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Investigation of the triplet doubly excited ${}^{3}P^{o}$ states of the Li⁺

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ABSTRACT

We report in this paper accurate computed data of the energy positions and widths of the triplet doubly excited ${}^{3}P^{o}$ states of the He-like Li⁺ ion lying below the N = 2 and N = 3 hydrogenic thresholds by using a *B*-spline based spectral approach of configuration interaction type combined with the complex rotation method. The method has been successfully applied in our previous works (Albert et al., 2018, 2019) to locate the singlet doubly excited states of the ion. We also demonstrate in the present paper the efficiency of our approach for the straightforward classification of the doubly excited states into distinct series.

1. Introduction

Two-electron excitation leading to the formation of the doubly excited ${}^{3}P^{o}$ states can be triggered in metastable He-like $(1s2s {}^{3}S^{e})$ ions by extreme ultraviolet (EUV) and x-ray laser pulses. The states form resonances that can decay by electron emission (autoionization) induced by electron correlation. Metastable He-like ions in the $1s2s {}^{3}S^{e}$ state can be produced by using electron-cyclotron-resonance ion sources (Müller et al., 2014, Müller et al., 2018a; Müller et al., 2018b). The ions with only two bound electrons occupying two different shells are perfect targets for studying the formation and decay of the ${}^{3}P^{o}$ resonance states.

The doubly excited ${}^{3}P^{o}$ states investigated in the present paper are accessible from the 1*s*2*s* ${}^{3}S^{o}$ level of the Li⁺ ion by a single EUV photon transition. The recent development in the generation techniques of laser pulses in the EUV spectral range and with attosecond durations (Attwood and Sakdinawat, 2016) opens the possibility to observe and control the autoionization dynamics. Accurate theoretical data of the energy positions *E* and the autoionizing widths Γ of the doubly excited ${}^{3}P^{o}$ states in the Li⁺(1*s*2*s* ${}^{3}S^{e}$) ion will be useful to the future experimental investigation of these states by attosecond EUV laser pulses.

In this work, we present accurate theoretical data of *E* and Γ for the doubly excited ${}^{3}P^{o}$ states of the Li ${}^{+}$ ion lying below the N = 2 and N = 3 Li²⁺(*Nl*) hydrogenic thresholds. The results are obtained by using our spectral method of configuration interaction type which combines a discretization technique based on *B*-spline functions with the complex rotation method. The approach has been successfully applied to locate the singlet ${}^{1}S^{e}$ and ${}^{1}P^{o}$ resonance states of the Li⁺ ion (Albert et al., 2018, 2019). In the present work, we extend the calculation to locate the triplet ${}^{3}P^{o}$ resonance states in the energy spectrum of

the ion. We also show how the present approach allows the straightforward classification of the states into distinct series.

The accuracy of the calculated resonant parameters (E, Γ) is demonstrated by comparing our results with the other available data. Only the experimental measurements of the energy positions E of few doubly excited ${}^{3}P^{o}$ states of the Li + ion have been reported by using beam-foil techniques (Ziem et al., 1975), ejected electron spectroscopy experiment (Rodbro et al., 1979) and from the measurement of Auger decays (Diehl et al., 1999). Theoretical investigations of the low lying doubly excited ${}^{3}P^{o}$ states have been conducted by using diverse approaches such as the Feshbach formalism (Bhatia and Temkin, 1984; Macias and Riera, 1988; Seminario and Sanders, 1990), the truncated diagonalization method (Conneely and Lipsky, 1978), the density functional theory (Roy et al., 1997), the complex rotation method (Ho, 1979; Chen, 2007; Chung and Lin, 1998), a time dependent perturbation approach (Das and Mukerjee, 1993) or the screening constant by unit nuclear charge method (Sakho et al., 2008).

Atomic units (a.u.), i.e., $e = m = \hbar = 1$ and $c = 1/\alpha$, are used throughout this paper unless otherwise stated.

