Relativistic spectroscopy of plasma-embedded Li-like systems with screening effects in two-body Debye potentials

Madhulita Das\textsuperscript{1}, B K Sahoo\textsuperscript{2} and Sourav Pal\textsuperscript{1}

\textsuperscript{1}National Chemical Laboratory, Pune 411008, India
\textsuperscript{2}Theoretical Physics Division, Physical Research Laboratory, Navrangpura, Ahmedabad 380009, India

E-mail: bijaya@prl.res.in

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Abstract

The spectroscopic properties of Li atoms and Li-like Ca and Ti ions in the plasma environment are investigated using a relativistic coupled-cluster (RCC) method. Assuming that the plasma is of low density and very hot, we consider the Debye model with two approximations to account for the screening effects: (i) in the nuclear potential alone and (ii) in both the nuclear and the electron–electron interaction potentials. Also, calculations for the energies and the lifetimes of the atomic states are carried out for plasma-free systems to check their accuracy, after which they are investigated in the plasma environment. It is observed that screenings in the electron–electron interaction potentials stabilize the systems more than when the screenings are present only in the nuclear potential. Similarly, the blue and red shifts in the $n_0\Delta n_0=0$ and $n_0\Delta n_0 \neq 0$ transition lines (with the principal quantum number $n$) of the Li-like ions observed in the (i) approximation are altered in the (ii) approximation. The level crossings among the energy levels are observed for large screening effects and are found to be prominent in the states of higher orbital angular momentum. The lifetimes of many low-lying states of the allowed transitions are estimated by considering different plasma screening strengths.

Keywords: Debye model, atomic Spectroscopy, relativistic method

1. Introduction

The knowledge of spectral properties of atomic systems immersed in the plasma environment is an important tool for plasma diagnostic processes and also has a wide range of applications in many research fields such as astrophysics, inertial confinement fusion (ICF), magnetic confinement fusion, laser–matter interaction, and x-ray lasers [1–5]. Usually, the spectral properties of plasma-embedded atomic systems change considerably in comparison with those of isolated systems due to the presence of other charged particles in the plasma confinement [6–8]. The radiations coming out from plasma-embedded atomic systems, through various excitations or ionization processes, play crucial roles in providing insights into physical phenomena happening inside the plasma [9, 10]. It has been found from laser-plasma experiments that the red shifts of the atomic emission lines are on the order of 3.7 eV [11, 12]. A detailed understanding of such findings requires proper characterization of the atomic spectral lines emitted from the systems. Therefore, theoretical investigation of atomic spectroscopy in hot plasma, where the atomic system is almost fully ionized, and dense plasma, in which the electron density is very high (greater than $10^{19}$ per cc), has become an exciting field of research. We, however, focus here only on the low-electron-density and high-temperature plasma where the electrons and the ions of the system are in the thermal equilibrium state.

The plasma environment mostly consists of ions and free electrons, which introduce screening effects into the Coulomb potentials of the embedded atomic systems. Thus, the atomic electrons are highly influenced by the external electromagnetic fields, compelling the atomic long-range electrostatic potentials to act as short-range screened potentials. For the theoretical study of the spectroscopy of a plasma-embedded atomic system, the screening effects due to the plasma can be conveniently accounted for, in such a scenario,
by defining suitable model potentials in the atomic Hamiltonian for the corresponding strength of the plasma. The strength of the plasma is defined by a coupling parameter \( \Gamma \) that measures the interactions among the particles inside the plasma environment. The Debye model \[13\] is the most conventional approach used for studying atomic spectroscopy in low-electron-density and high-temperature plasma (weakly coupled plasma, i.e., \( \Gamma < 1 \)).

The phenomenon of reduction of ionization potential (IP) of an atom or an ion in the plasma environment is known as ionization potential depression (IPD) \[14\text{–}17\]. Accurate determination of this quantity can provide much useful information, such as the equation of state of plasma, radiative opacity of stellar plasma, and inertial confinement fusion plasma. Recent, experimental studies by Hoarty et al \[18\] and Ciricosta et al \[19\] reveal the influence of the hot and dense plasma environment in atomic properties, and IPDs in the Al atom are reported. Thus, atomic structure probes in plasma have drawn experimentalists and theoreticians alike to make further attempts at yielding more accurate spectroscopic data. Many calculations with respect to H-like and He-like ions in the dense plasma environment have been performed \[6, 20\text{–}22\] for their simpler structures, but only a handful of theoretical investigations are available for Li-like systems \[7\]. Nonetheless, many emission spectra have been observed in both astrophysical and laboratory plasma corresponding to high nuclear charge \[23\text{–}33\]. For reliable identification of these spectral lines and to better understand the underlying physics of their origin, it is necessary to employ more accurate methods that can include both the relativistic and electron correlation effects appropriately in the theoretical analysis of atomic spectral properties.

The primary thrust of this work is to study theoretically the effects of plasma screenings in the spectroscopy of highly ionized Ca XVIII and Ti XX ions (Li-like) and compare them against the neutral Li atom. These ions are commonly used in laser-plasma experiments \[34, 35\] and are of particular interest for astrophysical-plasma studies \[36\]. Before evaluating the atomic properties in the plasma environment, we determine the IPs and the lifetimes of the atomic states in the plasma-free case to compare them with the available experimental values for the purpose of validating our calculations. Next we introduce the screening effects into the nuclear potential using the Debye model and then add them into the electron–electron interaction potential to find out how the results differ in these two approximations. To highlight the changes that transpire from one approximation to the other due only to Coulomb interactions, we do not take into account contributions from other relativistic corrections such as Breit interaction and QED effects. A relativistic coupled-cluster (RCC) many-body theory in the Fock-space representation has been employed for the calculations. We also give predicted values for the ratios of the line intensities among the atomic transitions.

