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Strong relativistic effects on dielectronic recombination of metastable Li^+ ions

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Dielectronic recombination (DR) of Li^+ ions in the metastable $1s2s\ ^3S$ state has been calculated by using the close-coupling *R*-matrix method and perturbation theory, and compared with the high-resolution experiment. Good agreement has been shown. The occurrence of the experimental double peak structure at energies of 0.1–0.2 eV can be surprisingly attributed to relativistic effects. A very strong radiation damping effect on the resonances in the second peak position was discovered. Furthermore, in the $1s2p(^1P)nl$ $(n=5-7)$ resonance energy region, our calculations have displayed that the contribution to DR from high-angular-momentum $(l>3)$ configurations is very small. This point is markedly different from the result of Saghiri *et al.* [Phys. Rev. A **60**, R3350 (1999)].

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Dielectronic recombination (DR) between electrons and ions can be referred to as an indirect two-step process. First one of bound electrons of the ion is excited by a free electron and correspondingly the free electron is captured so as to form so-called doubly excited states due to its energy loss. In the second step, these doubly excited states decay into nonautoionizing states by spontaneous radiative transitions. DR is not only of fundamental physical interest but also of practical importance. The precise description of this process is crucial to understanding electron correlation, relativistic and QED effects, radiation damping, and astrophysical and laboratory plasmas [1–4]. So far a great deal of experimental and theoretical efforts have been made to study dielectronic recombination (see, e.g., Ref. [5]). Many experimental observations have been satisfactorily reproduced by theoretical calculations; however, some measurements have not yet been deciphered [6–9]. This shows that further profound research on DR is required. Recently DR for the lightest He-like ion, Li^+, in both the ground and metastable states, has been observed at the Heidelberg ion-storage ring and electron cooler facility [9]. Meanwhile a close-coupling *R*-matrix calculation has been carried out to compare with the measurement. Their computational scheme, called the radiative optical potential method, has turned out to be successful in calculations of photorecombination [3]. However, the comparison showed that an experimental double peak structure of DR for the metastable Li^+ ions at the 0.1–0.2 eV energy region was not reproduced by the theory, and in the $1s2p(^1P)nl$ $(n=5-7)$ resonance energy region the theoretical results were up to a factor of 2 higher than the observation if involving the contribution from the $l\geqslant 3$ configurations. This prompted us to perform an investigation on the DR of Li^+. The theoretical method based on the rigorous continuum-bound transition theory of Davies and Seaton [10] and the perturbation theory, developed and applied to calculations of photorecombination for C^{4+} [11], has been employed in the present calculations. We found that the occurrence of the double peak at energies of 0.1–0.2 eV can surprisingly be attributed to relativistic effects, and radiation damping has a strong effect on the resonances in the second peak position. At first glance, it seems to be a little *abnormal*. In general, it is well known that the relativistic effect can be undoubtedly omitted for extremely low-*Z* atoms or ions, and it becomes significant only with increase of *Z* because of the higher velocity of electrons in medium- and high-*Z* atoms. Later we will give our calculated results and explain the reasons. Moreover, the identification of some states in Ref. [9] is not in agreement with our calculations, and we did not find any important contribution to DR of the metastable Li^+ ion from high-angular-momentum states in the $1s2p(^1P)nl$ $(n=5-7)$ resonance energy region (about 2.5–2.9 eV). This point markedly differs from the result of Saghiri *et al.* [9].

The theoretical method employed in this work has been detailed in Ref. [11]. Here we give only calculations and results. We first solved $Li^+ + e$ electron-ion systems in the framework of the close-coupling *R*-matrix approach (see Ref. [11] and references therein for details), neglecting interaction with the radiation field. Then the wave functions obtained were employed to evaluate the reduced dipole matrix and the *S* matrix. Finally the undamped and damped cross sections for photorecombination of Li^+ ions in the metastable $1s2s\ ^3S$ state were obtained. Our calculations were carried out in the *LS* coupling scheme, and the 11 lowest target states $1\ ^1S$, $2\ ^3S$, $2\ ^1S$, $2\ ^3P$, $2\ ^1P$, $3\ ^3S$, $3\ ^1S$, $3\ ^3P$, $3\ ^3D$, $3\ ^1D$, $3\ ^1P$ were included. The $2s$, $2p$, $3s$, $3p$, and $3d$ radial orbits were optimized on the $2\ ^{3,1}S$, $2\ ^{3,1}P$, $3\ ^{3,1}S$, $3\ ^{3,1}P$, and $3\ ^{3,1}D$ states, respectively. In Fig. 1, the partial cross sections for several symmetries $^2S^e$, $^2P^o$, $^2D^e$, and $^2F^o$ are plotted as a function of electron energy at the energy range 0–1.1 eV. The resonances with the $^2P^o$ and $^2D^e$ symmetries have been identified by comparison with the available experimental and theoretical energy levels. These data are listed in Table I together with earlier work [12–18]. All the energy levels were transferred to values relative to the $1s2s\ ^3S$ level. In the transfer, the exact energies of the $1s^22s\ ^2S$, and $1s2s\ ^3S$ states were used [14,19]. From Fig. 1 and Table I one can see that the experimental peak at the energy range 0.1–0.2 eV should be assigned to the state $1s2s(^1S)3d\ ^2D^e$, rather than $1s2p(^3P)3p\ ^2D^e$ identified by Saghiri *et al.* [9], and the peak at energy $\sim$0.43 eV should be the state $1s2p(^3P)3p\ ^2D^e$, rather than $1s2p(^3P)3p\ ^2S^e$ in Ref. [9], since Fig. 1 indicates that no resonance with