2. Theory

The nonrelativistic time-independent Schrödinger equation for a two-electron system is given by:

$$H\Phi^{SLM}(\mathbf{r}_1, \mathbf{r}_2) = E\Phi^{SLM}(\mathbf{r}_1, \mathbf{r}_2), \tag{1}$$

where the Hamiltonian H writes:

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$$H = \sum_{i=1}^{2} \left(-\frac{1}{2} \Delta_i - \frac{Z}{r_i} \right) + \frac{1}{r_{12}}.$$
 (2)

Z is the nuclear charge, $r_{12} = |\mathbf{r}_1 - \mathbf{r}_2|$ the interelectronic distance, and $1/r_{12}$ the electrostatic interaction potential treated by using the multipole expansion of the Coulomb repulsion between the two electrons (Zare, 1988):

$$\frac{1}{r_{12}} = \sum_{l=0}^{\infty} \frac{4\pi}{(2l+1)} \sum_{m=-l}^{l} \frac{r_{<}^{l}}{r_{>}^{l+1}} Y_{l}^{m^{*}}(\Omega_{1}) Y_{l}^{m}(\Omega_{2}),$$
(3)

with $r_{<} = \min(r_1, r_2)$, $r_{>} = \max(r_1, r_2)$ and $Y_l^m(\Omega_i)$ denotes a spherical harmonic with $\Omega_i = (\theta_i, \phi_i)$. The spatial wave function $\Phi^{SLM}(\mathbf{r}_1, \mathbf{r}_2)$ is expanded on the basis of two-electron configurations that are products of one-electron functions, as follows:

$$\Phi_{n}^{SLM}(\mathbf{r}_{1}, \mathbf{r}_{2}) = \sum_{\alpha \equiv l_{1}, l_{2}, i, j} c_{n, \alpha}^{SLM} \left(\frac{B_{l}^{k}(r_{1})}{r_{1}} \frac{B_{l}^{k}(r_{2})}{r_{2}} \mathscr{Y}_{l_{1}, l_{2}}^{L, M}(\Omega_{1}, \Omega_{2}) + (-1)^{S} \frac{B_{l}^{k}(r_{2})}{r_{2}} \right.$$
$$\left. \frac{B_{l}^{k}(r_{1})}{r_{1}} \mathscr{Y}_{l_{1}, l_{2}}^{L, M}(\Omega_{2}, \Omega_{1}) \right).$$
(4)

S is the total spin, *L* the total angular momentum, *M* the projection and $l_1(l_2)$ the orbital angular momentum quantum number of electron 1 (2). The radial part of Eq. (4) is defined by a basis of *B*-spline functions $B_i^k(r)|_{i=1,...,N_b}$ of order *k* (de Boor, 1978), with N_b the number of *B*splines used per electron in a box of radius r_0 . The angular part of Eq. (4) is described by the bipolar spherical harmonic function $\mathscr{Y}_{l_1,l_2}^{L,M}(\Omega_1, \Omega_2)$ (Zare, 1988):

$$\mathcal{Y}_{l_{1},l_{2}}^{L,M}(\Omega_{1},\,\Omega_{2}) = \sum_{m_{1}=-l_{1}}^{l_{1}} \sum_{m_{2}=-l_{2}}^{l_{2}} (-1)^{l_{1}-l_{2}+M} \sqrt{2L+1} \\ \times \begin{pmatrix} l_{1} & l_{2} & L \\ m_{1} & m_{2} & -M \end{pmatrix} Y_{l_{1}}^{m_{1}}(\Omega_{1}) Y_{l_{2}}^{m_{2}}(\Omega_{2}).$$
(5)

The angular configurations (l_1, l_2) employed in Eq. (5) are determined by the triangle condition $|l_1 - l_2| \le L \le |l_1 + l_2|$.

To locate the doubly excited ${}^{2S+1}L^{\pi}$ resonance states embedded between the Li²⁺(*Nl*) hydrogenic thresholds, we use the complex rotation method. The technique consists in applying a rotation by an angle θ to the radial coordinates $r_i \rightarrow r_i e^{i\theta}$ in the complex plane (Simon, 1972). The procedure transforms the Hamiltonian *H* defined in Eq. (2) into the following rotated Hamiltonian $H(\theta)$:

$$H(\theta) = \sum_{i=1}^{2} \left(-\frac{1}{2} \Delta_{i} e^{-2i\theta} - \frac{Z}{r_{i}} e^{-i\theta} \right) + \frac{1}{r_{12}} e^{-i\theta}.$$
 (6)

The diagonalization of $H(\theta)$ for S = 1, L = 1, M = 0 and pairs of (l_1, l_2) of odd parity $\pi = o$ provides an energy spectrum, see Fig. (1), in which the doubly excited ${}^{3}P^{o}$ resonance states are exposed and described by discrete complex eigenvalues of the form:

$$E_{res} = E - i\frac{\Gamma}{2},\tag{7}$$

where *E* is the energy position of the resonance and Γ its width.

