Doubly-excited 1,3De resonance states of two-electron positive ions Li+ and Be2+ in Debye plasmas

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Doubly-excited $^{1,3}D^6$ resonance states of two-electron positive ions Li$^+$ and Be$^{2+}$ in Debye plasmas

Sabyasachi Kar,1,a) Yang Wang,1 Zishi Jiang,2 Shuxia Li,2 and K. Ratnavelu3

1Center for Theoretical Atomic and Molecular Physics, The Academy of Fundamental and Interdisciplinary Sciences, Harbin Institute of Technology, Harbin 150080, People’s Republic of China
2College of Physical Science and Technology, Heilongjiang University, Harbin 150080, People’s Republic of China
3Institute of Mathematical Sciences, University of Malaya, Kuala Lumpur, Malaysia

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We investigate the bound $^{1,3}D$ states and the doubly-excited $^{1,3}D^6$ resonance states of two-electron positive ions Li$^+$ and Be$^{2+}$ by employing correlated exponential wave functions. In the framework of the stabilization method, we are able to extract three series ($2pnp$, $2snd$, $2pnf$) of $^{1}D^6$ resonances and two series ($2pnp$, $2snd$) of $^{3}D^6$ resonances below the $N = 2$ threshold. The $^{1,3}D^6$ resonance parameters (resonance energies and widths) for Li$^+$ and Be$^{2+}$ along with the bound-excited $1s^3d$ $^{1,3}D$ state energies are reported for the first time as functions of the screening parameter. Accurate resonance energies and widths are also reported for Li$^+$ and Be$^{2+}$ in vacuum. For free-atomic cases, comparisons are made with the reported results and few resonance states are reported for the first time. © 2014 AIP Publishing LLC. [http://dx.doi.org/10.1063/1.4862036]

I. INTRODUCTION

The study of atomic resonances in plasma environment has gained tremendous attention in the recent years and is one of the interesting topics of current research. Recently, resonance states of the helium atom and the hydrogen negative ion in Debye plasmas have been studied in the framework of the stabilization method and the complex-coordinate rotation method using the Hylleraas-type wave functions. Investigations on resonance states of helium in Debye plasmas have also been reported by Ordóñez-Lasso et al., using the configuration interaction method based on the explicitly correlated configurations. There have been a number of studies using the stabilization method to probe the existence of low-lying resonances in the s-wave channel of screened Coulomb potentials and pointed out likely importance of such phenomena for resonant radiative recombination processes in sufficiently dense plasmas. Applications of atomic processes in plasma environments can be found in detail from earlier articles. Recently, Chang et al. reported an interesting study related to photoionization of atoms in Debye plasmas.

In the present work, we have calculated the bound $^{1,3}D$ states and the doubly-excited $^{1,3}D^6$ resonance states of two-electron positive ions Li$^+$ and Be$^{2+}$ below the $N = 2$ thresholds of the respective subsystems. In the free-atomic cases, $^{1,3}D^6$ resonance states of Li$^+$ and Be$^+$ ion have been reported by Bhatia and Ho. In this work, we have employed the stabilization method to extract resonance parameters. Highly correlated exponential wave functions are used to describe the two-electron positive ions Li$^+$ and Be$^{2+}$. The convergence of the calculations has been examined with increasing number of terms in the basis functions. Atomic units (a.u.) are used throughout this work.

II. HAMILTONIAN AND WAVE FUNCTIONS

The non-relativistic screened Hamiltonian $H$ for the proposed systems can be written as

$$H = -\frac{1}{2} \left( \nabla_1^2 + \nabla_2^2 \right) - Z[V(r_1) + V(r_2)] + V(r_{12}), \quad (1)$$

$$V(r) = \frac{1}{r} \exp(-\mu r), \quad (2)$$

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 $\mu$ corresponds to the range of plasma conditions, as the Debye parameter is a function of electron density and electron temperature. $\mu = 0$ indicates the unscreened case. For the two-component plasma near thermodynamic equilibrium, the Debye screening length $\mu$ takes the form

$$\mu = \sqrt{\frac{4\pi(1 + Z^*)n}{k_B T}}, \quad (3)$$

where $k_B$ is the Boltzmann constant, $n$ and $T$ are the number density of the plasma electrons and temperature, respectively, and $Z^*$ is the effective charge of the ions in the embedded plasma.

