# THE GROUND STATE AND LOW-LYING EXCITED STATES OF THE HELIUM ATOM IN DENSE PLASMA

# ESTADO FUNDAMENTAL Y ESTADOS EXCITADOS DE BAJA ENERGÍA DEL ÁTOMO DE HELIO EN PLASMA DENSO

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## Abstract

In this paper, the energy eigenvalues of the helium atom and the helium-like ions up to Z=5 in dense plasma are investigated with screened interaction potentials using Debye-Hückel model and exponential cosine screened Coulomb potential using variational Monte Carlo method. The calculations which are carried out in this paper are based on using trial wave functions with different asymptotic behaviors, classified as polynomial correlation, exponential decreasing, and exponential increasing functions. Furthermore, the low-lying excited states of the helium atom were investigated under the same model potentials using trial wave functions for the lowest four excited states, corresponding to the configurations 1s2s and 1s2p. Interesting results are obtained in comparison with results obtained by using other trial wave functions.

**Keywords:** helium atom, dense plasma, exponential cosine screened Coulomb potential, variational Monte Carlo method.

## Resumen

En este trabajo se investigan los valores propios de energía del átomo de helio y de los iones helioides hasta

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Z = 5 inmersos en plasma denso, considerando potenciales de interacción apantallados descritos por el modelo de Debye–Hückel y por el potencial de Coulomb apantallado exponencial-coseno. Los cálculos se realizan mediante el método de Monte Carlo variacional empleando funciones de onda de prueba con distintos comportamientos asintóticos, clasificadas como de correlación polinómica, exponencial decreciente y exponencial creciente. Además, se estudian los estados excitados de baja energía del átomo de helio bajo los mismos potenciales modelo, utilizando funciones de onda de prueba para los cuatro estados excitados más bajos correspondientes a las configuraciones 1s2s y 1s2p. Se obtienen resultados interesantes en comparación con los obtenidos mediante otras funciones de prueba.

**Palabras clave:** átomo de helio, plasma denso, potencial de Coulomb apantallado exponencial-coseno, método de Monte Carlo variacional.

## Introduction

The theoretical studies of atomic systems in dense plasmas at different temperatures play very important role in some physical situations and have gained considerable interest in recent years [1–11]. To study the effect of the plasma environment on atoms, it is recommended to investigate the screened interaction potentials using Debye–Hückel model (DHM) [12], which provides a suitable treatment of non-ideality in plasma via the screening effect. This model is used to simulate plasma screening effect of weakly coupled plasmas. Furthermore, it was shown that the study of effective screened potential in dense quantum plasmas can be represented by using modified Debye–Hückel model (MDHM) [13] or exponential cosine screened Coulomb potential (ECSCP).
It should be noticed that extensive efforts have been focused on the screened Coulomb potentials and exponential cosine screened Coulomb potential in field theory, nuclear, and plasma physics [14–19]. Within the framework of the B-spline configuration interaction (BSCI) method, Yen-Chang Lin, Chih-Yuan Lin and

Yew Kam Ho studied the spectral/structural data of helium atom with exponential-cosine-screened Coulomb potentials [20]. Moreover, Amlan K. Roy discussed the critical parameter in three screened potentials, namely Hulthen, Yukawa, and exponential-cosine-screened Coulomb potentials and spherical confinement of H Atom [21]. Also, Arijit Ghoshal and Y. K. Ho [22] had made investigations on the two-electron system in the field of generalization screened potential within the framework of highly correlated and extensive wave functions in Ritz's variational principle, where they have been able to determine accurate ground state energies and wave functions of the two-electron system for different values of the screening parameter.

Furthermore, many studies have been attempted to construct trial wave function for helium atom. V. V. Nasyrov [23] considered a numerical method for constructing a model wave function for the helium atom. Moreover, D. Bressanini and G. Morosi [24] studied a compact boundary-condition determined wave function for the two-electron atomic systems. In addition, K. V. Rodriguez, G. Gasaneo and D. M. Mitnik [25] presented accurate and simple wave functions for the helium isoelectronic sequence with correct cusp conditions. Moreover, some attempts to study the ground state of the helium atom in dense plasmas were carried out by S. Kar and Y. K. Ho [4], who investigated the bound states of the helium atom in dense plasmas. Also, A. Ghoshal and Y. K. Ho [5] studied the ground state of the helium atom in exponential cosine screened Coulomb potentials.

The variational Monte Carlo (VMC) method provides us with an accurate technique for evaluating multidimensional integrals by transforming them to the evaluation of expectation values of operators over certain region of space, which can be handled well by a suitably application of the Metropolis algorithm [26].

Accordingly, in this paper we apply the VMC method to study the effect of the plasma environment by using the DHM and the MDHM to determine the accurate ground state energy $E_{\mathrm{He}(1s1s)}$ of the helium atom, the helium-like ions up to $Z = 5$, and the low-lying excited states of the helium atom by using trial wave functions with different asymptotic behaviors.

