The $^1P^o$ Resonant States of Li$^+I$ Between the N=2 and 3 Thresholds

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Abstract. We studied the lowest five doubly excited $^1P^o$ resonant states of Li$^+$ between the N=2 and 3 thresholds by the saddle-point complex rotation method with B-spline functions. The doubly excited states are grouped in Rydberg series labeled by the quantum numbers K, T, A. Our results of energies and widths are in good agreement with other theoretical and experimental results.

1. Introduction

Doubly excited states of two-electron atom and ions have attracted physicists to study experimentally and theoretically. The doubly excited $^1P^o$ resonant states of Li$^+$ have been observed firstly by Dual Laser Plasma technique [1]. They were also studied experimentally by beam-foil techniques[2, 3], and using the ejected electron spectroscopy method[4]. After high-resolution monochromators at synchrotron-radiation facilities have been developed, high-resolution measurements on Li$^+$ ion were performed at the Advanced Light Source [5] and Super-ACO [6]. Diehl et al [6] have measured the doubly excited states of Li$^+$ below n=2 threshold. More recently, absolute cross-section measurements for the double photoexcitation of Li$^+$ ion have been performed by using the photo-ion merged-beam endstation. Accurate measurements on several members of the $^1P^o$ Li$^+$ (2(0,1)$^+$ n , 3(1,1)$^+$ n ) ion have been made [7, 8, 9]. On the theoretical side, some resonances have been studied by the complex rotation method [10], the diagonalization approximation[11], the pseudo-potential-Feshbach method [12], the saddle-point complex-rotation method[13],the variation method with combining Hylleraas and incomplete hydrogenic wave functions [15], the density-functional method [14], the R-matrix method [7, 8, 9], the saddle-point complex rotation method [16], and the SCUNC method [17].

2. Theory

In the present work, we studied doubly excited $^1P^o$ states of Li$^+$ between the n=2 and 3 thresholds by saddle-point complex rotation method with B-spline functions[18]. In a Configuration Interaction scheme [19, 20, 21, 22], we constructed the wave functions in terms of B splines of order k and total number N, defined between two end points, $r_{min}=$0 and $r_{max}=$ R, and built vacancies into the wave functions. With an exponential sequence, we have the trial wave function for a two-electron system

$$\Psi = A(1 - P(r_1))(1 - P(r_2)) \sum_{i,j,l_1,l_2} C_{i,j,l_1,l_2} \Phi_{i,j}(r_1,r_2) Y_{l_1,l_2}^{L,M} \chi(1,2)$$ (1)
with
\[ \Phi_{i,j}(\vec{r}_1, \vec{r}_2) = \frac{B_{i,k}(r_1) B_{j,k}(r_2)}{r_1 r_2}, \]

\[ Y_{LM}^{1,2} = \sum_{m_1, m_2} <l_1 l_2 m_1 m_2|LM > Y_{l_1,m_1}(\vec{r}_1) Y_{l_2,m_2}(\vec{r}_2), \]

and
\[ i \geq j - j m, \]

where \( L \) is the total angular momentum and the numbers \( i \) and \( j \) are positive integers, which are not larger than \( N \), and \( jm \) is a specific selected integer. \( A \) is the antisymmetrization operator, \( \chi(1, 2) \) is the spin wave function, and \( P(\vec{r}) \) is a projection operator. For the present, 1s, 2s and 2p orbitals are the vacancy orbitals.

\[ P(\vec{r}) = P_{1s}(\vec{r}) + P_{2s}(\vec{r}) + P_{2p}(\vec{r}) \]

\[ P_{nl}(\vec{r}) = |\phi_{nl} > < \phi_{nl}| \]