For $^{1,3}D^6$ states, we employ highly correlated wave functions

[1]Author to whom correspondence should be addressed. Electronic addresses: skar@hit.edu.cn and karsabyasachi@yahoo.com

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In the present study, we compute the energy levels prescribed in the previous articles on the stabilization method. According to computational procedure described in the previous articles, we select the optimized values of the scaling factor, \( N_b \), the number of basis terms, and the non-linear vibrational parameters \( \alpha_i, \beta_i, \) and \( \gamma_i \) determined using a quasi-random process.

### III. RESULTS

We have mentioned earlier that we intend, in this work, to calculate the doubly-excited \( ^1\text{D}^\pi \) resonance states of two-electron positive ion Li\(^{2+}\) and Be\(^{2+}\) by employing the stabilization method. According to computational procedure prescribed in the previous articles on the stabilization method, in the present study, we compute the energy levels \( E(\omega, \mu) \) of the proposed systems by diagonalizing the atomic Hamiltonian (1) using the exponential correlated wave functions (4) in which exponent is generated by a quasi-random process. We have selected the optimized values of the

#### TABLE I

<table>
<thead>
<tr>
<th>( 1/\mu )</th>
<th>( \text{Li}^{+}(1s3d\ 1^3\text{D}) )</th>
<th>( \text{Li}^{+}(1s3d\ 1^3\text{S}) )</th>
<th>( \text{Be}^{2+}(1s^3\ 1^3\text{S}) )</th>
</tr>
</thead>
<tbody>
<tr>
<td>( \infty )</td>
<td>(-4.72239098976)</td>
<td>(-4.72252691378)</td>
<td></td>
</tr>
<tr>
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<td>(-4.72252691377^a)</td>
<td>(-4.50000000000)</td>
<td></td>
</tr>
<tr>
<td>(-4.7223909884^a)</td>
<td>(-4.7225269124^a)</td>
<td></td>
<td></td>
</tr>
<tr>
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</tr>
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<td>(-4.48639985130)</td>
<td>(-4.315846295)</td>
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<tr>
<td>10</td>
<td>(-4.4750495922)</td>
<td>(-4.4751427890)</td>
<td>(-4.2073405204)</td>
</tr>
</tbody>
</table>

\(^a\)Using 800-term wave functions.  
\(^b\)Reference 46.

\[
\psi = \sum_{i_j} \sum_{l_i=0}^2 \sum_{l_2=2}^2 A_i [Y_{LM}^{l,l_1}(r_1, r_2)] \chi(r_1, \alpha, \omega) \chi(r_2, \beta_1, \gamma_1, \omega) \\
+ S_{pn} Y_{LM}^{l,l_1}(r_1, r_2) \chi(r_1, \beta_1, \omega) \chi(r_2, \alpha, \omega) \chi(r_2, \gamma_1, \omega), \tag{4}
\]

and the bipolar harmonics \( Y_{LM}^{l,l_1}(r_1, r_2) \) can be written as

\[
Y_{LM}^{l,l_1}(r_1, r_2) = i_1 i_2 \sum_{m_1, m_2} \langle l_1 l_2 m_2 | LM > Y_{l,m_1}(\tilde{r}_1) Y_{l,m_2}(\tilde{r}_2), \tag{6}
\]

where \( Y_{l,m}(\tilde{r}) \) denotes the usual spherical harmonics, \( S_{pn} = +1 \) for singlet states, \( S_{pn} = -1 \) for triplet states, \( \omega \) is a scaling factor, \( N_b \) is the number of basis terms, and the non-linear vibrational parameters \( \alpha_i, \beta_i, \) and \( \gamma_i \) are determined using a quasi-random process.