The paper is organized as follows: In section 2, we introduce the screening models that are considered in the calculations of the atomic spectral properties and describe the employed RCC method briefly in section 3. We give the obtained results in section 4 along with their comparison with the other available results and discuss them before summarizing the work in section 5. Throughout the paper, the units given for IP, excitation energies (EE), and fine structure (FS) splittings are in cm\(^{-1}\), line strength (S) and the Debye screening length (D) are in atomic units (a.u.); transition rates (A) are in sec\(^{-1}\); and lifetimes (\( \tau \)) of the atomic states are in sec.

## 2. Debye model potentials

The atoms or ions embedded in a plasma are largely perturbed by the electromagnetic fields produced by the neighboring ions and the freely moving electrons of the plasma. The effectiveness of the interactions is usually approximated by considering appropriate models that can explain the systems with reasonable accuracy for all practical purposes. In a hot and low-density plasma, the atomic systems get screened due to the penetration of the slowly moving free electrons of the plasma into the systems. This will also affect the net relativistic effects observed for the electrons; hence, investigating such corrections from the Breit interaction and lower-order QED effects are also important. We do not investigate the roles of these interactions, however, because they are not relevant to the objective of this work. Using the Poisson-Boltzmann equation, the effective potential under these conditions can be approximated well in the Debye model for a point nuclear system as

\[
V_{\text{eff}}(r_i) = \frac{Z}{r_i} e^{-r_i/D} + \sum_{j \neq i} \frac{1}{r_{ij}} e^{-r_{ij}/D} = V_{\text{nuc}}(r_i) + \sum_{j \neq i} V_{\text{ee}}(r_{ij}),
\]

where \( D = \left[ \frac{k_B T_e}{4\pi (1 + Z)n_e} \right]^{1/2} \)

is the Debye screening length, \( Z \) is the nuclear charge, \( n_e \) is the number of electrons, \( k_B \) is the Boltzmann constant, \( T_e \) is the plasma temperature, and \( n_e \) represents the electron number density, which is a constant but whose magnitude depends on \( T_e \) and the plasma density.

In equation (1), \( V_{\text{nuc}}(r) \) represents the screened electron–nucleus potential, whereas \( V_{\text{ee}}(r) \) is the screened electron–electron interaction potential. Due to the computational difficulties, a majority of the previous studies on the spectroscopy of Li-like systems have been carried out only by accounting screenings in \( V_{\text{nuc}}(r) \), where the electron–electron potential \( V_{\text{ee}}(r) \) is truncated at its first term of exponential expansion for its dominant contribution \[37\]. We refer to this approximation as ‘Model A’ in this work. It is also important to determine roles of screening effects in the electron–electron interactions for large plasma strengths, which are considered to be more realistic in terms of the search for the stability of atomic structures in the plasma medium.
Instead of considering the point nucleus in the evaluation of $V_{\text{nuc}}(r)$, we use the standard Fermi-charge distribution to take into account the finite size of the nucleus by using the expression [38]

$$V_{\text{nuc}}(r) = \frac{Ze^{-r/R}}{Nr} \left( \frac{1}{b} \left( \frac{3}{2} + \frac{a^2 \pi^2}{2b^2} - \frac{r^2}{2b^2} + \frac{3a^2}{b^2} P_3^z + \frac{6a^3}{b^3} (S_3 - P_3^z) \right) \right)$$

for $r \leq b$

$$\times \left( \frac{1}{r} \left( 1 + \frac{a^2 \pi^2}{b^2} - \frac{3a^2r^2}{b^3} + \frac{6a^3}{b^3} (S_3 - P_3^z) \right) \right)$$

for $r > b$

where the factors are

$$N = 1 + \frac{a^2 \pi^2}{b^2} + \frac{6a^3}{b^3} S_3$$

with $S_3 = \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l^2} e^{-b/a}$

and $P^z_3 = \sum_{l=1}^{\infty} \frac{(-1)^{l-1}}{l^2} e^{-2l(r-b)/a}$.

Here parameter $b$ is known as the half-charge radius, and $a$ is related to the skin thickness of the nucleus. These two parameters are evaluated by

$$a = 2.3/4(m \lambda)$$

and

$$b = \sqrt{\frac{5}{3} f_{\text{rms}}^2 - \frac{7}{3} a^2 \pi^2}$$

with the appropriate values of the root mean square radius, $r_{\text{rms}}$, of the nucleus.

To add the screening effects into the electron-electron interactions, we adopt the approximation that has been made in [39–43] as

$$V_{\text{eff}}(r_i) = V_{\text{nuc}}(r_i) + e^{-r_i/b} \sum_{j \neq i} N_e \frac{1}{r_{ij}}.$$  \hspace{1cm} (6)

This approximation is labeled ‘Model B’ in this work.

### 3. Method of calculations

We employ the one-valence electron attachment RCC method that we developed (e.g., see [44–46]) for carrying out calculations of the atomic wave functions in the considered systems; this method is briefly described here. The four-component Dirac–Hamiltonian (along with the effective potentials) that is used for the wave-function calculations of the plasma-embedded atomic systems is given by

$$H = \sum_{i=1}^{N_e} \left( \bar{c} \bar{a}_i \cdot \bar{p}_i + (\beta - 1) c^2 + V_{\text{eff}}(r_i) \right).$$  \hspace{1cm} (7)

where $N_e$ is the number of electrons in the atomic system, $\bar{a}_i$ and $\beta$ are the Dirac matrices, and $c$ is the velocity of light.