The demonstration of the efficiency of the *B*-spline functions for the calculation of atomic structures can be found in the work of Van der Hart and Hansen (1992) and in our previous works (Barmaki et al., 2014, 2018, 2019). The details about the computational implementation for the diagonalization of rotated Hamiltonian are given in our previous work (Albert et al., 2018).

3. Results and discussion

3.1. Localization and classification of the doubly excited states into distinct series

The energy positions *E*, the widths Γ and other expectation values



Fig. 1. Schematic description of the energy spectrum of the Li + ion. The indicated ³*p*^o states are doubly excited states located below the *N* = 2 and *N* = 3 thresholds. An *N* hydrogenic threshold is in the energy spectrum located at the exact energy position $I_N = -\frac{z^2}{2N^2}$.

for the doubly excited ${}^{3}P^{o}$ resonance states are obtained by considering for the diagonalization of $H(\theta)$ (Eq. (6)) the ion confined in a spherical box of radius $r_{0} = 90$ a.u. In the radial part of the expansion (4), $N_{b} = 110$ *B*-spline functions of order k = 7 are used per electron. In the angular part of the expansion, we took into account the following pairs $(l_{1} = 0, l_{2} = 1)$, $(l_{1} = 1, l_{2} = 2)$, $(l_{1} = 2, l_{2} = 3)$, $(l_{1} = 3, l_{2} = 4)$, $(l_{1} = 4, l_{2} = 5)$ that satisfy the odd parity $\pi = (-1)^{l_{1}+l_{2}} = (-1)^{L} = o$.

Due to the strongly correlated nature of doubly excited states, they cannot in general be described by the spectroscopic notation (Nl_1, nl_2) ${}^{2S+1}L^{\pi}$ based on the independent particle model, with N the innerelectron quantum number associated with the ionic threshold and *n* the outer-electron radial quantum number (n = N, N + 1, ...). The problem of the description and the classification of the doubly excited ${}^{2S+1}L^{\pi}$ states in two-electron systems has been addressed in the pioneer works of Sinanoglu and Herrick (1975), Conneely and Lipsky (1978) and Lin (1984, 1986) using different theoretical approaches. The notation $_{N}(K, T)_{n}$ ^{2S+1}L^{π} introduced by Sinanoglu and Herrick (1975) to label the doubly excited states is the most widely used. In the present paper, the investigated ${}^{3}P^{o}$ states below an N threshold are classified and each state is assigned a symbol $_{N}(K, T)_{n}$. K and T are integer numbers that describe the angular correlations of the electron-electron interaction. The calculations of Sinanoglu and Herrick (1975) to obtain K and T are based on the group theoretical method that consisted in the diagonalization of the operator $\mathbf{B}^2 \equiv (\mathbf{c}_1 - \mathbf{c}_2)^2$, where \mathbf{c}_1 and \mathbf{c}_2 are Runge-Lenz vectors for electron 1 and electron 2, respectively. For a given N, L, and $\pi = (-1)^L$, the allowed values for *K* and *T* are:

$$T = 0,1,2, \dots, \min(L, N-1)$$
 (8)

$$K = (N - 1 - T), (N - 3 - T), \dots, -(N - 1 - T).$$
(9)

