu = 0.05$, $\mu = 0.5$, and $\mu = 1$. In addition, they show the comparison between SCP and ECSCP models, with the energy values shifted to a higher position than the SCP model. Also, the crossovers are shown in Tables 4 and 5 between $1s^2np$ and $1s^2nd$ states at different magnetic field strengths. Accordingly, it is clear that the different impacts of the two models were interpreted graphically and the confined (ECSCP) model showed remarkable results compared to the SCP model.

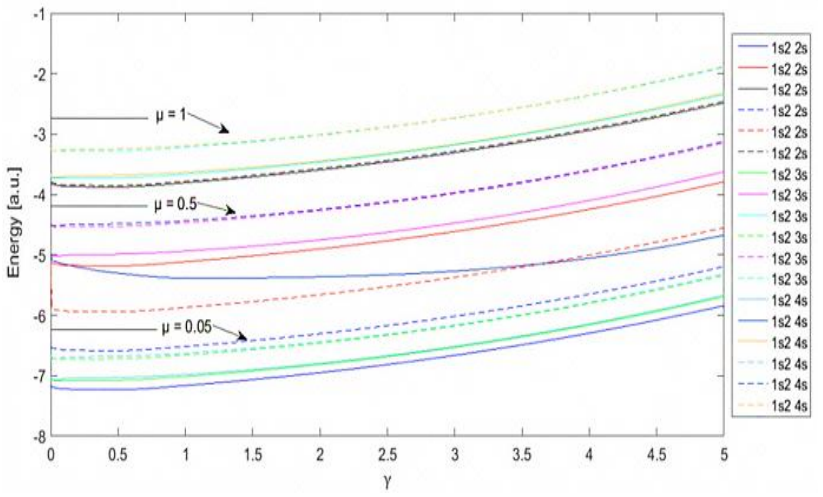

Fig. 1 – Energies of $1s^2ns$ states at $\mu = 0.05$, $\mu = 0.5$, and $\mu = 1$ using the SCP (-) and ECSCP (---) models, at various values of γ.

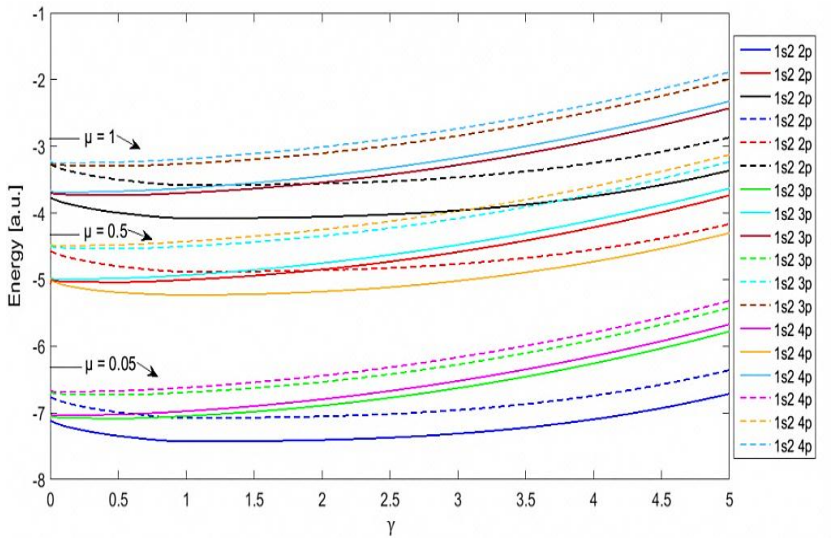

Fig. 2 – Energies of $1s^2np$ states at μ = 0.05, μ = 0.5, and μ = 1 using the SCP (-) and ECSCP (---) models, at various values of γ.