## The Used Plasma Models

The collective effects of correlated many-particle interactions lead to screened Coulomb interactions in hot and dense plasmas which are represented by the DHM and it is given by

$$V_{DH}(r) = -\frac{Ze^2}{r}\exp(-\mu r), \tag{1}$$

where $\mu = \frac{1}{\lambda_D}$ represents 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 in the following form [27]

$$\mu = \frac{1}{\lambda_D} = \sqrt{\frac{4\pi e^2 N_e}{KT_e}}, \tag{2}$$

where, $\lambda_D$ 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.
Furthermore, it was shown that the study of effective screened potential in dense quantum plasmas can be represented by using MDHM [13] or ECSCP, which is given by

$$V_{MDH}(r) = -\frac{Ze^2}{r}\exp(-\mu r)\cos(\mu r) \tag{3}$$

Usually, in quantum plasmas, $\mu$ is related to the quantum wave number of the electron, which is related to the electron plasma frequency. Furthermore, the definitions of $\mu$ in the two model potentials are different. In this work, we are dealing with $\mu$ as a parameter so that physical difference of $\mu$ between these model potentials [17, 21, 28] are not discussed.

## Variational Monte Carlo Method

Quantum Monte Carlo methods have already been used for quantum mechanical systems. There are several quantum Monte Carlo techniques such as VMC, Diffusion Monte Carlo and Green's function Monte Carlo methods. We will concentrate in this paper on the VMC method, which is used to approximate the ground state of the Hamiltonian $\hat{H}$ of quantum mechanical systems by some trial wave function $\psi_T(\mathbf{R})$ whose form is chosen from the analysis of the quantum mechanical system under study. Therefore, the expectation value of the Hamiltonian $\hat{H}$ is written as [29]

$$\begin{aligned}\langle \hat{H} \rangle = E_{\text{VMC}} &= \frac{\int \psi_T^*(\mathbf{R})\, \hat{H}\, \psi_T(\mathbf{R})\, d\mathbf{R}}{\int \psi_T^*(\mathbf{R})\, \psi_T(\mathbf{R})\, d\mathbf{R}} \\ &= \frac{\int d\mathbf{R}\, \psi_T^2(\mathbf{R})\, E_L(\mathbf{R})}{\int d\mathbf{R}\, \psi_T^2(\mathbf{R})} = \int d\mathbf{R}\, \rho(\mathbf{R})\, E_L(\mathbf{R}), \end{aligned} \tag{4}$$

where $E_L(R) = \frac{H\,\psi(R)}{\psi(R)}$ is the local energy depending on the $3N$ coordinates $\mathbf{R}$ of the $N$ electrons, and $\rho(\mathbf{R}) = \frac{\psi_T^2(\mathbf{R})}{\int d\mathbf{R}\, \psi_T^2(\mathbf{R})}$ is the normalized probability density. The variational energy can be calculated as the average value of $E_L(\mathbf{R})$ on a sample of $M$ points, $\mathbf{R}_k$, sampled from the probability density $\rho(\mathbf{R})$ as follows

$$E_{\text{VMC}} \approx \langle E_L \rangle = \frac{1}{M} \sum_{k=1}^{M} E_L(R_k). \tag{5}$$

In practice, the points $R_k$ are sampled using the Metropolis–Hastings algorithm [23]. When evaluating the energy of the system it is important to calculate the standard deviation of this energy, given by [29]

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

Since $\langle E_L \rangle$ will be exact when an exact trial wave function is used, then the standard deviation of the local energy will be zero for this case. Thus, in the Monte Carlo method, the minimum of $\langle E_L \rangle$ should coincide with a minimum in the standard deviation.

## Theoretical Details

The non-relativistic Hamiltonian in Hylleraas coordinates [30] for the two-electron systems, under effective screened potential in dense plasmas, is given, in atomic units, by

$$H_1 = -\tfrac{1}{2}\sum_i^2 \nabla_i^2 - 2\left[\frac{exp(-\mu r_1)}{r_1} + \frac{exp(-\mu r_2)}{r_2}\right] + \frac{exp(-\mu r_{12})}{r_{12}}, \quad (6)$$

where $r_1 = |\mathbf{r}_1|$ and $r_2 = |\mathbf{r}_2|$, in which $\mathbf{r}_1$ and $\mathbf{r}_2$ are the radius vectors of the two electrons relative to the nucleus, and $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ is their relative distance. Moreover, the non-relativistic Hamiltonian in the effective ECSCP is given by

$$H_2 = -\frac{1}{2}\sum_i^2 \nabla_i^2 - 2\left[\frac{\exp(-\mu r_1)}{r_1}\cos(\mu r_1) + \frac{\exp(-\mu r_2)}{r_2}\cos(\mu r_2)\right] + \frac{\exp(-\mu r_{12})}{r_{12}}\cos(\mu r_{12}) \quad (7)$$

Our calculations for the two electron systems depend on several different types of trial wave functions with different asymptotic behaviors classified as polynomial correlation, exponential decreasing and exponential increasing functions where all the considered wave functions satisfy Kato cusp conditions [24, 31]. Firstly, we consider a trial wave function with polynomial correlation in the form [20]

$$\psi_1(r_1, r_2, r_{12}) = C_1 e^{-Z(r_1+r_2)}\left(1 + \tfrac{1}{2}r_{12} + C_2 r_{12}^2\right), \quad (8)$$

where $Z$ is the nuclear charge and $C_1$ and $C_2$ are variational parameters.