#### FIG. 1

(a) The Stabilization diagram for the \( 2p^2\ 1^3\text{D}^\pi \) state of Li\(^+\) for \( \mu = 0.1 \). (b) The best fittings (solid line) of the density of states (circles) corresponding to the \( 2p^2\ 1^3\text{D}^\pi \) state of Li\(^+\) for \( \mu = 0.1 \).
non-linear variational parameters by observing optimum values of the bound states energies of the atomic systems under consideration. The bound $^1S^3D$ state energies of Li$^+$ and Be$^{2+}$ are presented in Table I, along with the threshold values of the respective subsystems. In the unscreened cases, the bound state energies obtained from this work are comparable with reported results and the comparisons are also made in Table I. To calculate threshold values for Li$^{2+}$ and Be$^{3+}$, we have employed the Slater-type basis functions of the form

$$\varphi_{nlm} = r^{n+\frac{1}{2}} e^{-\alpha r} Y_{n}^{\pm}(\theta,\phi), \quad n = 1, 2; l = 0, 1, 2, \ldots$$

We have used 900-term wave functions to calculate bound $1s3d$ $^1S^3D$ states energies of Li$^+$ and Be$^{2+}$ and 15-term wave functions for Li$^{2+}$($1s^2S$) and Be$^{3+}$($1s^2S$). We then construct the stabilization diagrams for Li$^+$ and Be$^{2+}$ by plotting $E(\omega, \mu)$ versus $\omega$ for each $\mu$. From stabilization plots, one can identify the resonance position by observing the stabilization plateau. A stabilization diagram for the $2p^2^1D^\pi$ state is depicted in Figure 1(a) for Li$^+$ for $\mu = 0.1$ ($1/\alpha_0$). Then to extract resonance energy and width ($E_r, \Gamma$) for a particular resonance state, we calculated the density of the resonance states for each single energy level in the stabilization plateau using the formula

$$\rho_n(E) = \left| \frac{E_n(x_j) - E_n(x_{j-1})}{x_j - x_{j-1}} \right|^{-1},$$

where the index $j$ is the $j$-th value for $x$ and the index $n$ is for the $n$-th resonance. After calculating the density of resonance states $\rho_n(E)$ using formula (8), we fit it to the following Lorentzian form that yields resonance energy $E_r$ and a total width $\Gamma$, with:

$$\rho_n(E) = y_0 + \frac{A}{\pi} \frac{\Gamma/2}{(E - E_r)^2 + (\Gamma/2)^2},$$

where $y_0$ is the baseline offset, $A$ is the total area under the curve from the baseline, $E_r$ is the centre of the peak, and $\Gamma$ denotes the full width of the peak of the curve at half height.

We obtained the desired results for a particular resonance state by observing the best fit (with the least chi-square and with the best value of the square of the correlation coefficient) to the Lorentzian form.

Figure 1(b) shows the best fitting of the density of states for the $2p^2^1D^\pi$ state of Li$^+$ for $\mu = 0.1$ ($1/\alpha_0$). Resonance parameters ($E_r, \Gamma$) obtained from the present work for each Debye screening parameter are presented in Tables II–V and are depicted in Figs. 2–6 along with the $N = 2$ thresholds of the respective two-body subsystems. In the unscreened cases, our results are comparable with other calculation available in the literature. Comparisons are made in Table V. It is clear from Table V that few resonance parameters are reported for the first time in the literature. In the screening environments, our results are reported for the first time. It is evident from Figures 2–6 and Tables II–V that the resonance energy increases with increasing $\mu$ and ultimately approaches the threshold. Resonance width as a function of $\mu$ exhibits decreasing behavior. Final results presented in the

<table>
<thead>
<tr>
<th>$^1D^\pi$ resonance states of Li$^+$ for different screening parameter, along with the $L^2(2s^22S)$ threshold energies.</th>
</tr>
</thead>
<tbody>
<tr>
<td>$^1D^\pi$ resonance states of Li$^+$ for different screening parameter, along with the $L^2(2s^22S)$ threshold energies.</td>
</tr>
</tbody>
</table>
TABLE III. The $^1D^e$ resonance states of Be$^{2+}$ for different values of the screening parameter, along with the Be$^{3+}$ (2s$^2$S) threshold energies.