The ground states of the considered atomic systems have the $[1s^2]^1$ closed-shell configuration and $2s$ valence orbital. Also, many of the low-lying excited states in these systems have the same closed-shell configuration with an electron in one of the virtual orbitals instead of in the $2s$ orbital. To calculate these states, we express the atomic wave functions in our RCC method as

$$|\Psi_i\rangle = e^T \left( e^{S_i} |\Phi_i\rangle \right).$$  \hspace{1cm} (8)

where we define the reference state $|\Phi_i\rangle$ by appending the appropriate valence orbital $\nu$ of the corresponding state to the Dirac–Fock (DF) wave function of the $[1s^2]$ configuration (denoted by $|\Phi_i\rangle$). Here $T$ is the core excitation operator and $S_i$ is the normal-order excitation operator from core and valence to the virtual orbitals. Because the states have only one valence orbital in their configurations, the exponential form $\{e^{S_i}\}$ naturally reduces to $\{1 + S_i\}$, yielding the form

$$|\Psi_i\rangle = e^T \left( 1 + S_i \right) |\Phi_i\rangle.$$  \hspace{1cm} (9)

Considering the singles and doubles approximation in the RCC theory (CCSD method), the cluster operators $T$ and $S_i$ are defined by

$$T = T_1 + T_2$$

and

$$S_i = S_1 + S_2.$$  \hspace{1cm} (10)

The amplitudes of these excitation operators are obtained by solving the following equations:

$$\langle \Phi^K_0 | T \Phi \rangle = \delta_{K,0} \Delta E_{\text{corr}}$$  \hspace{1cm} (11)

and

$$\langle \Phi^K_0 | T (1 + S_i) \Phi \rangle = \langle \Phi^K_0 | \delta_{K,\nu + S_i} | \Phi \rangle \Delta E_{\text{corr}}.$$  \hspace{1cm} (12)

where the values of the superscripts $K = 1, 2$ represent the (singly and doubly) excited hole-particle states, and $T \Phi$ is the dressed part of the normal-order Hamiltonian $(H_\Phi)$. $\Delta E_{\text{corr}}$ and $\Delta E_{\text{coul}}$ are the correlation energy and attachment energy (also equivalent to the negative of the IP), respectively, of the valence electron $\nu$. The advantage of considering the CCSD method in the current calculations is that it takes care of both the pair-correlation and core-polarization effects for all orders and that a significant number of contributions from triple excitations are included through the non-linear terms [47].

The lifetime of a given state $f$ is defined by the reciprocal of the total transition rate of that state due to all possible transition channels, i.e.,

$$\tau_f = \frac{1}{\sum_{i,j} A_{f \rightarrow i}^O A_{f \rightarrow j}^O},$$  \hspace{1cm} (13)

for the transition rate $A_{f \rightarrow i}^O$ due to a radiative operator $O$. The transition rates via various multipole channels are given by

$$A_{f \rightarrow i}^{E1} = \frac{2.02613 \times 10^{18}}{\lambda^3(2f + 1)} S_{f \rightarrow i}^{E1}.$$  \hspace{1cm} (14)
Table 1. Comparison of our calculated ionization potentials (IPs), excitation energies (EEs), and fine-structure splittings (FS) in Li I, Ca XVIII, and Ti XX with the National Institute of Science and Technology (NIST) data [50] in cm⁻¹. The uncertainties in our calculations are estimated by comparing them with the NIST data and are given for the quantity x in percentages as \( \delta = \frac{|x_{\text{NIST}} - x_{\text{CCSD}}|}{x_{\text{NIST}}} \times 100 \). Because the FS fall within the uncertainties, their \( \delta \) values are not quoted.

|         | Li I         | Ca XVIII      | Ti XX       |
|---------|--------------|---------------|-------------|
|         | Current      | NIST          | Current     | NIST          | Current     | NIST          |
| IP      | 43482.67     | 43487.11      | 9340603.58  | 9337690      | 11499573.80 | 11495470     |
| EE      |              |               | 290372.20   | 290057       | 323898.05   | 323521       |
| FS      | 14909.23     | 14903.66      | 30923.81    | 30925.38     | 6577736.86  | 6574040      |
|         | 14909.19     | 14904         | 30923.81    | 30925.38     | 6577736.86  | 6574040      |
|         | 27202.15     | 27206.12      | 30923.81    | 30925.38     | 6577736.86  | 6574040      |
|         | 31277.94     | 31283.08      | 30923.81    | 30925.38     | 6577736.86  | 6574040      |
|         | 31277.95     | 31283.12      | 30923.81    | 30925.38     | 6577736.86  | 6574040      |
|         | 36466.32     | 36469.55      | 30923.81    | 30925.38     | 6577736.86  | 6574040      |
|         | 36466.31     | 36469.55      | 30923.81    | 30925.38     | 6577736.86  | 6574040      |

\[
A_{\xi \rightarrow i}^{M1} = \frac{2.69735 \times 10^{13}}{\lambda^3 (2J_f + 1)} S_{\xi \rightarrow i}^{M1}
\]

(15)

and

\[
A_{\xi \rightarrow i}^{E2} = \frac{1.11995 \times 10^{18}}{\lambda^5 (2J_f + 1)} S_{\xi \rightarrow i}^{E2}
\]

(16)

where \( \lambda \) is the wavelength (Å) and \( S_{\xi \rightarrow i}^{\text{EE}, \text{FS}} = |\langle \text{f} || \text{O} || \text{i} \rangle|^2 \) is the line strength due to the corresponding transition operator \( O \), and \( J_f \) is the total angular momentum of the \( f \) state. \( E1, M1, \) and \( E2 \) represent the electric dipole, magnetic dipole, and electric quadrupole transition channels respectively. Because the matrix elements calculated using the length gauge expressions converge faster than the velocity gauge expressions with respect to the configuration space of the orbital bases [48, 49], we considered the length gauge expressions for evaluating the foregoing transition properties.

We used Gaussian type of orbitals (GTOs) to construct the single particle orbitals. The large and small radial components of a Dirac orbital in this case are expressed by

\[
P_{\kappa} (r) = \sum_{\nu} c_{\kappa, \nu}^P r^{l_{\nu}} e^{-\zeta_{\nu} r^2}
\]

(17)

and

\[
Q_{\kappa} (r) = \sum_{\nu} c_{\kappa, \nu}^Q r^{l_{\nu}} \left( \frac{d}{dr} + \frac{\kappa}{r} \right) e^{-\zeta_{\nu} r^2},
\]

(18)

respectively, where the summation over \( \nu \) stands for the total number of GTOs used in each orbital angular momentum \( l_{\nu} \) symmetry with the relativistic quantum number \( \kappa \), \( c_{\nu}^P \) and \( c_{\nu}^Q \) are the normalization constants, and \( \zeta_{\nu} \) are the guessed parameters chosen appropriately for different symmetries. To optimize the exponents, we use the even tempering condition

\[
\zeta_{\nu} = \zeta_0 \eta^{\nu - 1}
\]

(19)

with two unknown parameters \( \zeta_0 \) and \( \eta \).

