An $R$-matrix with pseudo-state approach to the single photon double ionization and excitation of the He-like Li$^+$ ion

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Abstract
The success of the $R$-matrix with pseudo-state (RMPS) method to model single photoionization processes, benchmarked against dedicated synchrotron light source measurements, is exploited and extended to investigate, single photon double ionization cross-sections for the He-like, Li$^+$ ion. We investigate these processes from both the ground state and the excited 1s2s 1$^S$ and 3$^S$ metastable levels of this He-like system. Comparisons of the results from the RMPS method are made with other state-of-the-art theoretical approaches such as time-dependent close-coupling (TDCC), B-splines and the convergent close-coupling (CCC). Excellent agreement with various other theoretical approaches are achieved but differences occur which are highlighted and discussed. For the ground state the peak of the cross-section is $\sim$2 kilo-barns (Kb), that for the 1s2s 1$^S$ state is $\sim$6 and $\sim$1 Kb for the corresponding 1s2s 3$^S$ state. All the cross-sections for single photon double ionization are extremely small, being in the region of 2–10 Kb, or less, rendering their experimental determination extremely challenging.

(Some figures may appear in colour only in the online journal)

1. Introduction

Photoionization is one of the most important processes within the interstellar medium (ISM). It dominates the heating of the ISM and produces the majority of the ionized medium. Photoionization is known to be the excitation mechanism in planetary nebulae, H II regions, starburst galaxies and Seyfert narrow line regions. Thus modelling photoionization is an important theoretical study as it not only can provide a physical insight into these emission line regions but can also give us a better understanding of the ISM as a whole. The photoionization process is one of the important radiative feedback processes in astrophysics [1, 2]. The increase in pressure caused by it can trigger strong dynamic effects: photoionization hydrodynamics. The challenge in combining hydrodynamics with photoionization lies in the difference in time scales between the two processes.

The situation for single photon double photoionization of ions of the He-like isoelectronic sequence are of importance in plasma physics and astrophysics, is far less advanced than that of single photoionization. This is due to major difficulties in attaining target densities sufficient to carry out experiments. The majority of our knowledge on this topic has been provided mainly by theoretical studies. The present study on the single photon double ionization of Li$^+$ ions, a proto-typical two-electron system, provides an essential benchmark for future photoionization studies on more astrophysically abundant highly ionized He-like species such as C, N, O and Ne which are of great importance, in determining the mass of missing baryons in the x-ray forest of the warm–hot intergalactic medium (WHIM) [3, 4].

We note that x-ray spectra obtained by Chandra, from sources such as Capella, Procyon, and HR 1099, are used as standards to benchmark plasma spectral modelling codes.
He-like ions of O, Ne, Mg, Si, S, and Ar were first discovered in the x-ray spectra of the Seyfert 1 galaxy NGC 3783, obtained with the High Energy Transmission Grating Spectrometer on the Chandra X-Ray Observatory [5]. Strong He-like, carbon [C VI] lines have been detected in the Chandra HRC-S/LETG x-ray grating spectrum of the blazar H 2356–309 [4] at 44.8 Å. He-like, nitrogen [N VI] lines have also been observed with Chandra and XMM-Newton in the x-ray spectra of Capella and Procyon [6, 7], the M dwarf binary YY Gem [8], and the recorded outburst of the recurrent nova RS Oph [9], in the wavelength region 28.7–29.6 Å (420 eV) that is attributed to 1s → 2s transitions. XMM-Newton observations of the fast classical nova V2941 Cyg [10] have also indicated the N VI, Kα and Kβ lines are present at about 28.78 and 24.90 Å. The He-like series lines of N VI and O VII are detected up to 1s → 5p, and for O VII, the recombination/ionization continuum at 16.77 Å (739.3 eV) is present between 16.6–16.8 Å. The intra-cluster medium (ICM) is the few 10^6–10^8 K, x-ray emitting plasma which fills the potential wells of objects ranging in scale from galaxy clusters down to massive elliptical galaxies. He-like oxygen [O VIII] has been revealed in stacked high spectral resolution, XMM-Newton Reflection Grating Spectrometer (RGS) spectra from galaxy clusters, groups of galaxies and elliptical galaxies [11]. Therefore, He-like C, N, O, Ne, and Fe are all of interest. The n = 2 to n = 1 x-ray lines are all used as diagnostics of photoionized and collisionally ionized gas. Typically, for He-like systems, the line ratios (R, L, and G) are studied and for double photoionization, high energy photons are required for applications in active galactic nuclei (AGNs) where all elements between, He, Li, Be, B, C, . . . , Zn can be treated [12, 13].

