Doubly-excited $2s^2 \, ^1S^e$ resonance state of helium embedded in Debye plasmas

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Abstract

We have made a first investigation on the resonances in two electron systems in various model plasma environments. The $2s^2 \, ^1S^e$ autoionization resonance state in the helium atom is determined by calculating the density of resonance states using the stabilization method. A screened Coulomb potential obtained from the Debye model is used to represent the interaction between the charged particles. A correlated wave function has been used to represent the correlation effect between the three charge particles. The calculated resonance energies and widths for various Debye parameters ranging from infinity to a small value along with the ground state energies are reported.

1. Introduction

In recent years, there is an upsurge of interest to study atomic processes in plasma environments. The investigations on two electron systems in the plasma networks play an important role because correlation effects between the charged particles can be studied. In such environments, the interaction between the electrons with atomic nucleus is screened, as well as that between the electrons. Several investigations on two-electron systems have been performed in a variety of model plasmas. The ground state energies of $\text{H}^-$ and He embedded in a variety of Debye plasmas have been reported by Winkler [1] and Zhang and Winkler [2]. In such environments, pair-function calculations for two electron systems have been reported by Wang and Winkler [3]. In their pair function calculations, Wang and Winkler [3] have reported the stability of $\text{H}^-$ and the energy splitting of several $1s\,n$ and $1s\,np$ states of the He atom. Dai et al. [4] have reported a calculation of the properties of the screened He-like systems using correlated wave functions. Saha et al. [5] have performed variational calculations for the energy levels of confined two-electron systems in the framework of the Debye plasmas. The electron affinity of positronium embedded in Debye plasmas has been presented by Saha et al. [6]. Mukherjee et al. [7] have reported the energies of the ground state and of the first three excited states of He-like atoms under plasma-type confinements. The ground state energy of helium atom in Debye plasma has also been presented by Lam and Varshni [8] using a simple form of wave functions. It should be mentioned in this regard that, Roussel and O’Connell [9] have performed a variational calculation of the Schrödinger’s equation for atomic hydrogen in static screened Coulomb potentials, and Rogers et al. [10] have investigated the bound eigenstates for a two-particle system interacting through a static screened Coulomb potential. The importance of the screened Coulomb potentials in modeling of atomic potentials has been discussed in the work of Stein et al. [11].

In the present work, a first investigation has been made on the $2s^2 \, ^1S^e$ autoionization resonance of He in the Debye plasma environments. To our knowledge,
no investigation on the S-wave autoionization states of He in Debye plasmas has been reported in the literature. It is also worthy of mention in this context that an investigation on resonances of a model screened Coulomb potential was carried out by Wang and Winkler [12]. They have presented an analytic method for a calculation of shape resonances for a model problem. In our earlier study on an S-wave resonance in H− [13], the screening effect was applied only to the electron–nucleus pairs, but not on the electron–electron pair. In our present work, the screening effect is applied to all the pairs of charged particles. We use a model screened Coulomb potential [1,2,6–8] of Debye-type, and employ the stabilization method proposed by Mandelshtam et al. [14] to calculate the resonance energy, \( E_r \), and the width, \( \Gamma \), of the 2s \(^1\)S\(_e\) autoionization state of He embedded in Debye plasmas. The details of this simple and powerful method to calculate resonance parameters are available in the works of Kar and Ho [15]. The correlated wave function expanded in terms of product basis sets involving inter-particle coordinates has been used to represent the correlation effect between the three charge particles. The convergence of our calculations has been examined with increasing number of terms in the basis expansion. The atomic unit (a.u.) has been used throughout the present work.

2. The method

The non-relativistic Hamiltonian describing the helium atom embedded in Debye plasmas characterized by a parameter \( D \) is given by [1]

\[
H = -\frac{1}{2} \nabla^2 - \frac{1}{2} \nabla_2^2 - 2 \left[ \frac{\exp(-r_1/D)}{r_1} + \frac{\exp(-r_2/D)}{r_2} \right] + \frac{\exp(-r_{12}/D)}{r_{12}},
\]

where \( r_1 \) and \( r_2 \) are the radial coordinates of the two electrons and \( r_{12} \) is their relative distance. A particular value of the screening parameter \( D \) corresponds to the range of plasma conditions, as the Debye parameter is a function of electron density and electron temperature. The smaller values of \( D \) are associated with stronger screening. A parameterized screening potential approximated the effects of the plasma charges on the interaction between the bound electron and the atomic nuclei.