4. Results and discussion

We first study the spectroscopic properties of plasma-isolated atomic systems by considering \( D = \infty \) in equation (7). The rationale for carrying out these calculations is to verify the accuracy of our results by comparing them with the available experimental values. The obtained IPs and FS splittings of Li I, Ca XVIII, and Ti XX from the CCSD method are given in Table 1 along with the recommended values from the National Institute of Science and Technology (NIST) database [50]. The NIST data listed are from many high-precision measurements that are tabulated in [51]. We found good agreement between our results and the NIST data, and the differences between these results are given in percentages as \( \delta \), which can be treated as the estimated uncertainties of the calculations. Due to large magnetic effects in the highly charged Ca XVIII and Ti XX ions, the FS splittings are large in these systems compared with the Li atom. In Tables 2 to 4, we give the values of \( S \) and \( A \) along with their estimated uncertainties from the E1, M1, and E2 channels from the excited states to the low-lying states of Li I, Ca XVIII, and Ti XX, respectively. Using these values, we have calculated the lifetimes of the excited states, which are given in the same
Table 2. Line strengths ($S$), transition probabilities ($A$), and lifetimes ($\tau$ in ns) of the excited states in a Li atom. Numbers given in the square brackets represent powers of 10, and the estimated uncertainties are given inside the parentheses of the calculated results.

| Transition | $S_{k \rightarrow i}$ | $A_{k \rightarrow i}$ | This work | Experiment |
|------------|------------------------|------------------------|------------|------------|
| $2p_{3/2} \rightarrow 2s_{1/2}$ | 11.019(5) | 3.70(1)[7] | 27.03(2) | 27.102 [52] |
| $2p_{3/2} \rightarrow 2s_{1/2}$ | 22.024(7) | 3.70(1)[7] | 27.05(2) | 27.102 [52] |
| $3p_{3/2} \rightarrow 3s_{1/2}$ | 1.33(1) | 6.05(1)[-16] | | |
| $3p_{3/2} \rightarrow 3s_{1/2}$ | 8.10(0)[-9] | 2.21(0)[-6] | 29.83(2) | 29.72 [53] |
| $E1 \rightarrow 2P_{1/2}$ | 5.936(2) | 1.12(1)[7] | | |
| $E1 \rightarrow 2P_{1/2}$ | 11.877(3) | 2.24(1)[7] | | |
| $3p_{1/2} \rightarrow 2s_{1/2}$ | 0.033(1) | 9.9(2)[5] | 211(2) | 203 [54] |
| $3p_{1/2} \rightarrow 2s_{1/2}$ | 3.60(0)[-8] | 1.99(0)[-6] | | |
| $E2 \rightarrow 2P_{3/2}$ | 448.4(8) | 2.64(1)[1] | | |
| $E2 \rightarrow 2P_{3/2}$ | 71.7(5) | 3.75(1)[6] | | |
| $3p_{1/2} \rightarrow 2s_{1/2}$ | 3.20(0)[-8] | 8.80(0)[-7] | | |
| $E2 \rightarrow 2P_{3/2}$ | 448.3(6) | 1.32(1)[1] | | |
| $E2 \rightarrow 2P_{3/2}$ | 143.5(6) | 3.75(1)[6] | | |
| $3d_{5/2} \rightarrow 2s_{1/2}$ | 301.130(1) | 2.52(1)[2] | 14.58(2) | 14.60 [52] |
| $E1 \rightarrow 2P_{1/2}$ | 25.7(3) | 5.71(1)[7] | | |
| $E1 \rightarrow 3s_{1/2}$ | 5.14(5) | 1.14(1)[7] | | |
| $E2 \rightarrow 3s_{1/2}$ | 11.31(3)[3] | 3.56(1)[-1] | | |
| $E2 \rightarrow 3p_{1/2}$ | 136.95(0) | 3.08(0)[3] | | |
| $E3 \rightarrow 3p_{1/2}$ | 24.65(6) | 3.70(1)[-1] | | |
| $2d_{3/2} \rightarrow 2s_{1/2}$ | 451.743(1) | 2.52(1)[2] | 14.58(2) | | |
| $E1 \rightarrow 3p_{3/2}$ | 46.3(4) | 6.86(1)[7] | | |
| $E2 \rightarrow 3p_{3/2}$ | 16.9(0)[3] | 3.56(0)[-1] | | |
| $E3 \rightarrow 3p_{3/2}$ | 246.5(6) | 3.70(1)[-1] | | |
| $M1 \rightarrow 3d_{3/2}$ | 2.40(8) | 2.04(1)[-18] | | |
| $4s_{1/2} \rightarrow 2s_{1/2}$ | 2.80(0)[-8] | 1.62(0)[-4] | 56.1(5) | 56 [55] |
| $E1 \rightarrow 2P_{1/2}$ | 0.420(7) | 3.46(5)[6] | | |
| $E1 \rightarrow 2P_{3/2}$ | 0.84(1) | 6.92(7)[6] | | |
| $E1 \rightarrow 3p_{1/2}$ | 36(0) | 2.49(1)[6] | | |
| $E1 \rightarrow 3p_{3/2}$ | 72.1(6) | 4.97(1)[7] | | |
| $E2 \rightarrow 3d_{3/2}$ | 8.5(0)[3] | 3.45(0)[-1] | | |
| $E2 \rightarrow 3d_{5/2}$ | 12.8(0)[3] | 5.17(0)[-1] | | |
Table 3. Line strengths ($S$), transition probabilities ($A$), and lifetimes ($\tau$ in ps) of the excited states in a Ca XVIII ion. Numbers given in the square brackets represent powers of 10, and the estimated uncertainties are given inside the parentheses of the calculated results.