As one of the most basic and fundamental three-body Coulomb problems, single photon double ionization of the two-electron (He-like) system requires an accurate description of the correlated motion of two electrons in the long-range Coulomb field of the residual stripped ion. As this process comprises the interaction of just three charged particles, it can only be properly handled numerically. With the advancement of computational power over the past decade or more, this has opened the doorway to investigate large scale numerical studies of this fundamental three-bodied problem using the R-matrix with pseudo-states (RMPS) method [14–18] allowing detailed convergence studies to be made. We note that the RMPS was first introduced into the literature, in the late 1960s, by Burke, Gallagher and Geltman [19] in studying electron scattering from atomic hydrogen with great success reproducing the earlier highly accurate work of Schwartz [20].

Single photon double ionization of the Li^+ ion has been studied theoretically by Kornberg and Miraglia [21] using two and three screened Coulomb wavefunctions and more recently using the eigenchannel R-matrix method by Meyer [22]. Wehltz and co-workers [23] have measured triple photoionization of lithium and related their experimental triple-to-single photoionization cross-sections ratio to the theoretical double-to-single ratio of the Li^+ ion reported by Kornberg and Miraglia [21]. A two-stage mechanism of triple photoionization was proposed. In the first stage double photoionization of the valence 1s^2 shell of the Li atom takes place followed by the shakeoff of the remaining 2s electron into the continuum. It is assumed that the double photoionization of the 1s^2 shell in the Li atom and the Li^+ ion are quite similar and the resulting triple-to-single photoionization cross-section ratio for the Li atom can be calculated as the double-to-single ratio of the Li^+ ion multiplied by the probability of the shakeoff 0.001 74 according to Wehltz et al [24]. This serves as a useful check on various theoretical models.

Various theoretical methods have been used to explore and study single photon double ionization of He-like systems, these are the two screened Coulomb method [25–27], the time-dependent close-coupling (TDCC) approach [28, 29, 18, 30], convergent close-coupling (CCC) [31–34], many-bodied perturbation (MBPT) [35, 36], B-spline with R-matrix, exterior complex scaling B-spline [37], intermediate energy R-matrix (IERM) method [38], and presently now using the RMPS method [14–18]. It has been shown by Forrey and co-workers [39] that in the limit of high photon energies double ionization of the excited singlet metastable state of Li^+ ions has a larger cross-section ratio than double ionization of the ground state [40]. McCurdy and co-workers [41] have used a finite-element discrete-variable representation (DVR) and exterior complex scaling to study excited state single photon double ionization of Li and Be with excellent agreement obtained with results from the RMPS approach. Forre [42] has shown (for single photon double ionization of helium) a heuristic formula for the double ionization of Li^+ compared with detailed ab initio calculations suggests the methodology is valid for the entire helium sequence [42].

We note in passing for He-like systems, Scott and co-workers [38] recently have shown that the IERM results for single photon, single and double ionization and detachment are in excellent agreement with those obtained from experiment and the RMPS method for He [43, 44] and H^- [2, 1] giving enhanced confidence in the existing theoretical data on H^- for astrophysical applications in the early universe [45]. Projected experimental measurements [46] on this He-like ion is one of the major motivations for undertaking the present theoretical study.