K is a measure of the angle θ_{12} between the two electrons position vectors. In a state with positive value of *K*, the electrons are located at opposite sides of the nucleus ($\langle \cos\theta_{12} \rangle < 0$). In a state with negative value of *K*, the electrons are located at the same side of the nucleus ($\langle \cos\theta_{12} \rangle > 0$). The two electrons in a state with K = 0 have their position vectors nearly perpendicular to each other ($\langle \cos\theta_{12} \rangle \simeq 0$). *K* is proportional to the average value of $r_{<}\cos\theta_{12}$ where $r_{<}$ is the radius of the inner electron $r_{<} = \min(r_1, r_2)$. *T* describes the relative orientation between the orbitals of the two electrons. When T = 0, the two electrons move in the same plane. According to the conditions (8) and (9), the allowed values of (*K*, *T*) for N = 2 and L = 1 are (*K*, *T*) = (1,0), (0,1) and (-1,0) and for N = 3 and L = 1, the allowed pairs are (*K*, *T*) = (2,0), (1,1), (0,0), (-1,1) and (-2,0). The doubly excited ${}^{3}P^{0}$ states lying below the N = 2 threshold can be separated in three series while

Table 1

Calculated values of n^* , $\langle r_< \cos\theta_{12} \rangle$, $\langle \cos\theta_{12} \rangle$ and $n^{*3}\Gamma$ for the doubly excited ${}^3P^o$ resonance states of Li⁺ below the N = 2 threshold. The integer number M indicates the orders of appearance of the states counting from the lowest ${}^3P^o$ state. The numbers in the square brackets denote the power of ten.

$^{3}P^{o}(M)$	n*	$\langle r_{<}\cos\theta_{12}\rangle$	$\langle \cos \theta_{12} \rangle$	$n^{*3}\Gamma$	$_N(K, T)_n$
${}^{3}P^{o}(1)$	1.629	- 0.577	- 0.336	0.001	2(1,0)2
${}^{3}P^{0}(2)$	2.666	- 0.824	- 0.395	0.002	$_{2}(1,0)_{3}$
${}^{3}P^{o}(5)$	3.654	- 0.840	- 0.410	0.002	$_{2}(1,0)_{4}$
³ P ⁰ (8)	4.649	- 0.843	- 0.416	0.002	2(1,0)5
${}^{3}P^{o}(11)$	5.646	- 0.847	- 0.419	0.002	2(1,0) ₆
³ <i>P</i> ⁰ (3)	2.704	- 0.005	- 0.003	6.7[-5]	2(0, 1) ₃
${}^{3}P^{o}(6)$	3.733	- 0.010	- 0.011	8.4[-5]	$_{2}(0, 1)_{4}$
${}^{3}P^{o}(9)$	4.743	- 0.010	- 0.010	9.4[-5]	₂ (0, 1) ₅
³ <i>P</i> ^o (4)	3.077	0.608	0.310	2.4[-6]	2(-1,0)3
${}^{3}P^{0}(7)$	4.067	0.772	0.384	3.1[-6]	$2(-1,0)_4$
³ <i>P</i> ^o (10)	5.063	0.834	0.413	3.6[-6]	2(-1,0)5

those located between the N = 2 and N = 3 can be grouped in five series.

Since our theoretical approach is different from that of Sinanoglu and Herrick (1975), the identification to which series $_N(K, T)$ a state will belong is made in the present work from the examination of the following calculated values (Chung and Lin, 1998):

- 1. The effective quantum number n^* of the outer electron calculated by using the Rydberg-Ritz formula that parameterizes the energy of the state as $E = -Z^2/2N^2 (Z 1)^2/2n^{*2}$ (Burgers et al., 1995). n^* differs from n by the quantum defect μ ($n^* = n \mu$).
- 2. The reduced width $n^{*3}\Gamma$.
- 3. The average value of $\cos\theta_{12} = \mathbf{r}_1 \cdot \mathbf{r}_2 / r_1 r_2$, where \mathbf{r}_1 and \mathbf{r}_2 are the position vectors of electron 1 and electron 2.
- 4. The average value of $r_{<}\cos\theta_{12}$, with $r_{<} = \min(r_{1}, r_{2})$.

In Tables 1 and 2, we present the results of the computed values of

Table 2

Calculated values of n^* , $\langle r_< \cos\theta_{12} \rangle$, $\langle \cos\theta_{12} \rangle$ and $n^{*3}\Gamma$ for the doubly excited ${}^3P^o$ resonance states of Li⁺ located between the N = 2 and N = 3 thresholds. The numbers in the square brackets denote the power of ten.