| Transition | $S_{k \rightarrow i}$ | $A_{k \rightarrow i}$ | This work | Others [56] |
|------------|----------------------|----------------------|-----------|-------------|
| $2p_{1/2} \rightarrow 2s_{3/2}$ | 5.28(7)\([-2]\) | 1.3(2)[9] | 763(17) | 753 |
| $2p_{1/2} \rightarrow 2s_{3/2}$ | 1.07(2)[4] | 2.00(3)[9] | 501(8) | 504 |
| $M_1 \rightarrow 2p_{1/2}$ | 1.33(1) | 7.00(1)[12] | | |
| $E^2_2 \rightarrow 2p_{1/2}$ | 6.35(0)[12] | 2.54(0)[12] | | |
| $3s_{1/2} \rightarrow 2s_{3/2}$ | 1.04(0)[5] | 2.04(0)[4] | 1.08(1) | 1.09 |
| $E^1_1 \rightarrow 2p_{1/2}$ | 2.42(0)[3] | 3.01(0)[11] | | |
| $E^2_1 \rightarrow 2p_{1/2}$ | 5.13(0)[12] | 6.22(0)[12] | | |
| $3p_{1/2} \rightarrow 2s_{3/2}$ | 1.52(1)[2] | 2.4(1)[12] | 0.43(3) | 0.4286 |
| $M_1 \rightarrow 2p_{1/2}$ | 8.39(0)[7] | 1.46(0)[3] | | |
| $M_1 \rightarrow 2p_{1/2}$ | 3.99(0)[5] | 6.76(0)[4] | | |
| $E^2_2 \rightarrow 2p_{1/2}$ | 4.78(0)[3] | 8.42(0)[8] | | |
| $E^1_1 \rightarrow 3s_{1/2}$ | 3.23(5)[1] | 1.70(3)[8] | | |
| $3p_{1/2} \rightarrow 2s_{3/2}$ | 2.96(2)[2] | 2.3(1)[12] | 43.4(4) | 43.7 |
| $M_1 \rightarrow 2p_{1/2}$ | 1.39(0)[5] | 1.22(0)[4] | | |
| $E^2_2 \rightarrow 2p_{1/2}$ | 4.56(0)[3] | 4.24(0)[8] | | |
| $M_1 \rightarrow 2p_{3/2}$ | 3.25(0)[5] | 2.77(0)[11] | | |
| $E^2_2 \rightarrow 2p_{3/2}$ | 4.71(0)[3] | 4.20(0)[8] | | |
| $E^1_1 \rightarrow 3s_{1/2}$ | 6.49(6)[1] | 2.65(3)[8] | | |
| $M_1 \rightarrow 3p_{1/2}$ | 1.332(4) | 1.80(1)[1] | | |
| $E^2_2 \rightarrow 3p_{1/2}$ | 2.35(1)[1] | 2.11(1)[1] | | |
| $3d_{3/2} \rightarrow 2s_{3/2}$ | 1.52(0)[6] | 1.60(0)[3] | 0.14(2) | 0.1434 |
| $E^2_2 \rightarrow 2s_{3/2}$ | 1.74(2)[2] | 2.20(1)[9] | | |
| $E^1_1 \rightarrow 2p_{3/2}$ | 8.71(6)[2] | 5.84(6)[12] | | |
| $E^1_1 \rightarrow 2p_{3/2}$ | 1.77(2)[2] | 1.16(1)[12] | | |
| $E^2_2 \rightarrow 3s_{1/2}$ | 1.51(1)[1] | 1.22(1)[2] | | |
| $E^2_2 \rightarrow 3s_{1/2}$ | 1.51(1)[1] | 1.22(1)[2] | | |
| $M_1 \rightarrow 3s_{1/2}$ | 4.01(0)[8] | 5.11(0)[4] | | |
| $E^1_1 \rightarrow 3p_{1/2}$ | 4.18(2)[1] | 1.71(1)[7] | | |
| $E^1_1 \rightarrow 3p_{1/2}$ | 8.33(6)[2] | 1.21(9)[6] | | |
| $3d_{3/2} \rightarrow 2s_{3/2}$ | 2.61(4)[2] | 2.21(5)[9] | 0.14(1) | 0.1444 |
| $E^1_1 \rightarrow 2p_{3/2}$ | 1.59(1)[1] | 6.93(5)[12] | | |
| $E^2_2 \rightarrow 3s_{1/2}$ | 2.28(1)[1] | 1.43(1)[2] | | |
| $E^1_1 \rightarrow 3p_{3/2}$ | 7.52(1)[1] | 1.03(1)[7] | | |
| $M_1 \rightarrow 3d_{3/2}$ | 2.40(5) | 5.99(1)[1] | | |
| $E^2_2 \rightarrow 3d_{3/2}$ | 5.14(4)[2] | 7.86(6)[7] | | |
| $4s_{1/2} \rightarrow 2s_{3/2}$ | 3.62(0)[6] | 1.72(0)[4] | 1.61(7) | 1.612 |
| $E^1_1 \rightarrow 2p_{1/2}$ | 3.81(0)[4] | 1.20(0)[11] | | |
tables. Our theoretical estimated lifetimes of the excited states in Li I match well with the experimental values [52–55]. Experimental results for the lifetimes of the excited states of Ca XVIII are not available. So we compare the results with the previously reported theoretical results [56] (see table 3) and find reasonably good agreement between these results as well. In fact, neither any measurements nor any theoretical values of the lifetimes of the excited states of Ti XX are known. Nevertheless, we foresee similar levels of accuracy of these results, which are given in table 4, based on the calculations in Li I and Ca XVIII.