The single photon double ionization processes investigated here on the 1s^2 S ground state of the Li^+ ion are

\[ hv + Li^+(1s^2 1S) \rightarrow Li^3+ + e^- + e^- . \]

We extend our investigation also to the excited n = 2 metastable levels

\[ hv + Li^+(1s2s1S) \rightarrow Li^3+ + e^- + e^-, \]

as the Li^+ (1s2s 1S) metastable states are of prime interest. In both cases we have a fully stripped Li nucleus with the two out going electrons in the continuum whereas in the case of the single photoionization process the resulting H-like Li^2+ (n^t) ion may be left in its ground or excited state with one electron in the continuum. Figure 1 shows a schematic diagram of the Li^+ and Li^2+ spectrum adapted from the work of Kleiman and co-workers [28]. In the previous investigations on this system we note that for the case of single photon single ionization [47, 48]
calculations were carried out using the RMPS method [14–18]. In that work, the RMPS results were shown to be in excellent agreement with the high resolution measurements made at the Advanced Light Source synchrotron radiation facility in Berkeley, California. Here we concentrate our efforts on photo-excitation and double ionization processes for this He-like system above the ionization threshold from the ground and metastable 1s2s1S states. We note preliminary investigations for the case of the ground state have been carried out by McLaughlin and Ballance [49] using this same RMPS method. Here we use this same RMPS method and apply it to the case of single photon double ionization for both the ground state and the excited metastable states of the He-like Li ion and to photo-excitation, comparing and contrasting our results with previous theoretical approaches and investigate convergence issues.

We note that the eigenchannel R-matrix technique and the CCC method give similar results for electron impact ionization of H and He⁺ [50]. Owing to the success of the CCC approach a comparison of this method with the present R-matrix calculations permits a more conclusive evaluation of the reliability of the R-matrix method. Therefore we expect to have similar agreement between the RMPS and the CCC methods for the case of photon impact in the above half collision process with this He-like complex.

The layout of this paper is as follows. Section 2 presents a brief outline of the theoretical work. Section 3 details the results obtained. Section 4 presents a discussion and a comparison of the results obtained between various theoretical methods as limited experimental measurements are available. Finally in section 5 conclusions are drawn from the present investigation.

2. Theory

Photoionization cross-section calculations were performed in LS-coupling on the two-electron He-like Li⁺ ion using the R-matrix methodology [51–54]. We use an efficient parallel version of the R-matrix codes. Details of the atomic structure employed in the present calculations have been published before [47, 48] and only a brief summary will be presented here. The ionization cross-sections are determined by summing over all excitations above the ionization threshold, including all single-electron excitations to the pseudo-states as well as doubly excited states. Single photon double ionization from the ground state has been reported on previously using the same method [49]. In the present work we use 65 and 80 levels respectively of the residual Li²⁺ ion states using the RMPS method introduced by Burke, Bartschat and co-workers [19, 14, 55–57] and further extended by Badnell and co-workers [15, 58, 16] for the close-coupling calculations. The basis sets consist of n = 4 spectroscopic orbitals and nℓ = 5̂ℓ ... 18̂ℓ (ℓ = 0, 1, 2, 3, and 4, i.e. s, p, d, f and g angular momentum) correlation/pseudo orbitals of Li²⁺ to represent the target wavefunctions. Basis set RMPS1 has n = 4 spectroscopic orbitals and nℓ = 5̂ℓ ... 18̂ℓ, correlation/pseudo orbitals, whereas for basis set RMPS2, we have expanded the pseudo-state representation of the continuum as, nℓ = 5̂ℓ ... 18̂ℓ, correlation/pseudo orbitals along with retaining the n = 4 spectroscopic orbitals in the basis. All of these hydrogenic orbitals were determined using the AUTOSTRUCTURE program [59, 60] for the Li²⁺ ion.

For photoionization of this He-like system, 120 continuum orbitals were used and double-electron promotions from specific base configuration sets described the (Li²⁺ + e⁻) scattering wavefunction in the RMPS calculations. In our previous work on single photon, single electron ionization [47, 48] an energy mesh size of 13.6 μeV was required in order to resolve all the fine resonances in the PI cross-sections for resonances lying below the single ionization threshold. Here since we are interested in processes above the ionization threshold a broader mesh size was used of 0.02 Rydbergs (272 meV). For the excitation and ionization processes studied here we use models differing only in the size of the basis included in the close-coupling calculations, as a means of checking the convergence of our results. These basis sets we designate as follows: RMPS1, in which we restrict the pseudo-state basis to nℓ = 15̂ℓ and RMPS2, where we extend the pseudo-state basis to nℓ = 18̂ℓ, thus allowing for checks to be made on convergence of the method. For the case of a two-electron system and the single photon double detachment process in H⁻, we note that a smaller pseudo-state basis set (n = 1–4 physical, 5–14 pseudo-states, with s, p, d, f and g angular momentum) within the RMPS approach reproduced cross-section results obtained using an extended pseudo-state basis (n = 1–4 physical, 5–38 pseudo-states, with s, p, d and f angular momentum) within the IERM method [38].