The second type of trial wave function with exponential increasing behavior is written as [25]

$$\psi_2(r_1, r_2, r_{12}) = (1 + P_{12})\exp\left(\tfrac{-Zr_1+b_1r_1^2}{1+r_1}\right)\exp\left(\tfrac{-Zr_2+b_2r_2^2}{1+r_2}\right)\exp\left(\tfrac{dr_{12}}{1+er_{12}}\right), \quad (9)$$

where $P_{12}$ is the operator that permutes the two electrons, and $b_1, b_2, d$ and $e$ are variational parameters. The third type of trial wave function with exponential decreasing is written as [32]

$$\psi_3(r_1, r_2, r_{12}) = \frac{A}{2}\, e^{-Z(r_1+r_2)} \left[\cosh(ar_1) + \cosh(ar_2)\right] \left(1 + \tfrac{g}{2} r_{12} e^{-br_{12}}\right), \tag{10}$$

with $Z$ the atomic number of the system and $A = 0.702534$ is the normalization constant of the wave function. Here $a$ and $b$ are variational parameters. The case corresponding to $g = 1$ gives the wave function of Le Sech [33], while for $g = 0$ and $a = 0$ we get the well-known separable two-electron wave function [34].

## The Trial Wave Functions for the Low-Lying Excited States of Helium Atom

The study of the low-lying excited states of the helium atom has received considerable attention in the theoretical investigations. Therefore, for the lowest four excited states, corresponding to the configurations $1s2s$ and $1s2p$, we used the following trial wave functions:

a. For the lowest ortho (space-antisymmetric) state $2\,^3S$, corresponding to the configuration $1s2s$, we consider the following simple trial wave function

$$\Psi_{2^3S}(r_1, r_2) = N \left[\psi_{1s}(r_1)\, \psi_{2s}(r_2) - \psi_{1s}(r_2)\, \psi_{2s}(r_1)\right] f(r_{12}), \tag{11}$$

b. The state $2\,^1S$ is a para (space-symmetric) state corresponding to the configuration $1s2s$ and its trial wave function is, then, taken of the form

$$\Psi_{2^1S}(r_1, r_2) = N \left[\psi_{1s}(r_1)\, \psi_{2s}(r_2) + \psi_{1s}(r_2)\, \psi_{2s}(r_1)\right] f(r_{12}). \tag{12}$$

For the $2^1P$ state, which is the lowest para-state corresponding to the configuration $1s2p$, we consider the trial wave function

$$\Psi_{2^1P}(r_1, r_2) = N \Big[\psi_{1s}(r_1)\, \psi_{2pm}(r_2) + \psi_{1s}(r_2)\, \psi_{2pm}(r_1)\Big] f(r_{12}) \tag{13}$$

For the $2^3P$ state, which is the lowest ortho state corresponding to the configuration $1s2p$, the trial wave function takes the form

$$\Psi_{2^3P}(r_1, r_2) = N\Big[\psi_{1s}(r_1)\,\psi_{2pm}(r_2) - \psi_{1s}(r_2)\,\psi_{2pm}(r_1)\Big] f(r_{12}), \quad (14)$$

where

$$\psi_{1s}(r) = \exp(-z_0 r),$$

$$\psi_{2s}(r) = \Big(1 - \frac{z_i r}{2}\Big)\exp\Big(-\frac{z_i r}{2}\Big),$$

and

$$\psi_{2pm}(r) = r\exp\Big(-\frac{z_i r}{2}\Big)\,Y_{1,m}(\theta, \phi), \quad m = 0, \pm 1.$$

In the above equations, $z_0$ and $z_i$ are variational parameters, and $N$ is the normalization constant. The function $f(r_{12})$ is the Jastrow correlation function given by [35].

$$f(r_{12}) = e^{\frac{r_{12}}{\alpha(1+\beta r_{12})}}$$

For the relationship of the electron-electron interaction, one obtains the cusp conditions

$$\left.\begin{aligned} \frac{1}{\Psi}\frac{\partial\Psi}{\partial r_{ij}}\Big|_{r_{ij}=0} &= \frac{1}{2}, \quad \text{for unlike spins} \\ \frac{1}{\Psi}\frac{\partial\Psi}{\partial r_{ij}}\Big|_{r_{ij}=0} &= \frac{1}{4}, \quad \text{for like spins} \end{aligned}\right\}$$

The numerical method, which is used in the calculations, the VMC method, is based on a combination of the well-known variational method and the Monte Carlo technique of calculating the multi-dimensional integrals. By a suitable choice of the trial wave function, it is then possible to obtain minimum energy eigenvalues in agreement with the exact values for the ground as well as the excited states of the given atom. These minimum energies are associated with the least values of the standard deviation. In all our calculations, the resulting values of the standard deviation for the ground-state and the four low-lying excited states of helium are less than 0.0001.