After establishing the accuracy of various quantities of interest to us in the isolated atomic systems, we now proceed to present these properties of the plasma-embedded systems by considering finite values of $D$ in equation (7). The calculations are assumed to be within the reported uncertainties of their corresponding observables as discussed in the preceding paragraph; however accuracy of the final results is substantially limited by the accounting for screening effects via the considered Debye models. Unlike the isolated system, the IP of the plasma-embedded system is no longer stable, and it changes depending on the strength of the plasma environment. As can be seen from equation (2), $D$ is a function of the plasma electron density ($n_e$) and plasma temperature ($T_e$). It is, therefore, possible to generate various plasma conditions by varying these parameters. For this purpose, we have varied the values of $D$ from 0.5 to 200 a.u., 0.045 to 7.52 a.u., and 0.04 to 8.33 a.u. in the calculations of the foregoing quantities in Li I, Ca XVIII, and Ti XX, respectively. In figure 1, we plot the variation in the IPs of the ground states of Li I, Ca XVIII, and Ti XX against the $D$ values, considering both the Model A and Model B approximations. As expected, the IPs decrease with the decrease in $D$ values in both the models, which is one of the unique characteristics of the plasma-embedded atomic systems and referred to as IPD or continuum lowering [14–17]. In Model A, the lower values of $D$ around which the systems exist are 14 a.u., 0.3 a.u., and 0.25 a.u. in Li I, Ca XVIII, and Ti XX, respectively; and below these critical values of $D$, the systems are supposed to be unbounded. After introducing the screenings in the repulsive interactions through Model B, the above critical values change from 14 a.u. to 0.4 a.u., 0.3 a.u. to 0.043 a.u., and 0.25 a.u. to 0.04 a.u., respectively, in Li I, Ca XVIII, and Ti XX. It is evident from figure 1 that the IPs obtained in both models are almost the same for large $D$ values but differ for smaller values of $D$ (large plasma couplings). To show this more prominently, we plot the differences in IPs from Model B and Model A ($\Delta$IP = IPB – IP) in figure 2 against the $D$ values. It is obvious from this figure that $\Delta$IP shows slow variation for large $D$ values, whereas there are drastic differences that are positive for the smaller values of $D$ (large screening). This indicates high stability of the systems in the presence of screening effects through electron–electron repulsion.

We also plot the variations in EEs of the first six low-lying excited states of Li I, Ca XVIII, and Ti XX against the $D$ values in figures 3, 4, and 5, respectively, for both Model A and Model B. First we discuss the effects of plasma on EEs in the aforementioned systems using Model A. Figure 3 shows that the EEs of the $2p_{1/2,3/2}$, $3p_{1/2,3/2}$, $3d_{3/2,5/2}$, $4s_{1/2}$, and $4p_{1/2}$ states in the Li atom decrease with the decrease in $D$ values, and finally, the states are merged into the continuum. Similar features are also observed in the highly charged Ca XVIII and Ti XX ions except for the $2p$ states (see figures 4 and 5). In these states, the EEs of the $2p$ states increase toward the strong screening strengths. Such signatures were also reported earlier in the H-like systems [57], He-like systems [58], and Li-like systems [8]. Therefore, Model A suggests that there are blue shifts in the $2s–2p$ transitions in the plasma-embedded Ca XVIII and Ti XX ions, whereas all the EEs in Li I show red shifts for the reducing values of $D$. The figures also indicate that the embedded systems lose their capability to hold the bound states with an increase in plasma strength and hence possess only a finite number of energy levels as compared with the corresponding isolated systems.

Now, with respect to the EEs obtained from Model B, it is clear from figures 3, 4, and 5 that the EEs of all the states except for the $2p$ states decrease with a decrease in the $D$ values. Thus, these transitions show red shifts and finally move to the continuum at the critical values of $D$. The EEs of the $2p$ states show different behavior; they are blue-shifted for the larger $D$ values (smaller screening), and then gradually become red-shifted toward the smaller $D$ region (higher screening). To realize these behaviors extensively, we plot the EEs of the $2s–2p_{1/2}$, $2s–3p_{1/2}$, $3s–3p_{1/2}$, and $3s–4p_{1/2}$ transitions of Li I and Ca XVIII against the $D$ values in figures 6 and 7, respectively, by considering Model B. It is
Table 4. Line strengths ($S$), transition probabilities ($A$), and lifetimes (in $\text{ps}$) of the excited states in a Ti XX ion. Numbers given in the square brackets represent powers of 10, and the estimated uncertainties are given inside the parentheses of the calculated results.