3. Results

All of the photoionization cross-sections were determined in LS-coupling with an efficient parallel version [61] of the R-matrix programs [52, 51, 62]. Length and velocity forms of the cross-sections were seen to be in excellent agreement and virtually indistinguishable. We have therefore chosen to plot
only the length form. Figure 2 shows a sample of the RMPS (using basis set RMPS1 as defined previously) results for the ground state compared to those from the TDCC approach [28], the close-coupling to the continuum method (CCC) [31–34] and the B-spline method [37]. A best fit (sixth-order polynomial fit) to the raw results was used. Consistent with other complexes studied such as Li, Be, Mg, and Ne, for single photon double ionization [63–65] using the RMPS method, we find that the present cross-section results are larger than those obtained from the TDCC approach. In figure 2 it can be seen that the present RMPS results are in closer agreement with the CCC approach and the B-splines methods at all energies above 250 eV and merge to the CCC and B-splines results at photon impact energies above about 500 eV.

To illustrate the convergence of the model employed here, we carried out double ionization calculations varying the size of the basis set used in the close-coupling approach for the single photon double ionization from the Li$^+$ (1s2s $^1$S) metastable state. In figures 3(a) and (b), cross-section results are presented from calculations using different sized basis sets, which are designated respectively as RMPS1 and RMPS2. We found that results from larger basis sets gave similar results to those from the smaller basis. Details of the two basis sets have been outlined above. As clearly seen from figures 3(a) and (b), the RMPS results for the single photon double ionization from the Li$^+$ (1s2s $^1$S) metastable state using the two different basis (RMPS1 and RMPS2 respectively) give comparable results. In figure 3(a) there appears to be more scatter in the raw results from the larger basis (RMPS2) resulting from pseudo resonances. To guide the eye we present a best fit (tenth-order polynomial fit) to the raw results from the RMPS close-coupling calculations in figure 3(b). For the double ionization process we conclude from our results presented in figures 3(a) and (b) (for all energies considered) that the cross-sections obtained from the larger (80 level RMPS2) calculation are adequately represented by those from the smaller (65 level RMPS1) model. Subsequently in the remaining figures we present only the results of our work from the 65-state model (RMPS1).

4. Discussion

In the case of electron impact ionization of the metastable states of Li$^+$ (1s2s $^3$S) [66] the cross-section from the singlet state is larger than those for the corresponding triplet metastable state. From the results presented in figure 4, the situation is similar for the case of single photon impact double ionization as the singlet metastable state cross-section is about a factor of 6 larger at the peak (in cross-section) than that from the corresponding triplet metastable state. We note that cross-sections obtained from both the RMPS and TDCC methods tend to the same value at impact energies of about 500 eV and beyond, for each of the individual 1s2s $^1$S metastable states but to different limits. Forrey and co-workers [39] have determined the different asymptotic limits of the ratio $R$ (i.e. double to single photoionization cross-sections) for the He-like ground state and the metastable (1s2s $^1$S) states. They have shown that the ratio $R$ (i.e. double to single photoionization, expressed as a percentage) behaves for large $Z$ as,

$$R_{Z→∞} \sim \frac{9}{Z^2} - \frac{3}{Z^3}$$

for the 1s$^2$ $^1$S ground states,

$$R_{Z→∞} \sim \frac{32}{Z^2} - \frac{66}{Z^3}$$

for the 1s2s $^1$S metastable states, and

$$R_{Z→∞} \sim \frac{6}{Z^2} - \frac{9}{Z^3}$$

for the 1s21 $^3$S states.
Single Photon Double Ionization of $\text{Li}^+(1s2s\,^{1,3}S)$

$$\text{Li}^2+(n): \text{Photoexcitation from } \text{Li}^+(1s2s\,^1S)$$

**Figure 4.** Theoretical cross-sections (Kb) for the single photon double ionization from the $\text{Li}^+(1s2s\,^{1,3}S)$ metastable states for the photon energy range 100 to 500 eV. RMPS results (solid line) along with the TDCC (dashed line) method are illustrated and included for comparison purposes.