For the \(^1\)S\(_e\) states of He atom, we have considered the wave function

\[
\Psi = (1 + P_{12}) \sum_{i=1}^{N} C_i \exp \left[ \left( -\alpha_{r_1} - \beta_{r_2} + \gamma_{r_{12}} \right) \omega \right],
\]

where \( \alpha, \beta, \gamma \) are the non-linear variational parameters, \( C_i \) (\( i = 1, \ldots, N \)) are the linear expansion coefficients, \( \omega \) is a scaling constant to be discussed later in the text, and \( P_{12} \) is the permutation operator defined by \( P_{12} f(r_1, r_2, r_{12}) = f(r_2, r_1, r_{12}) \). To obtain the ground-state energy of He we first set \( \omega = 1 \). The wave functions of Eq. (2) have been widely used in several bound states calculations of two electron systems in model plasma environments ([1,2,6,7] and references therein). It is worthy to mention in this regard that Thakkar and Smith [16] has used this wave function in their calculations of the \(^1\)S ground states of helium-like ions from H\(^{-}\) through Mg\(^{10+}\). Frolov [17] and Frolov and Smith [18] have used this wave function in their calculations of the bound states properties for the He-like ions. Following the work of Frolov [19], we have used a quasi-random process to choose the non-linear variational parameters \( \alpha, \beta, \gamma \). According to the multi-box strategy for constructing highly accurate bound state wave functions for three body systems [19], the parameters \( \alpha, \beta, \gamma \) will be chosen from the three positive interval \([A_1^{(k)}, A_2^{(k)})\), \([B_1^{(k)}, B_2^{(k)})\] and \([C_1^{(k)}, C_2^{(k)})\]; where \( k = \text{mod}(i,3) + 1 \), \( 1 \leq i \leq N \).

\[
\alpha_i = \eta_1^{(k)} \left[ \left\langle \left( \frac{1}{2} (i(i+1))^{1/2} \right) \right\rangle \right] \left( A_1^{(k)} - A_2^{(k)} \right) + A_1^{(k)},
\]

\[
\beta_i = \eta_2^{(k)} \left[ \left\langle \left( \frac{1}{2} (i(i+1))^{1/3} \right) \right\rangle \right] \left( B_1^{(k)} - B_2^{(k)} \right) + B_1^{(k)},
\]

\[
\gamma_i = \eta_3^{(k)} \left[ \left\langle \left( \frac{1}{2} (i(i+1))^{1/5} \right) \right\rangle \right] \left( C_1^{(k)} - C_2^{(k)} \right) + C_1^{(k)},
\]

where the symbol \( \langle \ldots \rangle \) designates the fractional part of a real number. The positive scaling factors \( \eta_1^{(k)}, \eta_2^{(k)} \) and \( \eta_3^{(k)} \) will be equal to 1 in the first stage and in the second stage it will be varied. But for the present problem we have set \( A_1^{(k)} = 0, A_2^{(k)} = \alpha, B_1^{(k)} = 0, B_2^{(k)} = \beta, C_1^{(k)} = 0, C_2^{(k)} = \gamma \) and \( \eta_1^{(k)} = \lambda_1, \eta_2^{(k)} = \lambda_2, \eta_3^{(k)} = \lambda_3 \). Ultimately, six variation parameters \( \alpha, \beta, \gamma, \lambda_1, \lambda_2, \lambda_3 \) are used in the entire calculations.

3. Results and discussion

We have used the stabilization method [14] to extract the resonance energies and widths by calculating the density of resonance states. After diagonalization of the Hamiltonian (1) using the basis functions (2) with different \( \omega \) values, we obtained the energy levels \( E(\omega) \) which leads to a stabilization plot from which resonance position can be identified. The scaling parameter \( \omega \) in the wave function (Eq. (2)) can be considered as the reciprocal range of a ‘soft’ wall [15]. Detail discussions can be available in the recent work of Kar and Ho [15]. Varying the Debye length \( D \) from infinity to small values, different resonance parameters (energy and width) have been obtained.

To extract the resonance energy \( E_r \) and the resonance width \( \Gamma \), we have calculated the density of resonance...
states for a single energy level with the help of the following formula,

\[
\rho_n(E) = \left| \frac{E_n(\omega_{i+1}) - E_n(\omega_{i-1})}{\omega_{i+1} - \omega_{i-1}} \right|^{-1},
\]

where the index \( i \) is the \( i \)th value for \( \omega \) and the index \( n \) is for the \( n \)th resonance. After calculating the density of resonance states \( \rho_n(E) \) with the above formula (4), we fit it to the following Lorentzian form that yields resonance energy \( E_r \) and a total width \( \Gamma \), with

\[
\rho_n(E) = y_0 + \frac{A}{\pi} \frac{\frac{E}{2}}{(E - E_r)^2 + \left( \frac{\Gamma}{2} \right)^2},
\]

where \( y_0 \) is the baseline offset, \( A \) is the total area under the curve from the base line, \( E_r \) is the center of the peak and \( \Gamma \) denotes the full width of the peak of the curve at half height.