| Transition | $S_{k \rightarrow i}$ | $A_{k \rightarrow i}$ | $\tau_k$ |
|------------|----------------------|----------------------|----------|
| $2p_{3/2} \rightarrow 2s_{1/2}$ | 4.15(4)$\times 10^{-2}$ | 1.4(1)$\times 10^{0}$ | 700(75) |
| $2p_{3/2} \rightarrow 2s_{1/2}$ | 8.40(2)$\times 10^{-2}$ | 2.50(6)$\times 10^{0}$ | 400(10) |
| $M^1 \rightarrow 2p_{3/2}$ | 1.33(1) | 2.43(1)$\times 10^{0}$ | | |
| $E^2 \rightarrow 2p_{3/2}$ | 4.17(0)$\times 10^{-3}$ | 1.33(0)$\times 10^{0}$ | | |
| $3s_{1/2} \rightarrow 2s_{1/2}$ | 3.33(0)$\times 10^{-5}$ | 1.22(0)$\times 10^{0}$ | 0.634(1) |
| $E^1 \rightarrow 2p_{3/2}$ | 2.19(0)$\times 10^{-3}$ | 5.14(0)$\times 10^{0}$ | | |
| $E^1 \rightarrow 2p_{1/2}$ | 4.66(0)$\times 10^{-3}$ | 1.06(0)$\times 10^{1}$ | | |
| $3p_{1/2} \rightarrow 2s_{1/2}$ | 1.31(2)$\times 10^{-2}$ | 3.7(5)$\times 10^{0}$ | 0.27(5) |
| $M^1 \rightarrow 2p_{3/2}$ | 1.27(0)$\times 10^{-0}$ | 4.15(0)$\times 10^{0}$ | | |
| $M^1 \rightarrow 2p_{1/2}$ | 6.01(0)$\times 10^{-5}$ | 1.90(0)$\times 10^{0}$ | | |
| $E^2 \rightarrow 2p_{3/2}$ | 3.16(0)$\times 10^{-3}$ | 1.58(0)$\times 10^{0}$ | | |
| $E^1 \rightarrow 3s_{1/2}$ | 2.59(1)$\times 10^{-3}$ | 1.90(1)$\times 10^{0}$ | | |
| $3p_{3/2} \rightarrow 2s_{1/2}$ | 2.54(2)$\times 10^{-3}$ | 3.7(3)$\times 10^{0}$ | 0.27(3) |
| $M^1 \rightarrow 2p_{3/2}$ | 2.10(0)$\times 10^{-3}$ | 3.47(0)$\times 10^{0}$ | | |
| $E^2 \rightarrow 2p_{3/2}$ | 2.00(0)$\times 10^{-3}$ | 2.00(0)$\times 10^{0}$ | | |
| $M^1 \rightarrow 2p_{1/2}$ | 2.00(0)$\times 10^{-3}$ | 2.00(0)$\times 10^{0}$ | | |
| $E^2 \rightarrow 2p_{1/2}$ | 4.89(0)$\times 10^{-3}$ | 7.82(0)$\times 10^{0}$ | | |
| $E^1 \rightarrow 3s_{1/2}$ | 5.21(1)$\times 10^{-3}$ | 3.41(1)$\times 10^{0}$ | | |
| $M^1 \rightarrow 3p_{1/2}$ | 1.33(1) | 6.28(1)$\times 10^{0}$ | | |
| $E^1 \rightarrow 3p_{3/2}$ | 1.54(1)$\times 10^{-3}$ | 1.10(1)$\times 10^{0}$ | | |
| $3d_{3/2} \rightarrow 2s_{1/2}$ | 2.48(0)$\times 10^{-6}$ | 4.85(0)$\times 10^{0}$ | 0.094(7) |
| $E^2 \rightarrow 2s_{1/2}$ | 1.16(3)$\times 10^{-2}$ | 2.85(0)$\times 10^{0}$ | | |
| $E^1 \rightarrow 2p_{3/2}$ | 7.04(4)$\times 10^{-2}$ | 1.43(2)$\times 10^{0}$ | | |
| $E^1 \rightarrow 2p_{1/2}$ | 7.04(4)$\times 10^{-2}$ | 1.43(2)$\times 10^{0}$ | | |
| $E^2 \rightarrow 3s_{1/2}$ | 9.89(2)$\times 10^{-2}$ | 1.67(2)$\times 10^{0}$ | | |
| $E^1 \rightarrow 3p_{3/2}$ | 3.38(1)$\times 10^{-3}$ | 2.62(1)$\times 10^{0}$ | | |
| $E^1 \rightarrow 3p_{1/2}$ | 6.74(4)$\times 10^{-2}$ | 1.39(9)$\times 10^{0}$ | | |
| $3d_{5/2} \rightarrow 2s_{1/2}$ | 1.73(2)$\times 10^{-2}$ | 4.1(0)$\times 10^{0}$ | 0.095(1) |
| $E^1 \rightarrow 2p_{3/2}$ | 1.29(1)$\times 10^{-1}$ | 1.06(1)$\times 10^{1}$ | | |
| $E^2 \rightarrow 3s_{1/2}$ | 1.49(1)$\times 10^{-1}$ | 2.05(2)$\times 10^{0}$ | | |
| $E^1 \rightarrow 3p_{3/2}$ | 6.09(1)$\times 10^{-1}$ | 1.33(1)$\times 10^{0}$ | | |
| $M^1 \rightarrow 3d_{3/2}$ | 2.39(5) | 2.1(0) | | |
| $E^2 \rightarrow 3d_{3/2}$ | 1.82(4)$\times 10^{-2}$ | 2.2(5)$\times 10^{-2}$ | | |
| $4s_{1/2} \rightarrow 2s_{1/2}$ | 1.24(0)$\times 10^{-5}$ | 1.10(0)$\times 10^{0}$ | 1.4(1) |
| $E^1 \rightarrow 2p_{3/2}$ | 2.03(0)$\times 10^{-4}$ | 1.20(0)$\times 10^{0}$ | | |
| $E^1 \rightarrow 2p_{3/2}$ | 4.32(0)$\times 10^{-4}$ | 2.51(0)$\times 10^{0}$ | | |
clear from these figures that the EEs of the $2s \rightarrow 3p$ and $3s \rightarrow 4p$ transitions decrease with the decrease in $D$ values in accordance with the findings in Model A [8]. However, the quantities for the $2s \rightarrow 2p$ and $3s \rightarrow 3p$ transitions increase initially with the decrease in $D$ values and then fall suddenly in the lower $D$ region. Similar trends are also observed in the Ti XX ion. We infer from this behavior that the $\Delta n \neq 0$ transition spectra are red-shifted with the decrease in $D$ values for both Model A and Model B but that the $\Delta n = 0$ transition spectra are red-shifted in the Li atom and blue-shifted in the Ca XVIII and Ti XX ions with decreasing $D$ values for Model A. In contrast, the spectra for $\Delta n = 0$ transitions show blue shifts at the higher values of $D$ and red shifts for the lower values of $D$ in all the atomic systems embedded in plasma when Model B is taken into account. This indicates that the effects of the two-electron screenings become less important

| Transition | $S_{k\rightarrow i}$ | $\Delta S_{k\rightarrow i}$ | $\tau_k$ |
|------------|----------------------|---------------------|--------|
| $E_1 \rightarrow 3p_{3/2}$ | 1.22(3) $[-2]$ | 1.20(1) $[11]$ |
| $E_1 \rightarrow 3p_{1/2}$ | 2.59(4) $[-2]$ | 2.5(4) $[11]$ |
| $E_2 \rightarrow 3d_{3/2}$ | 1.35(2) $[-2]$ | 2.9(4) $[7]$ |
| $E_2 \rightarrow 3d_{5/2}$ | 2.05(2) $[-2]$ | 4.40(1) $[7]$ |

Figure 1. Variation of ionization potentials with Debye screening length ($D$).

Figure 2. Differences in the ionization potentials from Model B and Model A with Debye screening length ($D$).

Figure 3. Variation in the excitation energies of Li I with Debye screening length obtained from Model A, shown in panel (a), and from Model B, shown in panel (b).