**Figure 5.** Theoretical cross-sections (Kb) for the single photon impact on the $\text{Li}^+(1s2s\,^1S)$ ground state leaving the residual $\text{Li}^2+$ ion in an excited state for the photon energy range 100 to 600 eV. The TDCC [28] and CCC [31] results are included for comparison purposes.

**Figure 6.** Theoretical cross-sections (Kb) for the single photon impact on the $\text{Li}^+(1s2s\,^3S)$ metastable state leaving the residual $\text{Li}^2+$ ion in an excited state for the photon energy range 100 to 600 eV. The TDCC results [28] are included for comparison purposes.

**Figure 7.** Theoretical cross-sections (Kb) for the single photon impact on the $\text{Li}^+(1s2s\,^3S)$ metastable state leaving the residual $\text{Li}^2+$ ion in an excited state for the photon energy range 100 to 600 eV. The TDCC results [28] are included for comparison purposes.

for the $1s2s\,^3S$ metastable states. Detailed calculations by these authors, for $R$, using explicitly correlated Frankowski–Perkeris-type functions, gave a value of 0.856 for the ground state, 1.204 for the $1s2s\,^1S$ metastable state and 0.304 for the corresponding $1s2s\,^3S$ state. The present RMPS results are compatible with these results. Furthermore, for He-like systems, table III of Forrey and co-workers [39] clearly showed by explicit calculation that the values of $R$ for the $1s2s\,^1S$ states exceed those of the corresponding $1s2\,^1S$ ground states for $Z \geq 3$.

Figure 5 illustrates the present RMPS results for photoexcitation into the $n = 1–4$ excited levels of the residual $\text{Li}^2+$ ion from the initial $\text{Li}^+(1s^2\,^1S)$ ground state. Whereas, in figures 6 and 7 we present the RMPS results for photoexcitation into the $n = 1–4$ excited levels of the residual $\text{Li}^2+$ ion from the $\text{Li}^+(1s2s\,^1S)$ and $\text{Li}^+(1s2s\,^3S)$ metastable states using the RMPS method. Figures 5–7 compare the present RMPS cross-section results with similar ones obtained from both the CCC and TDCC methods of photoexcitation of the residual ion for the ground and metastable states. For the ground state, as can be seen from the cross-section results presented in Figure 5, excitation into the ground residual level of $\text{Li}^2+(1s\,^1S)$ ion dominates over all others. Excellent agreement between all three vastly different theoretical approaches is obtained. Such comparisons provide confidence in our current theoretical results. In the case of
the Li$^+$ (1s2s $^1$S) metastable states shown respectively in figures 5 and 6, it is clearly seen that excitation into the residual ion $n = 2$ levels predominate over all other levels. For these metastable states only the TDCC results [28] are available for comparison purposes and only for excitation into the $n = 1–3$ levels of the residual Li$^+$ ion. From the limited data available to compare with, it is seen that the present RMPS results are in excellent accord with previous results obtained using the TDCC method [28, 29, 18, 30], providing additional confidence in our data for applications.

5. Conclusion

State-of-the-art theoretical methods were used to study the single photon double ionization of Li$^+$ ions within the $R$-matrix with pseudo-states (RMPS) approach. Due to the lack of experimental data on these processes we compare the results of our study with those from previous theoretical studies using a variety of different methods in order to gauge the accuracy and quality of our work. Given the validation with experiment of our previous RMPS cross-section results on the ground state [47, 48], photo-absorption of Li$^+$ ions for this He-like system, and the close agreement with the convergent close-coupling (CCC), the time-dependent close-coupling (TDCC), and B-splines methods, for the ground and excited states, we expect that the present results for single photon double ionization to be of comparable quality to those for single photoionization. We hope that this current work might provide a stimulus for future experimental work on this complex.

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