To construct the stabilization plot, we have used an expansion length of \( N = 500 \) in the basis function (2). The stabilization diagram (in Fig. 1a) corresponding to the Debye length \( D = 10 \) (a.u.) in the range of \( \omega = 0.4-1.0 \) shows the stabilization character near \( E = -0.51 \) (a.u.). We use 301 points to cover the range of \( \omega \) from 0.4 to 1.0 in the mesh size of 0.002. We have calculated the density of resonance states for the individual energy levels in the range \( \omega = 0.4-1.0 \), with one energy level at a time. The calculated density of resonance states from the single energy eigenvalue is then fitted to Eq. (5), and the one that gives the best fit (with the least \( \chi^2 \)) to the Lorentzian form is considered as the desired results for that particular resonance. Fig. 1b shows the fitting of the density of the resonance states for the 25th eigenvalue of the stabilization plot. From the fit, we obtain the resonance energy \( E_r = -0.52179 \) a.u. and the corresponding width as \( \Gamma = 0.004159 \) a.u. The circles are the results of the actual calculations of the density of resonance states using formula (4), and the solid line is the fitted Lorentzian form of the corresponding \( \rho_n(E) \).

Table 1 shows the convergence of the resonance energies and the widths for \( N = 300, 400 \) and 500 basis terms corresponding to \( D = 3, 20 \) and infinity, respectively. For \( N = 300 \) and 400 terms we have used the same parameters as those for the 500-term basis functions. It is interesting to mention here that we have reproduced from our calculations the results for the eigenenergy of the ground state of He as reported by Thakkar and Smith [16] considering \( D \) tends to infinity which corresponding to no screening, and \( \omega = 1 \). In the present work, we are interested to calculate resonances for He in the framework Debye plasmas and so we have first obtained accurate ground state energy of He. Our value of \(-2.903724373 \) a.u. reported in Table 2 is fairly comparable to the best results of \(-2.903724377 \) a.u. available in the literature [18,20]. The ground state energies of He for 300 and 400-term basis functions are \(-2.903724357 \) a.u. and \(-2.903724368 \) a.u., respectively, using the same set of parameters. All other ground state energies obtained from our calculations for various De-

![Fig. 1](image-url)
The resonance energy ($E_r$) and width ($\Gamma$) of the helium atom for various Debye parameters along with the ground state energy ($E_{1s}$) and the non-linear variational parameters

<table>
<thead>
<tr>
<th>$D$</th>
<th>Non-linear parameters</th>
<th>$-E_{1s}$</th>
<th>$-E_r$</th>
<th>$\Gamma$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\infty$</td>
<td>$b = 2.21$, $c = 0.22$, $\lambda_3 = 1.30$</td>
<td>2.903724373</td>
<td>0.77783</td>
<td>0.004549</td>
</tr>
<tr>
<td>100</td>
<td>$b = 2.21$, $c = 0.20$, $\lambda_3 = 1.30$</td>
<td>2.873838790</td>
<td>0.74819</td>
<td>0.004545</td>
</tr>
<tr>
<td>70</td>
<td>$b = 2.21$, $c = 0.18$, $\lambda_3 = 1.30$</td>
<td>2.86100412</td>
<td>0.73572</td>
<td>0.004540</td>
</tr>
<tr>
<td>50</td>
<td>$b = 2.21$, $c = 0.17$, $\lambda_3 = 1.30$</td>
<td>2.844180571</td>
<td>0.71929</td>
<td>0.004533</td>
</tr>
<tr>
<td>40</td>
<td>$b = 2.21$, $c = 0.16$, $\lambda_3 = 1.30$</td>
<td>2.829436045</td>
<td>0.70513</td>
<td>0.004531</td>
</tr>
<tr>
<td>30</td>
<td>$b = 2.21$, $c = 0.15$, $\lambda_3 = 1.30$</td>
<td>2.810486231</td>
<td>0.68188</td>
<td>0.004496</td>
</tr>
<tr>
<td>20</td>
<td>$b = 2.18$, $c = 0.10$, $\lambda_3 = 1.30$</td>
<td>2.756548806</td>
<td>0.63683</td>
<td>0.004450</td>
</tr>
<tr>
<td>7</td>
<td>$b = 2.15$, $c = 0.092$, $\lambda_3 = 1.30$</td>
<td>2.614852941</td>
<td>0.51279</td>
<td>0.004159</td>
</tr>
<tr>
<td>5</td>
<td>$b = 2.09$, $c = 0.06$, $\lambda_3 = 1.30$</td>
<td>2.347001674</td>
<td>0.31105</td>
<td>0.003191</td>
</tr>
<tr>
<td>4</td>
<td>$b = 2.09$, $c = 0.06$, $\lambda_3 = 1.28$</td>
<td>2.220468659</td>
<td>0.23151</td>
<td>0.002591</td>
</tr>
<tr>
<td>3</td>
<td>$b = 2.08$, $c = 0.05$, $\lambda_3 = 1.26$</td>
<td>2.109936908</td>
<td>0.12792</td>
<td>0.001569</td>
</tr>
</tbody>
</table>

Here $a = 2.82$, $\lambda_1 = 0.098$, $\lambda_2 = 0.14$. Results are in atomic units.