In Table 1, we present the values of the parameters of the trial wave functions which produced the best fit to the low-lying excited states of helium.

| State | $z_0$ | $z_i$ | $\alpha$ | $\beta$ |
|---|---|---|---|---|
| $2^3S$ | 2 | 1.620 | 2 | 0.30 |
| $2^1S$ | 2 | 0.865 | 4 | 0.65 |
| $2^1P$ | 2 | 1.000 | 4 | 1.00 |
| $2^3P$ | 2 | 1.200 | 2 | 0.40 |

TABLE 1. *The variational parameters for low-lying excited states of helium using the four trial wave functions.*

## Results and Discussions

It is impossible to find a complete analytical solution for the wave functions of the interaction of a system of two electrons because of the presence of the correlation of atomic electrons $r_{12}$. Therefore, we tended to solve it in an approximate manner. We used the well-known VMC method, to investigate the effect of the plasma environment using DHM and MDHM to determine the energy eigenvalues of the helium atom and helium-like ions up to $Z = 5$. The calculations, which are carried out in our investigation, are based on using the three trial wave functions with different asymptotic behaviors, as explained above.

First, we considered the trial wave function $\psi_1$ which contains a polynomial angular correlation, the variational parameters $C_1$ and $C_2$ are given the values 1.55134 and 0.03889, respectively [23]. In Table 2, we present the calculated ground state energies of the helium atom and the helium-like ions $(\mathrm{H}^-, \mathrm{Li}^+, \mathrm{Be}^{2+}, \mathrm{B}^{3+})$ under effective screened potential in dense quantum plasmas using the trial wave function $\psi_1$. Furthermore, in Table 3 we presented the calculated ground state energies of helium and helium-like ions $(\mathrm{H}^-, \mathrm{Li}^+, \mathrm{Be}^{2+}, \mathrm{B}^{3+})$ under ECSCP by using the same wave function.

Secondly, we considered the trial wave function $\psi_2$, which is classified as exponentially growing increasing behavior as $r_{12}$ increases. The value of the variational parameter $d$ is 0.5. It was fixed in order to satisfy all the cusp conditions, and the other parameters are given by the following relations: $b_1 = -1.0778 \times Z$, $b_2 = 0.4142 - 0.8287 \times Z$ and $e = 0.2247 \times Z$ [25]. The results of the calculations by using the trial wave function $\psi_2$ under effective

| $\lambda_D$ | | $Z = 1, \dots, 5$ | | | | |
|---|---|---|---|---|---|---|
| | | $-E_{H^-}$ | $-E_{He}$ | $-E_{Li^+}$ | $-E_{Be^{2+}}$ | $-E_{B^{3+}}$ |
| 1 | $\psi_1$ | — | 0.6583782 | 3.384993 | 7.779964 | 14.20784 |
| | $\psi_2$ | — | 0.8793133 | 3.269577 | 7.945492 | 14.20680 |
| | $\psi_3$ | 0.1357037 | 0.678469 | 3.258693 | 7.757832 | 13.91359 |
| | | — | 0.81704 [19] | — | — | — |
| 2 | $\psi_1$ | 0.1276934 | 1.618487 | 5.085995 | 10.45508 | 17.83788 |
| | $\psi_2$ | 0.1448210 | 1.688010 | 5.051023 | 10.50654 | 17.84351 |
| | $\psi_3$ | 0.1078920 | 1.63016 | 5.046806 | 10.45222 | 17.70252 |
| | | 0.15156 [19] | 1.65504 [19] | — | — | — |
| | | 0.15783 [36] | — | — | — | — |
| 10 | $\psi_1$ | 0.4253473 | 2.61339 | 6.793266 | 12.96514 | 21.13618 |
| | $\psi_2$ | 0.4323791 | 2.616365 | 6.791333 | 12.96878 | 21.14311 |
| | $\psi_3$ | 0.4047339 | 2.62304 | 6.789536 | 12.96792 | 21.06163 |
| | | 0.43192 [19] | 2.61451 [19] | — | — | — |
| | | 0.43295 [36] | 2.61471 [36] | — | — | — |
| 20 | $\psi_1$ | 0.4717589 | 2.756179 | 7.033276 | 13.30552 | 21.57625 |
| | $\psi_2$ | 0.4783779 | 2.756607 | 7.032549 | 13.30738 | 21.58320 |
| | $\psi_3$ | 0.4509977 | 2.75661 | 7.040529 | 13.30846 | 21.50382 |
| | | 0.47724 [19] | — | — | — | — |
| | | 0.47903 [36] | — | — | — | — |
| 40 | $\psi_1$ | 0.4958478 | 2.829343 | 7.155744 | 13.47809 | 21.79875 |
| | $\psi_2$ | 0.5023600 | 2.829113 | 7.155327 | 13.47950 | 21.80570 |
| | $\psi_3$ | 0.4750360 | 2.83896 | 7.153632 | 13.48107 | 21.72686 |
| 70 | $\psi_1$ | 0.5063561 | 2.861069 | 7.208744 | 13.55254 | 21.8946 |
| | $\psi_2$ | 0.5128439 | 2.860691 | 7.208398 | 13.55385 | 21.90157 |
| | $\psi_3$ | 0.4855415 | 2.87068 | 7.206707 | 13.55553 | 21.82285 |
| 100 | $\psi_1$ | 0.5105907 | 2.873823 | 7.230032 | 13.58241 | 21.93304 |
| | $\psi_2$ | 0.5170725 | 2.873407 | 7.229702 | 13.58369 | 21.9400 |
| | $\psi_3$ | 0.4897735 | 2.88343 | 7.228013 | 13.5854 | 21.86131 |
| $\infty$ | $\psi_1$ | 0.5205414 | 2.903724 | 7.279894 | 13.65228 | 22.0229 |
| | $\psi_2$ | 0.5270174 | 2.903272 | 7.279582 | 13.65353 | 22.02987 |
| | $\psi_3$ | 0.4997217 | 2.903761 | 7.277893 | 13.65527 | 21.95121 |
| | | 0.52644 [16] | 2.90337 [16] | 7.27948 [16] | — | — |
| approx [37] | | 0.527750974 | 2.903724311 | 7.279913341 | 13.65556617 | 22.03097151 |