<table>
<thead>
<tr>
<th>$1/\mu$</th>
<th>$E_r$ ($\times 10^{-5}$)</th>
<th>$\Gamma_r$ ($\times 10^{-5}$)</th>
<th>$E_r$ ($\times 10^{-5}$)</th>
<th>$\Gamma_r$ ($\times 10^{-5}$)</th>
<th>$E_r$ ($\times 10^{-5}$)</th>
<th>$\Gamma_r$ ($\times 10^{-5}$)</th>
<th>$E_r$ ($\times 10^{-5}$)</th>
<th>$\Gamma_r$ ($\times 10^{-5}$)</th>
<th>$Li^2+, (2s^2S)$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$\infty$</td>
<td>$-1.77058$</td>
<td>$3.8761$</td>
<td>$-1.37411$</td>
<td>$1.1034$</td>
<td>$-1.34617$</td>
<td>$1.611$</td>
<td>$-1.26170$</td>
<td>$4.670$</td>
<td>$-1.24941$</td>
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<td>$50$</td>
<td>$-1.67229$</td>
<td>$3.867$</td>
<td>$-1.27711$</td>
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<td>$-1.24937$</td>
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<td>$-1.16647$</td>
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<td>$-1.15454$</td>
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<td>$20$</td>
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<td>$3.82$</td>
<td>$-1.14221$</td>
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<td>$-1.11538$</td>
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<td>$0.947$</td>
<td>$-0.91907$</td>
<td>$0.773$</td>
<td>$-0.86425$</td>
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<td>$6$</td>
<td>$-1.04729$</td>
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<td>$-0.694888358$</td>
<td>$0.16$</td>
<td>$-0.6302120452$</td>
</tr>
<tr>
<td>$5$</td>
<td>$-0.92675$</td>
<td>$3.13$</td>
<td>$-0.62999$</td>
<td>$0.639$</td>
<td>$-0.62999$</td>
<td>$0.639$</td>
<td>$-0.694888358$</td>
<td>$0.16$</td>
<td>$-0.6302120452$</td>
</tr>
<tr>
<td>$4$</td>
<td>$-0.75978$</td>
<td>$2.77$</td>
<td>$-0.53923$</td>
<td>$0.591$</td>
<td>$-0.53923$</td>
<td>$0.591$</td>
<td>$-0.694888358$</td>
<td>$0.16$</td>
<td>$-0.6302120452$</td>
</tr>
<tr>
<td>$3$</td>
<td>$-0.51680$</td>
<td>$2.18$</td>
<td>$-0.39739$</td>
<td>$0.399$</td>
<td>$-0.39739$</td>
<td>$0.399$</td>
<td>$-0.694888358$</td>
<td>$0.16$</td>
<td>$-0.6302120452$</td>
</tr>
</tbody>
</table>

TABLE IV. The $^1D^e$ resonance states of Li$^+$ and Be$^{2+}$ for different values of the screening parameter, along with the Li$^{2+}$ (2s$^2$S) and Be$^{3+}$ (2s$^2$S) threshold energies.

<table>
<thead>
<tr>
<th>States</th>
<th>$Li^+$</th>
<th>Be$^{2+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2p3p, ^1D^e$</td>
<td>$E_r$ ($\times 10^{-5}$)</td>
<td>$\Gamma_r$ ($\times 10^{-5}$)</td>
</tr>
<tr>
<td>$2s3d, ^1D^e$</td>
<td>$E_r$ ($\times 10^{-5}$)</td>
<td>$\Gamma_r$ ($\times 10^{-5}$)</td>
</tr>
<tr>
<td>$2p4p, ^1D^e$</td>
<td>$E_r$ ($\times 10^{-5}$)</td>
<td>$\Gamma_r$ ($\times 10^{-5}$)</td>
</tr>
<tr>
<td>$2s4d, ^1D^e$</td>
<td>$E_r$ ($\times 10^{-5}$)</td>
<td>$\Gamma_r$ ($\times 10^{-5}$)</td>
</tr>
</tbody>
</table>

Li$^+$ threshold energy: $-1.1250000000$
Be$^{2+}$ threshold energy: $-0.6302120452$

TABLE V. Comparison of $^1D^e$ resonance parameters for Li$^+$ and Be$^{2+}$ for the unscreened case. The numbers in the square brackets denote the power of ten.