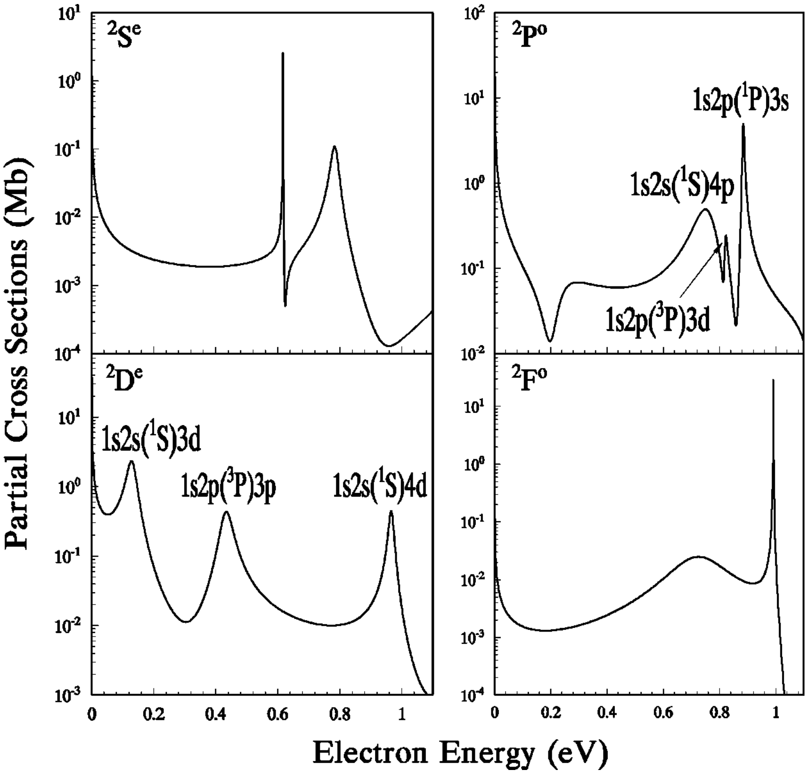

FIG. 1. Partial DR cross sections of Li^+ ions in the metastable $1s2s\ ^3S$ state in the 0–1.1 eV energy region.

symmetry $^2S^e$ appears in the vicinity of 0.4 eV. Moreover, Saghiri *et al.* [9] attributed the observed peak at about 0.72 eV to the contribution from the resonances $1s2p(^3P)3d\ ^2D^o$ and $1s2p(^3P)3s\ ^2S^o$. Obviously this is unreasonable, because there exists no continuum state $1s2s(^3S)\varepsilon l\ ^2L$ both of odd parity and of $L=0$ or 2 to interact with these two states in the LS coupling scheme that was adopted in their calculations, and thus it is impossible to engender dielectronic capture and autoionization. Only when relativistic effects are taken into account can dielectronic recombination happen. Cederquist and Mannervik [20] observed the position of the $1s2p(^3P)3d\ ^2D^o$ resonance to be 0.578 eV. We attempted to calculate the Auger rate Γ_a and the radiative rate Γ_r for the $1s2p(^3P)3d\ ^2D^o_{3/2,5/2}$ states by using the perturbation theory in the relativistic Breit-Pauli approximation (see Ref. [11] for details). We found that although the Γ_a is $\sim 3\times10^9$/s, the Γ_r is smaller by more than one order of magnitude. The corresponding DR cross sections displayed a negligible contribution from these two states.