Theoretical results of L. U. Ancarani et al. [19]
Theoretical results of S. Kar et al. [36]

TABLE 2. Ground state energies of helium and helium-like ions ($H^-$, $Li^+$, $Be^{2+}$, $B^{3+}$) under effective screened potential in dense quantum plasmas, given in Eq. (6), using the wave functions $\psi_1$, $\psi_2$ and $\psi_3$. Approximation energies are taken from [38]. All energies are in atomic units.

screened potential in dense quantum plasmas and effective ECSCP is presented in Tables 2 and 3, respectively.

Finally, we considered the trial wave function $\psi_3$, which is classified as exponentially growing decreasing behavior as $r_{12}$ increases. The variational parameters $a$, $g$ and $b$ are given by 0.72, 1 and 0.20, respectively. The calculations are carried out by using the trial wave function $\psi_3$ under effective screened potential in dense quantum plasmas and effective ECSCP and are presented in Tables 2 and 3, respectively.

It is worth mentioning that the evaluation of the ground state energies for He-like configurations are not directly observable in the plasma environment. Therefore, we studied the low-lying excited states of helium atom under effective screened potential in dense quantum plasmas and effective ECSCP using trial wave functions for the lowest four excited states, corresponding to the configurations $1s2s$ and $1s2p$. In Table 1, we present the variational parameters for the four trial wave functions, which are used.

In Figs.1, 2 and 3, we presented the bound state energies of helium and helium-like ions $(\mathrm{H}^-, \mathrm{Li}^+, \mathrm{Be}^{2+}, \mathrm{B}^{3+})$ with increasing screening effect. Moreover, in Figs. 4, 5 and 6, we presented the bound state energies of helium and helium-like ions $(\mathrm{H}^-, \mathrm{Li}^+, \mathrm{Be}^{2+}, \mathrm{B}^{3+})$ with decreasing screening effect.

We noticed from Figs. 1, 2 and 3 that the calculated ground state energies take logarithmic function behavior when we use the effective screened potential in dense quantum plasmas. In addition, for small screening length $\lambda_D = 1, 2$, the calculated ground state energies of helium and helium-like ions are low and far from approximations energies values which have been obtained in [38]. Furthermore, for large screening length $\lambda_D$, we find that the calculated ground state energies are close to the experimental values and they are in very good agreement with the experimental values when the screening length $\lambda$ tends to $\infty$.

On the other hand, in Figs. 4, 5 and 6, the calculated ground state energies take linear function behavior when we use the exponential cosine screened Coulomb effective potential; this is because of the oscillatory part (cosine). To be more precise, the calculated ground state energies increase with decreasing $\lambda_D$. Most accurate results of the calculated ground state energies are computed by using the presented three wave functions, which are collected in Table 4. However, it has been found from the computations presented that it is easy to deal with the trial wave function with polynomial correlation $\psi_1$, rather than the trial wave function with exponential increasing behavior $\psi_2$.

We note here that the results shown in Tables 5 and 6 are carried out by using the trial wave function for the lowest four excited states under effective screened potential in dense quantum plasmas and effective ECSCP, respectively.

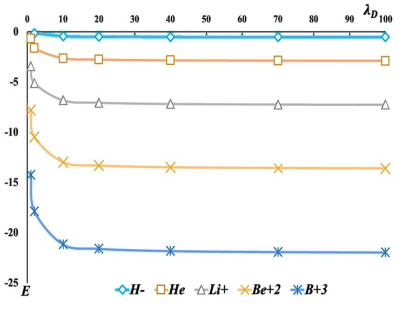


FIGURE 1.