$^{3}P^{o}(M)$	<i>n</i> *	$\langle r_{<}\cos\theta_{12}\rangle$	$\langle \cos \theta_{12} \rangle$	$n^{*3}\Gamma$	$_N(K, T)_n$
³ P ^o (1)	2.373	- 2.040	- 0.533	0.045	₃ (2,0) ₃
³ P ^o (3)	3.376	- 2.570	- 0.570	0.068	₃ (2,0) ₄
³ P ^o (8)	4.339	- 2.653	- 0.588	0.069	₃ (2,0) ₅
³ P ^o (13)	5.320	- 2.676	- 0.598	0.066	₃ (2,0) ₆
$^{3}P^{0}(4)$	3.377	- 1.244	- 0.287	0.004	$_{3}(1,1)_{4}$
³ P ^o (9)	4.396	- 1.240	- 0.274	0.005	$_{3}(1,1)_{5}$
$^{3}P^{o}(14)$	5.403	- 1.274	- 0.279	0.006	₃ (1,1) ₆
${}^{3}P^{o}(2)$	2.644	0.185	0.037	0.024	₃ (0,0) ₃
³ P ^o (5)	3.793	0.027	0.014	0.027	₃ (0,0) ₄
³ P ^o (10)	4.801	0.090	0.022	0.030	₃ (0,0) ₅
${}^{3}P^{o}(15)$	5.800	0.124	0.029	0.030	₃ (0,0) ₆
3 20(5)	3 807	1 103	0.270	2 0[-3]	(11).
³ P ⁶ (6)	4.965	1.195	0.270	2.9[-3]	$3^{(-1,1)}_{3}$
${}^{3}P^{0}(11)$	4.865	1.294	0.295	8.4[-4]	$3^{(-1,1)_5}$
${}^{3}P^{o}(16)$	5.888	1.350	0.304	7.2[-4]	$_{3}(-1,1)_{6}$
${}^{3}P^{0}(7)$	4.287	1.947	0.440	3.6[-5]	$_{2}(-2,0)_{4}$
³ P ^o (12)	5.255	2.342	0.525	3.4[-5]	₃ (-2,0) ₅

 n^* , $\langle r_< \cos\theta_{12} \rangle$, $\langle \cos\theta_{12} \rangle$ and $n^{*3}\Gamma$ for the lowest doubly excited ${}^{3}P^o$ states located below the N = 2 and N = 3 thresholds, respectively. The states that have similar values of $\langle \cos\theta_{12} \rangle$, $\langle r_< \cos\theta_{12} \rangle$, $n^{*3}\Gamma$ and the fractional part of n^* are put in the same group or series. According to the values of $\langle \cos\theta_{12} \rangle$ and $\langle r_< \cos\theta_{12} \rangle$, K and T numbers are assigned to each series. Each ${}^{3}P^o(M)$ state of a given series is designated by the unique notation ${}_N(K, T)_n$ with n the outer-electron radial quantum number. The values of n^* , $\langle r_< \cos\theta_{12} \rangle$, $\langle \cos\theta_{12} \rangle$ and $n^{*3}\Gamma$ obtained by our theoretical approach are similar to the values reported by Chung and Lin (1998) using the saddle-point complex rotation method.

3.2. Results of the energy positions and widths

The accuracy of the results of the energy positions *E* and the widths Γ is demonstrated by comparing in Table 3 and Table 4 our computed values obtained for the lowest doubly excited ${}^{3}P^{o}$ states of the Li + ion with other available data. The states are in the Tables arranged according to their orders of appearance. The data of (E, Γ) for the states located below the N = 2 threshold are in Table 3 compared to the available theoretical data reported by Conneely and Lipsky (1978) using the truncated diagonalization method with the open-channel close-coupling approximation, Bhatia and Temkin (1984) using the Feshbach formalism with Hylleraas functions, Ho (1981) using the complex rotation method with Hylleraas functions, Macias and Riera (1988) using the Feshbach formalism with a discretization method, Chen (2007) and Chung and Lin (1998) using the saddle-point complex rotation method. The approaches developed by these authors distinguish by their capacity to access not only the information about the energy position of a resonant state but also its width. We also compare our computed data with the experimental measurements obtained by Ziem et al. (1975) using beam-foil techniques, Rodbro et al. (1979) using ejected electron spectroscopy experiment and with the more recent data of Diehl et al. (1999) obtained from the measurement of Auger decays.