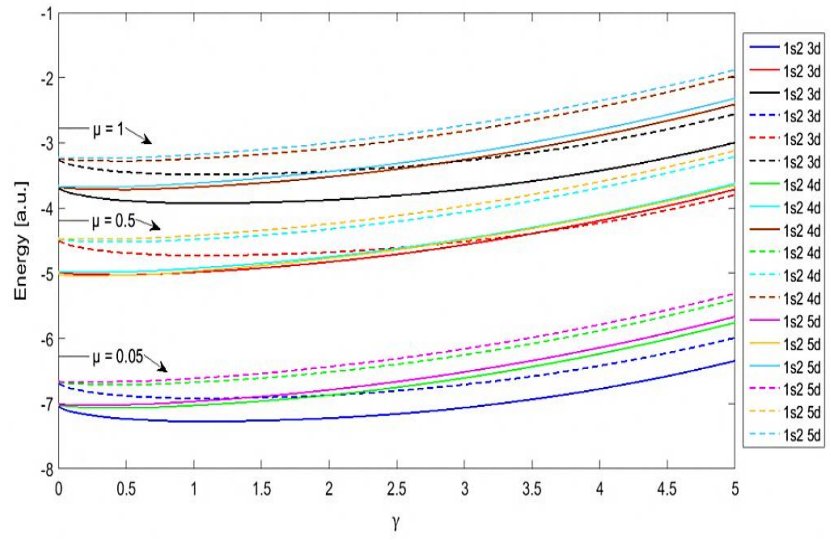

Fig.3 – Energies of $1s^2nd$ states at μ = 0.05, μ = 0.5, and μ = 1 using the SCP (-) and ECSCP (---) models, at various values of γ.

Table 4

The crossovers of $1s^2np$ states, state 1 to state 2, using the SCP and ECSCP models at a magnetic field strength γ.

γ	μ	Plasma model	State 1	μ	Plasma model	State 2
0.0037	0.5	SCP	$1s^2\ 3p$	1	SCP	$1s^2\ 4p$
0.0089	0.05	SCP	$1s^2\ 2p$	1	SCP	$1s^2\ 4p$
0.6108	0.05	ECSCP	$1s^2\ 2p$	1	SCP	$1s^2\ 4p$
0.8461	0.05	ECSCP	$1s^2\ 2p$	0.5	SCP	$1s^2\ 3p$
1.3230	0.05	ECSCP	$1s^2\ 2p$	1	SCP	$1s^2\ 4p$
1.3604	0.05	ECSCP	$1s^2\ 2p$	0.5	SCP	$1s^2\ 3p$
1.8941	0.05	ECSCP	$1s^2\ 2p$	0.5	SCP	$1s^2\ 3p$
3.0704	0.05	SCP	$1s^2\ 2p$	1	ECSCP	$1s^2\ 4p$
3.7457	0.05	SCP	$1s^2\ 2p$	1	ECSCP	$1s^2\ 3p$

Table 5

The crossovers of $1s^2nd$ states, state 1 to state 2, using the SCP and ECSCP models at a magnetic field strength γ.

γ	μ	Plasma model	State 1	μ	Plasma model	State 2
0.0014	0.5	SCP	$1s^2\ 4d$	1	SCP	$1s^2\ 5d$
0.0036	0.05	SCP	$1s^2\ 3d$	1	SCP	$1s^2\ 5d$
1.3685	0.05	ECSCP	$1s^2\ 3d$	1	SCP	$1s^2\ 5d$
2.0069	0.05	ECSCP	$1s^2\ 3d$	0.5	SCP	$1s^2\ 4d$
2.0294	0.05	ECSCP	$1s^2\ 3d$	1	SCP	$1s^2\ 5d$
2.5884	0.05	ECSCP	$1s^2\ 3d$	0.5	SCP	$1s^2\ 4d$
2.7394	0.05	ECSCP	$1s^2\ 3d$	1	SCP	$1s^2\ 5d$
2.8146	0.05	ECSCP	$1s^2\ 3d$	0.5	SCP	$1s^2\ 4d$

5. CONCLUSIONS

The current investigation provides valuable insights into the ground and excited doublet states of lithium atom embedded in two different plasma model

potentials when impacted by an external magnetic field. Low standard deviation results were produced by all the computations, which were performed using the Metropolis algorithm within the numerical VMC method. To perform that, appropriate trial wave functions were used with finely optimized variational parameters, considering the Landau orbital wave function as a magnetic part, in addition to the proposed effective-plasma factor for the ECSCP model exclusively.

As a result of varying magnetic field strengths, the characteristics of the electron systems embedded in each plasma model were revealed, besides the attributes of the ECSCP model, which exhibited a stronger plasma screening effect than the SCP potential model. Furthermore, by increasing the magnetic field, in addition to the effective roles of the diamagnetic and Zeeman terms for each system, the ECSCP model caused an increase in the kinetic energy of the entire system and a rapid decrease in the pure Coulomb and correlation potentials.

Also, the influence of the different plasma model potentials was investigated graphically by plotting the energy values as functions of the magnetic field strength at specific plasma screening parameters, and demonstrated multiple crossovers for the different excited states. Eventually, the obtained results imply that the adherence to the energy ordering $E_{SCP} < E_{ECSCP}$ is numerically validated using the VMC method for the lithium atom within various external potentials.

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