Figure 4. Variation in the excitation energies of Ca XVIII with Debye screening length obtained from Model A, shown in panel (a), and from Model B, shown in panel (b).
and states show a sharp rise in the high-screening region. A similar trend is observed by Bowen et al in He-like systems [43].

Figures 3, 4, and 5 also disclose that there appear to be changes in the energy level structures in the high-screening regions with Model B with respect to the isolated systems. In Li I, they show energy level crossings between the 2p and 3s states near the continuum edge. The 2p states move to the continuum toward very low D values, whereas the 3s state still exists there. Similar level crossings are also seen in the Li-like Ca and Ti ions near the high-screening regions. In the ionized systems, the level crossings become more obvious.

To demonstrate these level-crossing processes in the plasma-embedded systems, we present the Grotrian energy levels for higher values of D (lower screening strengths), for which the results of Model A and Model B show nearly the same behavior, but these screening effects play a significant role in influencing the results at the lower values of D (higher screening strength) by producing a humplike structure. It is worth pointing out here that similar features have also been observed by Bowen et al in He-like systems [43].

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Figure 5. Variation in the excitation energies of Ti XX with Debye screening length obtained from Model A, shown in panel (a), and from Model B, shown in panel (b).

Figure 6. Variation in the transition energies with Debye screening length in Li I using Model B. Panels (a) and (b) correspond to the 2s−2p_{1/2} and 2s−3p_{1/2} transitions, respectively, and panels (c) and (d) correspond to the 3s−3p_{1/2} and 3s−4p_{1/2} transitions, respectively.

Figure 7. Variation in the transition energies with Debye screening length in Ca XVIII using Model B. Panels (a) and (b) correspond to the 2s−2p_{1/2} and 2s−3p_{1/2} transitions, respectively, and panels (c) and (d) correspond to the 3s−3p_{1/2} and 3s−4p_{1/2} transitions, respectively.

diagram, particularly for Ca XVIII, for a few selected values of D in figure 8. This figure shows the change in the sequence of energy levels with the decrease in values of D. For lower screening lengths, a sequence alternative of the energy levels is found. As seen in this figure, the lower 3d_{3/2,5/2} levels of the Ca XVIII ion have moved to the continuum around D = 0.3 a.u. even when the 4s_{1/2} state is still bounded with the ion. This implies that there are level crossings between the 4s and 3d states. There are also crossovers among the 4s, 3s, 2p, and 3p states in this ion such that its energy level sequence becomes 2s, 3p_{1/2,3/2}, 2p_{1/2,3/2}, 3s, and 4s. A similar trend is also noticed in the Li-like Ti ion. Figure 8 also illustrates that the states with n = 3 in the Ca XVIII ion are nearly degenerate for the higher values of D, but the differences among the 3s, 3p, and 3d states increase with decreasing values of D. Gradually, toward the high-screening lengths, the crossovers occur among the 3s, 3p, and 3d energy levels, probably owing to the weaker attraction of bound electrons by the nucleus. It is, however, found from figure 8 that the FS splittings between the states are least affected by the plasma screening. Indeed, we find that the states with larger orbital angular momentum are more affected by the screenings, leading to the remarkable change in the energy level structures of the plasma-embedded atomic systems near the continuum edge.

Because the atomic systems are affected by the plasma environment, it is obvious that the radiative properties such as lifetimes of the excited states in these systems are different from their corresponding isolated systems. By calculating the line strengths for various allowed and forbidden transitions, we evaluate the lifetimes of the excited states in the considered systems with different values of D. The variations in the lifetimes of the 2p_{1/2,3/2}, 3s_{1/2}, 3p_{1/2,3/2}, and 4s_{1/2} states in Li I and Ca XVIII for different D values are listed in table 5. We plot them against the D values in figure 9, from which we find that the lifetimes of the 2p states in Li I decrease slowly with increasing plasma strengths. Moreover, the lifetimes of the 3s, 3d, and 4s states show a sharp rise in the high-screening region.
5. Concluding remarks

We have investigated the effects of plasma confinement on the electronic structure and spectroscopic properties of the Li atom and the highly charged Li-like Ca XVIII and Ti XX ions with two different approximations in the Debye model and using a relativistic coupled-cluster method. We find that the ionization potentials of the plasma-embedded systems decrease with decreasing values of the Debye length $D$ and that the energy levels of the embedded systems merge into the continuum at some critical values of $D$. Inclusion of the screening effects in the electron–nucleus interaction potentials destabilizes the systems, whereas inclusion of the screenings in the electron–electron potentials counteracts these effects by lowering the energies of the embedded systems, hence enhancing the stability of these systems. With Model A approximation, all the...
transition spectra in the Li atom show red shifts with increasing values of the plasma strengths. In the case of Ca XVIII and Ti XX ions, the spectra corresponding to the \( n s \rightarrow np \) transitions show blue shifts and the \( ns \rightarrow np \) transitions exhibit red shifts with increasing plasma strengths. However, the systems display some peculiar behavior in the presence of screenings in the electron–electron interactions via the Model B approximation. It is found that the \( \Delta n \neq 0 \) transition spectra of the plasma-embedded systems are red-shifted with increasing values of the plasma strengths and that this feature holds for both Model A and Model B. In the Model B approximation, the \( \Delta n = 0 \) transitions show blue shifts at higher screening lengths and red shifts at lower screening lengths due to the presence of the screenings in the electron–electron interactions. Change in the sequence of the atomic energy levels of the considered systems is noticed in both the approximations with respect to their corresponding plasma-isolated systems, and the level crossings between the states become more prominent in the highly ionized systems. The states with the same principal quantum number remain degenerate for the higher screening lengths, but the differences in the energy levels widen for decreasing values of \( D \). Due to the strong influence of the screenings in the energy spectra of the embedded atomic systems, the lifetimes of the excited states change in comparison with the corresponding plasma-free systems. The reported spectral properties in this work will be useful in studies of both laboratory and astrophysical plasma for identifying the spectral lines in the considered atomic systems and should motivate the experimentalists to verify their underlying physics.

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