Experimental values of the energy positions are only available for the first three states of the $_2(1,0)$ series which are ${}^3P^o(1)$, ${}^3P^o(2)$ and ${}^3P^o(5)$ states and the two first states of the $_2(0, 1)$ series: ${}^3P^o(3)$ and ${}^3P^o(6)$. Our theoretical values of their energy positions agree with the experimental data within the first 3 – 4 digits. As one can see in Table 3, all the theoretical approaches we compare with have provided values of the energy positions of the three lowest ${}^3P^o(1)$, ${}^3P^o(2)$ and ${}^3P^o(3)$ states. We note generally a good agreement between all the reported results. Our data of energy positions for these states and the other states compare best with the data reported by Chen (2007). The results agree within the first 5 – 7 digits.

Besides the calculation of the energy positions of the resonances, the information about their widths is also necessary in order to evaluate the lifetimes for their decay. Theoretical investigations are in this case of interest since experimental measurement of the widths of the ${}^{3}P^{o}$ resonances in Li⁺ are completely lacking. Our calculation indicates that the two lowest ${}^{3}P^{o}(1)$ and ${}^{3}P^{o}(2)$ states are the broadest among the other resonances in agreement with the other approaches. The present calculation evaluates their lifetimes:

$$\tau = \frac{n}{\Gamma},\tag{10}$$

to $\tau_1 = 77$ fs and $\tau_2 = 220$ fs, respectively. Our results indicate that the ${}^{3}P^{o}(4)$, ${}^{3}P^{o}(7)$ and ${}^{3}P^{o}(10)$ states belonging to the ${}_{2}(-1,0)$ series have the narrowest widths in agreement with Chen (2007) and Chung and Lin (1998). Once formed in the ion, these states have low probability to decay by emission of electrons which makes them longer-lived states.

In Table 4, we present the results of the resonant parameters for the lowest doubly excited ${}^{3}P^{o}$ states of Li + located between the N = 2 and N = 3 thresholds. To the best of our knowledge, no experimental investigations on the characterization of these resonant states have been conducted to date. The results are compared with the reported data of

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Table 3

Energy positions and widths of the doubly excited ${}^{3}P^{o}$ resonance states of Li ${}^{+}$ below the N = 2 threshold. The numbers in the square brackets denote the power of ten.

$^{3}P^{o}(M)$	${}^{3}P^{o}(1)$	${}^{3}P^{o}(2)$	${}^{3}P^{o}(3)$	${}^{3}P^{o}(4)$	${}^{3}P^{o}(5)$	³ <i>P</i> ⁰ (6)	${}^{3}P^{o}(7)$	${}^{3}P^{o}(8)$	³ <i>P</i> ⁰ (9)	${}^{3}P^{o}(10)$
-E (a.u.) Expt.										
а	1.8770± 0.0007	1.4048 ± 0.0007	1.3975± 0.0007		1.273 ± 0.002	1.267 ± 0.001				
b	1.877± 0.004	$1.402\pm$ 0.004	1.398± 0.004							
c	1.877 ± 0.001									
Theory										
Present	1.878174	1.406273	1.398511	1.336194	1.274756	1.268551	1.245908	1.217540	1.213899	1.203004
d	1.878174	1.406272	1.398511	1.336190	1.274755	1.268551	1.245906	1.217539	1.213898	1.203003
e	1.878263	1.406368	1.398632	1.336293	1.285887	1.268640	1.245997	1.217653	1.213993	1.203099
f	1.87869	1.40644	1.39865	1.33504						
g	1.878185	1.40627	1.398514	1.33621						
h	1.8746	1.4029	1.3972							
i	1.8794	1.4065	1.3985							
Γ (a.u.) Theory										
Present	3.131[-4]	1.101[-4]	3.387[-6]	8.249[-8]	4.385[-5]	1.610[-6]	4.563[-8]	2.121[-5]	8.809[-7]	2.778[-8]
d	3.145[-4]	1.110[-4]	3.624[-6]	2.76[-10]	4.444[-5]	2.238[-6]	9.96[-10]	2.154[-5]	6.46[-7]	2.92[-10]
e	3.231[-4]	1.137[-4]	3.408[-6]	5.667[-10]	4.55[-5]	1.559[-6]	2.896[-10]	2.200[-5]	8.655[-7]	4.245[-10]
f	3.146[-4]	1.117[-4]	2.848[-6]	1.948[-9]						
g	3.12[-4]	1.05[-4]								
ĥ	4.81[-4]	1.90[-4]	4.85[-6]							
i	3.28[-4]	1.16[-4]	3.494[-6]							