<table>
<thead>
<tr>
<th>States</th>
<th>Li$^+$</th>
<th>Be$^{2+}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>$2p^2, ^1D^e$</td>
<td>$E_r$</td>
<td>$\Gamma$</td>
</tr>
<tr>
<td>$2p3p, ^1D^e$</td>
<td>$E_r$</td>
<td>$\Gamma$</td>
</tr>
<tr>
<td>$2s3d, ^1D^e$</td>
<td>$E_r$</td>
<td>$\Gamma$</td>
</tr>
<tr>
<td>$2p4p, ^1D^e$</td>
<td>$E_r$</td>
<td>$\Gamma$</td>
</tr>
<tr>
<td>$2s4d, ^1D^e$</td>
<td>$E_r$</td>
<td>$\Gamma$</td>
</tr>
</tbody>
</table>

Li$^+$: $E_r$ | $\Gamma$
Be$^{2+}$: $E_r$ | $\Gamma$
Tables for $^{13}$D resonance states are obtained using 500-term wave functions. It is important to mention here that we are unable to extract resonance widths for the $2p4f^1D^e$ and $2p4p^3D^e$ states of Li$^+$, and the $2p5p^1D^e$ and $2s5d^1D^e$, $2pnp$ ($n = 4, 5$) $^3D^e$ and $2p4p^1D^e$ states of Be$^{3+}$ using 500-term wave functions. Behavior of the bound $1s3d^1,^3D$ state energies of Li$^+$ and Be$^{3+}$ as functions of the screening parameters $\mu$ are depicted in Fig. 7, along with the $1s^2S$ thresholds of the respective subsystems. According to the method and wave functions employed, it appears that the results obtained from the present calculations are reasonably accurate.

FIG. 2. The $^1D^e$ [in (a) and (b)] resonance energy of two-electron positive ions Li$^+$ and Be$^{3+}$ as a function of the Debye screening parameter $\mu$.

FIG. 3. The $^3D^e$ [in (a) and (b)] resonance energy of Li$^+$ and Be$^{3+}$ as a function of $\mu$.

FIG. 4. The $2pnp^1D^e$ [in (a)] and $2snp^1D^e$ [in (b)] resonance widths of two-electron positive ions Li$^+$ and Be$^{3+}$ below the $N = 2$ thresholds of the respective subsystems as a function of the Debye screening parameter $\mu$.

FIG. 5. The $2p4f^1D^e$ resonance width of Be$^{3+}$ below the $N = 2$ threshold of Be$^{3+}$ as a function of the Debye screening parameter $\mu$. 

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functions of the Debye screening parameter. We have used the stabilization method to extract resonance states of two-electron positive ions (Z = 2) as functions of the Debye parameter along with the hydrogenic threshold energies of the respective subsystems.

IV. CONCLUSIONS

In this paper, we have presented the doubly-excited 1,3D* resonance states of two-electron positive ions (Z = 3-4) in Debye plasmas using highly correlated exponential wave functions. We have used the stabilization method to extract resonance position and width for the 1,3D* states of Li* and Be2+. The bound 1s3d 1,3D* states energies are also presented as functions of the screened parameter. For the unscreened case, resonance parameters for 2pop (n = 4, 5) 1,3D*, 2sod (n = 4, 5) 1,3D*, and 2p4f 1,3D* states are reported for the first time in the literature. For the screened case, our results are also reported for the first time. We hope our findings will provide useful information for future studies on this topic.

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