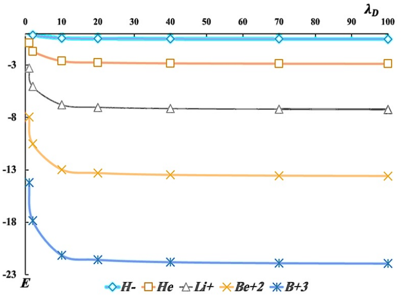


FIGURE 2.

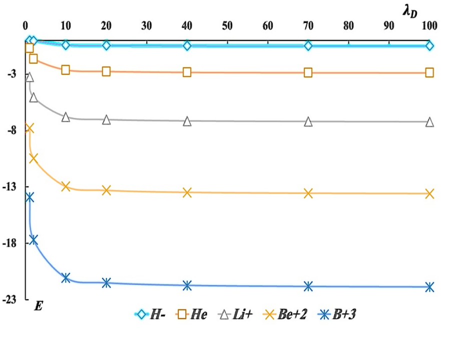


FIGURE 3.

*Figs. 1, 2 and 3 Ground state energies of helium and helium-like ions* ($H^-$, $Li^+$, $Be^{2+}$, $B^{3+}$) *under effective screened potential in dense quantum plasmas, given in Eq. (6), using the wave functions* $\psi_1$, $\psi_2$ *and* $\psi_3$.

| $\mu$ | | $Z = 1, \ldots, 5$ | | | | |
|---|---|---|---|---|---|---|
| | | $-E_{\mathrm{H}^-}$ | $-E_{\mathrm{He}}$ | $-E_{\mathrm{Li}^+}$ | $-E_{\mathrm{Be}^{2+}}$ | $-E_{\mathrm{B}^{3+}}$ |
| 0.0 | $\psi_1$ | 0.5205414 | 2.903724 | 7.279894 | 13.65228 | 22.0229 |
| | $\psi_2$ | 0.5270174 | 2.903272 | 7.279582 | 13.65353 | 22.02987 |
| | $\psi_3$ | 0.4997217 | 2.903761 | 7.277893 | 13.65527 | 21.95121 |
| | | 0.52644[19] | 2.90337[19] | 7.27948[19] | — | — |
| approx.[38] | | 0.527750974 | 2.903724311 | 7.279913341 | 13.65556617 | 22.03097151 |
| 0.01 | $\psi_1$ | 0.5105417 | 2.873724 | 7.229895 | 13.58228 | 21.93291 |
| | $\psi_2$ | 0.5170177 | 2.873273 | 7.229583 | 13.58354 | 21.93987 |
| | $\psi_3$ | 0.4897221 | 2.873762 | 7.227893 | 13.58527 | 21.86121 |
| 0.02 | $\psi_1$ | 0.5005434 | 2.843729 | 7.1799 | 13.51228 | 21.8429 |
| | $\psi_2$ | 0.5070199 | 2.843281 | 7.179585 | 13.51354 | 21.84987 |
| | $\psi_3$ | 0.4797247 | 2.843766 | 7.177896 | 13.51527 | 21.77121 |
| 0.05 | $\psi_1$ | 0.4705732 | 2.753802 | 7.029972 | 13.30233 | 21.57295 |
| | $\psi_2$ | 0.4770572 | 2.753397 | 7.02870 | 13.30361 | 21.57991 |
| | $\psi_3$ | 0.4497679 | 2.753834 | 7.027954 | 13.30532 | 21.50123 |
| | | 0.47643[19] | — | — | — | — |
| | | 0.47772[5] | — | — | — | — |
| 0.08 | $\psi_1$ | 0.4406728 | 2.664038 | 6.880208 | 13.09248 | 21.30308 |
| | $\psi_2$ | 0.4471828 | 2.663772 | 6.879829 | 13.09385 | 21.31006 |
| | $\psi_3$ | 0.4199104 | 2.664053 | 6.878138 | 13.09548 | 21.23131 |
| 0.1 | $\psi_1$ | 0.4207997 | 2.604330 | 6.780503 | 12.95267 | 21.12326 |
| | $\psi_2$ | 0.4273427 | 2.604236 | 6.780061 | 12.95414 | 21.13024 |
| | $\psi_3$ | 0.4000894 | 2.604325 | 6.778368 | 12.95568 | 21.05140 |
| | | 0.42650 [19] | 2.60409[19] | — | — | — |
| | | 0.42768[5] | 2.60444[5] | — | — | — |
| 0.15 | $\psi_1$ | 0.3714258 | 2.455702 | 6.531906 | 12.60360 | 20.67408 |
| | $\psi_2$ | 0.3781309 | 2.456417 | 6.531172 | 12.60553 | 20.68110 |
| | $\psi_3$ | 0.3509516 | 2.455612 | 6.529469 | 12.60664 | 20.60184 |
| | | — | — | 6.53007[19] | — | — |
| 0.25 | $\psi_1$ | 0.2746979 | 2.162305 | 6.038846 | 11.90822 | 19.77819 |
| | $\psi_2$ | 0.2822341 | 2.166879 | 6.03667 | 11.91242 | 19.7854 |
| | $\psi_3$ | 0.2552527 | 2.161887 | 6.034924 | 11.91141 | 19.70409 |
| | | 0.28049[19] | — | — | — | — |
| | | 0.28160[5] | — | — | — | — |
| 0.50 | $\psi_1$ | 0.05296836 | 1.462158 | 4.844694 | 10.19662 | 17.56252 |
| | $\psi_2$ | 0.06705844 | 1.495206 | 4.831298 | 10.21832 | 17.57109 |
| | $\psi_3$ | 0.03875005 | 1.460709 | 4.839085 | 10.20077 | 17.47341 |
| | | 0.04349[19] | 1.47653[19] | — | — | — |
| | | 0.08289[5] | 1.47696[5] | — | — | — |
| 0.70 | $\psi_1$ | — | 0.8224184 | 3.943935 | 8.867401 | 15.82618 |
| | $\psi_2$ | — | 0.9157847 | 3.911365 | 8.918591 | 15.83673 |
| | $\psi_3$ | — | 0.9445192 | 3.908388 | 8.872678 | 15.71030 |
| 1.00 | $\psi_1$ | — | 0.247953 | 2.703626 | 6.961212 | 13.30194 |
| | $\psi_2$ | — | 0.4316978 | 2.623409 | 7.084514 | 13.31631 |
| | $\psi_3$ | — | 0.255767 | 2.617936 | 6.967584 | 13.11581 |
| | | — | 0.40056[19] | — | — | — |
| | | — | 0.40526[5] | — | — | — |