aDiehl et al. (1999). ^bRodbro et al. (1979). ^cZiem et al. (1975). ^dChen (2007). ^eChung and Lin (1998). ^fMacias and Riera (1988). ^gHo (1981). ^hConneely and Lipsky (1978). ⁱBhatia and Temkin (1984).

Table 4

Energy positions and widths of the doubly excited ${}^{3}P^{o}$ resonance states of Li ${}^{+}$ located between the N = 2 and N = 3 thresholds. The numbers in the square brackets denote the power of ten.

${}^{3}P^{0}(M)$	${}^{3}P^{o}(1)$	³ <i>P</i> ⁰ (2)	³ <i>P</i> ⁰ (3)	³ <i>P</i> ⁰ (4)	${}^{3}P^{o}(5)$	³ <i>P</i> ^o (6)	${}^{3}P^{o}(7)$	${}^{3}P^{o}(8)$	³ <i>P</i> ^o (9)	${}^{3}P^{o}(10)$
-E (a.u.) Theory Present a b	0.855030 0.855082 0.8569	0.786097 0.786069 0.7878	0.675403 0.675441 0.6763	0.675333 0.675375 0.6754	0.638975 0.638972 0.6392	0.638002 0.638016 0.6374	0.608805 0.608839 0.6066	0.606204 0.606240 0.6060	0.603472 0.603491 0.6034	0.586761 0.586732 0.5867
c Γ (a.u.) Theory Present a b c	0.85505 3.384[-3] 3.405[-3] 4.040[-3] 3.3[-3]	0.786125 1.318[-3] 1.351[-3] 1.507[-3] 1.325[-3]	1.763[-3] 1.777[-3] 2.278[-3]	1.150[-4] 1.150[-4] 1.396[-4]	4.937[-4] 4.973[-4] 6.615[-4]	5.298[-5] 6.255[-5] 1.507[-5]	4.630[-7] 4.906[-7] 1.176[-3]	8.408[-4] 8.475[-4] 4.777[-6]	6.182[-5] 6.160[-5] 7.717[-5]	2.748[-4] 2.819[-4] 3.675[-4]

^aChung and Lin (1998).

^bBachau et al. (1991).

^cHo (1979).

Chung and Lin (1998), Ho (1979) and Bachau et al. (1991) using a pseudo potential Feshbach formalism. Our computed energy positions agree with the other data within the first 3 - 6 digits. Large differences in magnitude between the widths reported by Bachau et al. (1991) for the ${}^{3}P^{o}(6)$, ${}^{3}P^{o}(7)$ and ${}^{3}P^{o}(8)$ states and the other values are observed. The values of the widths we obtained for all the states agree best with the results of Chung and Lin (1998) and the available data of Ho (1979).

4. Conclusion

We have in this work investigated the triplet doubly excited ${}^{3}P^{o}$ states of the Li⁺ ion under the N = 2 and N = 3 hydrogenic thresholds by using a *B*-spline based spectral approach of configuration type combined with the complex rotation method. Our approach accurately locates the broad and narrow doubly excited ${}^{3}P^{o}$ resonance states in the energy spectrum of the ion. It also allows to extract a number of values of interest for each state which permits the straightforward classification of the states into distinct series.

In the future experimental investigations on the photoabsorption process in the Li⁺(1s2s ${}^{3}S^{e}$) ion by EUV laser pulses, the autoionizing ${}^{3}P^{o}$ states will manifest themselves as prominent resonant structures in the measured cross section. Accurate theoretical description of the doubly excited ${}^{3}P^{o}$ states is needed for a proper analysis of the photoabsorption process.

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