We assume \( \phi_{nl} \) to be nl hydrogenic orbital with effective nuclear charge, \( q \). The saddle-point variation is carried out by first minimizing the energy with respect to \( C_{i,j,l_1,l_2} \) and the set of B-spline basis functions, and then maximizing the energy with respect to the effective nuclear charge, \( q \), to obtain the saddle-point energy and wave function. After the saddle-point variation is carried out, we calculate the resonance energy and width by a complex-rotation method. The trial wave functions are composed of the saddle-point wave functions (eq.1) and the open-channel components. We choose the open-channel components to be:

\[ \Psi_{\text{open}} = A \sum_{i} \psi_i(\vec{r}_1) \sum_{k=1}^{KO} C_{kL} u_{kL}(\vec{r}_2) Y_{1,1}^{L,M} \chi(1, 2), \]

with
\[ u_{kL}(\vec{r}) = r_i e^{-\beta r_i}, \]

and
\[ Y_{1,1}^{L,M} = \sum_{m_1, m_2} <1LM|LM > Y_{l_1,m_1}(\vec{r}_1) Y_{l_2,m_2}(\vec{r}_2), \]

where \( \psi_i \) is the 1s, 2s and 2p radial wave function of hydrogen-like ions. The non-negative integer, KO, is chosen to be large enough to ensure the accuracy of the resonance energy and width in the calculation by the complex-rotation method. In the complex-rotation calculation, each radial coordinate \( r_i \) in \( u_{kL}(\vec{r}_i) \) of the open-channel components, \( \Psi_{\text{open}} \) takes the form \( r_i e^{i \theta} \).

3. Results

In the present, we studied the lowest five doubly excited \( ^1P_o \) resonant states of Li\(^{+}\) between the \( N=2 \) and 3 thresholds. The values of \( R \) for end points are chosen to be 400 a.u. so that the saddle-point energies of the lowest five doubly excited \( ^1P_o \) resonant states of Li\(^{+}\) between the \( N=2 \) and 3 thresholds are converged to within an uncertainty of \( 10^{-8} \) a.u. We included 8-15 partial waves in calculating \( ^1P_o \) states of Li\(^{+}\) for the saddle-point energies are converged to within an uncertainty of \( 10^{-7} \) a.u.. By examining convergence behaviors, it is believed that the accuracy of the present results is comparable with other theoretical results. We also calculated the expectation value of the angle between the two electrons, \( < \theta_{12} > \), the average values of \( r \) for the inner electron and outer electron, \( < r_< > \) and \( < r_> > \). The results are shown in Table.
Table 1. The expectation values of $\cos \theta_{12}$, $r_<$, $r_>$, $r$ and $r^2$.(in a.u.)

| n  | $\cos \theta_{12}$ | $r_<$ | $r_>$ | $r$ | $r^2$ | $\cos(\theta_{12})$ | $r_<$ | $r_>$ | $r$ | $r^2$ |
|----|------------------|------|------|-----|------|------------------|------|------|-----|------|
| 3  | -0.223           | 3.51 | 5.62 | 4.57| 24.1 | 0.262            | 3.49 | 5.94 | 4.72| 26.3 |
| 4  | -0.267           | 4.10 | 9.45 | 6.77| 59.6 | 3(1,1)$^+_n$     | 0.262| 3.49 | 5.94| 4.72 |
| 4  | -0.589           | 3.88 | 9.08 | 6.48| 52.5 | 3(0,0)$^-_n$     | 0.0064| 3.65 | 9.19| 6.42 |

Table 2. Non-relativistic energies and widths for doubly excited $^1P^o$ resonances of Li$^+$ between the n= 2 and 3 thresholds( in a.u.). A(-m) means A X $10^{-m}$. a: the present results, b: theory[8], and c: experiment[8].

| n  | E   | Width | E   | Width | E   | Width | E   | Width |
|----|-----|-------|-----|-------|-----|-------|-----|-------|
| a  | 3   | 0.828710|     | 9.81(-3) | 0.732843 | 2.46(-3) | 0.7328 | 2.5(-3) |
| [10]|     | 0.8297 |     | 1.0(-2) | 0.7320 | 2.5(-3) |
| [12]|     | 0.8288 |     | 1.1(-2) | 0.7320 | 2.5(-3) |
| [13]|     | 0.828755 |     | 1.040(-2) | 0.732690 | 2.484(-3) |
| [15]|     | 0.8359 |     |
| b  |     | 0.8275 |     | 1.036(-2) | 0.7325 | 1.036(-2) |
| c  |     | 0.8241±0.0026 |     |     |
| a  | 4   | 0.6871264 | 4.58(-5) | 6.59366 | 5.26(-3) | 0.655662 | 6.91(-5) | 0.655667 | 5.59(-3) |
| [12]|     | 0.6872 | 6.6(-5) | 0.6598 | 6.6(-3) | 0.6555 | 8.8(-5) |
| [13]|     | 0.6871259 | 4.563(-5) | 0.659379 | 5.278(-3) | 0.655667 | 6.957(-5) |
| b  |     | 0.6581 | 5.207(-3) |
| c  |     | 0.6566±0.002 |