Theoretical results of A. Ghoshal et al. [5]
Theoretical results of L. U. Ancarani et al. [19]

TABLE 3. *Ground state energies of helium and helium-like ions ($H^-$, $Li^+$, $Be^{2+}$, $B^{3+}$) under effective ECSCP, given in Eq. (7), by using the wave functions $\psi_1$, $\psi_2$ and $\psi_3$. Approximation energies are taken from Ref. [38]. All energies are in atomic units.*

| Energy | $-E_{H^-}$ | $-E_{He}$ | $-E_{Li^+}$ | $-E_{Be^{2+}}$ | $-E_{B^{3+}}$ |
|---|---|---|---|---|---|
| $\psi_1$ | 0.5205414 | 2.903724 | 7.279894 | 13.65228 | 22.0229 |
| $\psi_2$ | 0.5270174 | 2.903272 | 7.279582 | 13.65353 | 22.02987 |
| $\psi_3$ | 0.4997217 | 2.903761 | 7.277893 | 13.65527 | 21.95121 |
| approx. [38] | 0.527750974 | 2.903724311 | 7.279913341 | 13.65556617 | 22.03097151 |

TABLE 4. *Ground state energies of helium and helium-like ions* ($H^-$, $Li^+$, $Be^{2+}$, $B^{3+}$)*. All the quantities reported here are expressed in atomic units.*

| $\lambda_D$ | Bound-state energies | | | |
|---|---|---|---|---|
| | $-E_{He(1s2s^3S)}$ | $-E_{He(1s2p^1P)}$ | $-E_{He(1s2p^3P)}$ | $-E_{He(1s2s^1S)}$ |
| 1 | 0.446934<br>0.59258[4]<br>0.57636[19] | 0.455367<br>——- | 0.427100<br>——- | 0.524792<br>0.59255[4]<br>0.57388[19] |
| 2 | 1.097174<br>1.16384[4]<br>1.15629[19] | 1.086767<br>1.157886[39]<br>——- | 1.071526<br>1.158562[39]<br>——- | 1.157865<br>1.163745[4]<br>1.15339 |
| 10 | 1.892765<br>1.9010[4]<br>1.90082[19] | 1.851994<br>1.8527035[4] | 1.857288<br>1.8600978[4] | 1.880405<br>1.875036[4]<br>1.87481[19] |
| 20 | 2.025056<br>2.0320[4] | 1.981269<br>1.981437[4] | 1.988531<br>1.990211[4]<br>1.990202[39] | 2.005345<br>2.00368[4] |
| 40 | 2.095346<br>2.10197[4] | 2.050633<br>2.050802[4] | 2.058500<br>2.0599765[4] | 2.073310<br>2.072966[4] |
| 70 | 2.126397<br>2.13294[4] | 2.081453<br>2.081635[4] | 2.089471<br>2.090906[4] | 2.103776<br>2.103778[4] |
| 100 | 2.138983<br>2.14551[4] | 2.093977<br>2.094163[4] | 2.102033<br>2.1034598[4] | 2.116204<br>2.11630[4] |
| $\infty$ | 2.168892<br>2.175229[4]<br>2.17502[19] | 2.123652<br>2.1238430[4] | 2.131747<br>2.133164[4] | 2.145788<br>2.145974[4]<br>2.14571[19] |

Theoretical results of S. Kar et al. [4]
Theoretical results of L. U. Ancarani et al. [19]
Theoretical results of S. T. Dai et al. [39]