Table 2

Bye parameters are presented in Table 2 and these results are nicely comparable with the results of Zhang and Winkler [2], Saha et al. [5] and Lam and Varshni [8]. Our calculated ground state eigenenergy values reported in Table 2 for $D = 3, \ldots, 100$ are lower than those published in the literature. All the results presented in Table 2 are for the $N = 500$ basis function of Eq. (2). It seems from Table 1 that the convergence of the resonance energies and the widths are quite good.

Table 2 also presented the resonance energies and the widths for various Debye lengths ranging from infinity (corresponding to no screening) to a small value 3 (corresponding to strong screening) along with the non-linear parameters used in our calculations. The results for the $2s^2 \ 1S^0$ resonant state of He are comparable with the reported results of Ho [21]. During the study on the complex coordinate calculations for the doubly excited states of two-electron atoms, he has reported the resonance energy $E_r = -1.55574$ Ry (0.77787 a.u.) and the corresponding width as $\Gamma = 0.00908$ Ry (0.00454 a.u.), which are nicely comparable to our results $E_r = -0.77783$ a.u. and the corresponding width as $\Gamma = 0.004549$ a.u. Our resonance energy, converted to electronvolt and measured from the ground state of the helium atom, is 57.85 eV and the width is determined as 0.124 eV. Our values compare quite well with the measured results of $E_r = 57.82 \pm 0.04$ eV and $\Gamma = 0.138 \pm 0.015$ eV in an electron impact experiment [22].

When the density of the resonance states $q_n(E)$ is fitted to the Lorentzian form, it has been observed that the value of $\chi^2$ for each fitting is much less than 0.1. All the results shown in Figs. 1–3 and Table 2 are obtained using the 500-term wave functions. Our calculated resonance energies associated with the $N = 2$ He threshold are shown in Figs. 2 and 3a along with the $\text{He}^+(2S)$ threshold energies for different values of $D$ and $1/D$, respectively, with the corresponding widths are plotted in the Figs. 2 and 3b. The values of the $\text{He}^+(2S)$ energies are taken from the reported results of Rogers et al. [10].

Fig. 2. (a) The $2s^2 \ 1S^0$ resonance energy $E_r$ for different values of the Debye parameter $D$. Dashed line denotes the $\text{He}^+(2S)$ threshold energy. (b) Resonance width $\Gamma$ corresponding to the resonance energy in (a) for different values of the Debye parameter $D$. 


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From Fig. 2 band Table 2, it is seen that the resonance width $\Gamma$ decreases with decreasing value of $D$. The situation can be explained in the following way: The $2s^2 1S^e$ state in He is a $+^2S^e$ state, and the two electrons are located on the opposite sides of the nucleus. The movements of the two electrons are moving toward the nucleus ‘in phase’. The autoionization of such a state is through momentum transfer, as one of the electrons is ‘knocked out’ by the other via the nucleus. Apparently, when the electron-ion screening is increased (decreasing $D$, increasing $1/D$), the movement of the electrons will be slowed down. As a result, the lifetime of the autoionization process will be prolonged, leading to the narrowing of the resonance width, a consequence of the uncertainty principle.

It should be mentioned here that we have not found any resonance for $D = 1, 2$ and 2.5. For $D = 1, 2$ and 2.5, the resonance, if exist, would be located very near the He$^+$ (2S) threshold. However, such calculations would need more extensive basis sets. In our future calculations we shall search for such resonances.

4. Conclusions

This work presents a first calculation on the $2s^2 1S^e$ autoionization resonance for helium embedded in Debye plasma environments. The resonance energies and widths for various Debye parameters ranging from infinity to small values (up to 3) have been reported along with the accurate ground state energies. The stabilization method is used to extract resonance energies and widths. This method is a practical method to calculate resonance parameters ($E_r$, $\Gamma$). Our present work will provide useful information to the plasma physics research community.

Acknowledgement

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References


Fig. 3. (a) The $2s^2 1S^e$ resonance energy $E_r$ as a function of $1/D$. Dashed line denotes the He$^+$ (2S) threshold energy. (b) Resonance width $\Gamma$ corresponding to the resonance energy in (a) as a function of $1/D$. 