1. From $< \cos \theta_{12} >$, $< r_<$ > and with Lin’s results[23, 24], The doubly excited states are grouped in Rydberg series labeled by the quantum numbers K, T, A. The average value of K $\approx < r_<= \cos \theta_{12} >$. For the lowest five $^1P^o$ resonant states, there are two members in the $3(1,1)_n^+$ series, one member in the $3(2,0)_n^-$, $3(-1,1)_n^+$ and $3(0,0)_n^-$ series. The numbers, n in $3(K,T)_n^A$ are assigned according to the effective principal quantum numbers $n^*$, which are calculated from the equation $E_n=(-Z-1)^2/2n^*^2$. $E_n$ is measured from the 3l states of Li$^{+2}$. The resonant energies and widths for Li$^+$ are shown and compared with other theoretical[8, 10, 12, 13, 15] and experimental[8] results in Table 2. The agreement amongst the various theoretical and experimental results is not as good as that for the $^1P^o$ states of Li$^+$. Our results for energies agree with other theoretical results[13] within first 4-5 digits, with the theoretical results of pseudo-potential-Feshbach Method[12] within first 3-4 digits, but with the experimental and theoretical results[8] within first 2 digits. The agreement amongst the various theoretical results is better for $3(2,0)_n^-$ and $3(0,0)_n^-$ series than that for $3(1,1)_n^+$ and $3(-1,1)_n^+$ series. It may be due to the stronger electron-electron correlation in the $3(1,1)_n^+$ and $3(-1,1)_n^+$ Li$^+$. For the widths, our results agree well with other theoretical results[10, 12, 13, 8] except the theoretical results[12] for $3(2,0)_4^+$, $3(1,1)_4^+$ and $3(0,0)_4^-$ states. Scully et al[8] did not reported the experimental results of widths for these resonant states. The agreement amongst the various theoretical and experimental results is not as good as that for the $^1P^o$ states of Li$^+$. 


below n=2 threshold[16]. Therefore, we hope our present work will stimulate further theoretical and experimental results to understand these stats more.

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[1] Carroll P K and Kennedy E T 1977 Phys. Rev. Lett. 38 1068
[2] Bruch R, Paul G, Andra J and Lipsky L 1975 Phys. Rev. A 12 1808
[3] Ziem P, Bruch R and Stolterfoht N 1975 J. Phys. B 8 L480
[4] Rodbro M, Bruch R and Bisgaard P 1979 J. Phys. B 12 2413
[5] Diehl S et al 1997 J. Phys. B 30 L595
[6] Diehl S et al 1999 J. Phys. B 32 4193
[7] Scully S W J et al 2005 J. Phys. B 38 1967
[8] Scully S W J et al 2006 J. Phys. B 39 3957
[9] Scully S W J et al 2007 J. Phys. Conf. Ser. 58 387
[10] Ho Y K 1979 J. Phys. B 12 387
[11] Waghe A 1987 Z. Phys. D 6 337
[12] Tacchini H et al 1991 At. Data Nucl. Data Tables 48 167
[13] Chung K T 1998 At. Data Nucl. Data Tables 69 101
[14] Roy A K, Singh R and Deb B M 1997 J. Phys. B 30 4763
[15] Biaye M et al 2005 Phys. Scr. 72 373
[16] Chen M-K 2007 J. Phys. Conf. Ser. 58 125
[17] Sakho I et al 2008 Eur. Phys. J. D 47 37
[18] deBoor C 1978 A Practical Guide to Splines (New York: Springer)
[19] Chen M-K 2005 Chinese J. of Phys. 43 329
[20] Chen M-K 2003 Eur. Phys. J. D 21 13
[21] Chen M-K 1999 Phys. Rev. A 60 2565
[22] Chen M-K 1997 Phys. Rev. A 56 4537
[23] Lin C-D 1982 Phys. Rev. A 25 1535
[24] Lin C-D 1984 Phys. Rev. A 29 1019