TABLE 5. *Excited states $1s2s^3S$, $1s2p^1P$, $1s2p^3P$ and $1s2s^1S$ of the helium atom under effective screened potential in dense quantum plasmas. All the quantities reported here are expressed in atomic units.*

| $\mu$ | Bound-state energies | | | |
|---|---|---|---|---|
| | $-E_{\mathrm{He}(1s2s\,^3S)}$ | $-E_{\mathrm{He}(1s2p\,^1P)}$ | $-E_{\mathrm{He}(1s2p\,^3P)}$ | $-E_{\mathrm{He}(1s2s\,^1S)}$ |
| 0.0 | 2.168892<br>2.17502[19] | 2.123652 | 2.131747 | 2.145788<br>2.14571 [19] |
| 0.01 | 2.138791 | 2.093663 | 2.101756 | 2.115807 |
| 0.02 | 2.108828 | 2.063734 | 2.071805 | 2.085933 |
| 0.05 | 2.019466 | 1.974792 | 1.982598 | 1.997761 |
| 0.08 | 1.931473 | 1.887868 | 1.894943 | 1.912852 |
| 0.1 | 1.873670<br>1.88096[19] | 1.831351 | 1.837650 | 1.858399<br>1.85374[19] |
| 0.15 | 1.733492 | 1.695194 | 1.699100 | 1.729997 |
| 0.25 | 1.473183 | 1.448405 | 1.443456 | 1.501125 |
| 0.5 | 0.931384<br>1.03402[19] | 0.936718 | 0.909911 | 1.016984<br>1.03327[19] |
| 0.70 | 0.578183 | 0.593538 | 0.557661 | 0.675692 |
| 1.00 | 0.133539<br>0.29092[19] | 0.153774 | 0.111808 | 0.226527<br>0.28772[19] |

Theoretical results of L. U. Ancarani et al. [19]

TABLE 6. *Excited states $1s2s^3S$, $1s2p^1P$, $1s2p^3P$ and $1s2s^1S$ of the helium atom under effective ECSCP. All the quantities reported here are expressed in atomic units.*

## Conclusion

The present study is a potentially relevant contribution to the understanding of the ground state of one of the smaller atoms in the periodic table. The model used in this paper describes the screening of charges in a plasma where both positive and negative charges are present, and where their motion is thermal. Furthermore, we have carried out an investigation to determine the effect of Debye plasma and dense quantum plasmas on the low-lying excited states of the helium atom using trial wave functions for the lowest four excited states, corresponding to the configurations $1s2s$ and $1s2p$. The computations presented in the present paper were verified, to high accuracy, by using the VMC method, which has been applied successfully to the case of light atoms in dense plasma states, by suitably chosen theoretical models and trial wave functions.

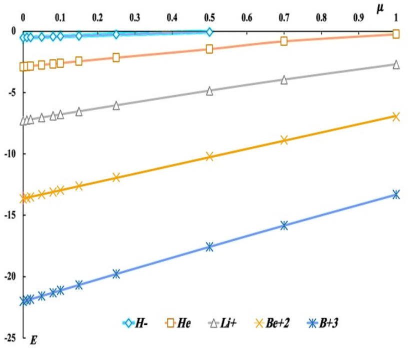


FIGURE 4.

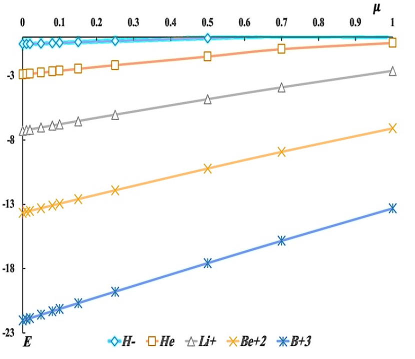


FIGURE 5.

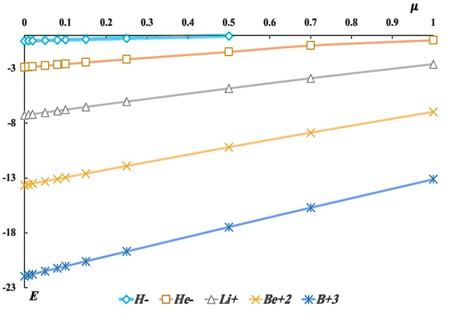


FIGURE 6.

*Figs. 4, 5 and 6 Ground state energies of helium and helium-like ions (*$H^-$*,* $Li^+$*,* $Be^{2+}$*,* $B^{3+}$*) under effective ECSCP, given in Eq. (7), by using the wave functions* $\psi_1$*,* $\psi_2$ *and* $\psi_3$*.*

By analyzing the data presented in Tables 2 and 3, we see that the most accurate results of the calculated ground state energies are obtained by using the trial wave function with polynomial correlation $\psi_1$ and with exponential increasing behavior $\psi_2$, rather than the trial wave function with exponential decreasing behavior $\psi_3$. Also, it has been found, from the computations presented, that it is easy to deal with the trial wave function with polynomial correlation, rather than the trial wave function with exponential behavior.

In addition, the calculated low-lying excited states of the helium atom using the chosen trial wave functions in the framework of the VMC method are in very good agreement with the results used in the already published papers.

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