Based on the measurements and evaluations, which are listed in Table I, by several experimental and theoretical groups, there is a resonance $1s2p(^3P)3p\ ^2P^e$ (exactly $^2P^e_{1/2,3/2}$) in the vicinity of about 0.16 eV. It probably contributes to the second peak of the double peak in the 0.1–0.2 energy region observed by Saghiri *et al.* [9]. In the LS coupling scheme, there is no such resonance. Only when the relativistic interaction is considered can this resonance emerge, as analyzed in the above paragraph. In general, as made in Ref. [9], it is thought that relativistic effects can

TABLE I. Energy levels of resonances $1s2lnl'$ relative to the $1s2s\ ^3S$ state in LiI in units of eV.

	Experiment		Theory			
State	Ref. [12]	Ref. [13]	This work	Refs. [14–16] [b]	Ref. [17]	Ref. [18]
$1s2s(^1S)4p\ ^2P^o$			0.748	0.728	0.733	
$1s2p(^3P)3d\ ^2P^o$		0.825 [a]	0.822	0.833	0.843	
$1s2p(^1P)3s\ ^2P^o$		0.870	0.884	0.880	0.882	
$1s2p(^3P)3p\ ^2P^e$	0.167			0.158		0.176
				0.173		
$1s2s(^1S)3d\ ^2D^e$	0.126		0.128	0.164		0.131
$1s2p(^3P)3p\ ^2D^e$	0.415		0.433	0.505		0.485
$1s2s(^1S)4d\ ^2D^e$	0.947		0.965	0.993		0.974

[a]A different identification from the experiment.
[b]The energy levels of $^2P^o$ are taken from Ref. [14]; the relativistic (above) and nonrelativistic (below) ones of $^2P^e$ from [15]; and the nonrelativistic ones of $^2D^e$ from [16].

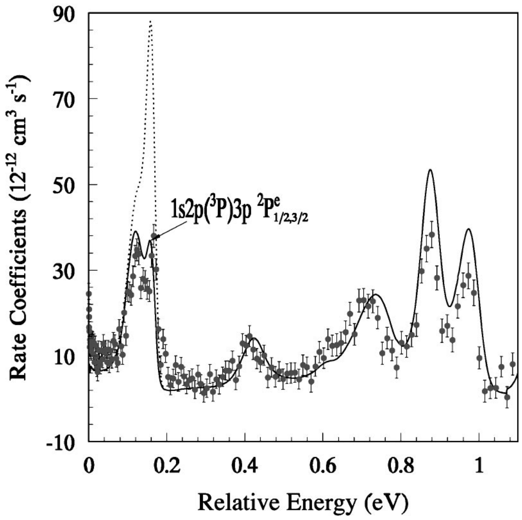

FIG. 2. The theoretical DR rate coefficients (solid line) of Li^+ ions in the metastable $1s2s\ ^3S$ state, calculated in the close-coupling *R*-matrix method and perturbation theory, along with the experimental measurements (dots with error bars).

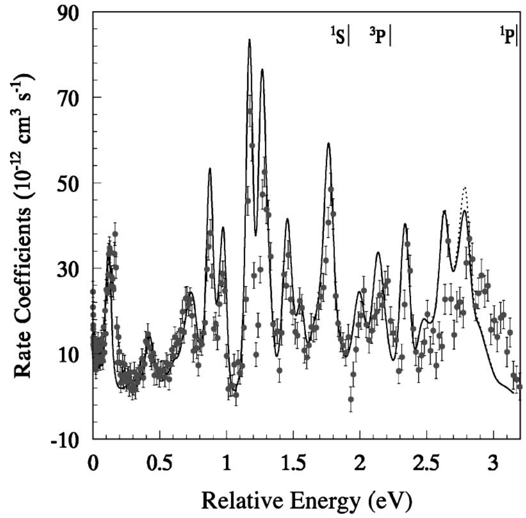

FIG. 3. Comparison between the *R*-matrix *LS* coupling DR rate coefficients of Li^+ ions in the metastable $1s2s\ ^3S$ state and the experimental measurements (dots with error bars). The solid and dotted lines denote the contribution from all states of configurations $1s2p(^1P)nl$ (all l), and that only from the states with $l=0-3$, respectively.

undoubtedly be omitted for very low-*Z* ions. We have found, however, that for DR of Li^+ ions in the $1s2s\ ^3S$ state, this is not the case. By employing the developed perturbative theoretical method [11], we calculated DR through this resonance in the framework of the semirelativity. The Auger and radiative widths evaluated are 1.97×10^{-3} meV and 2.86×10^{-3} meV, respectively, for the state $1s2p(^3P)3p\ ^2P^e_{1/2}$; and 1.31×10^{-3} meV and 2.55×10^{-3} meV for $1s2p(^3P)3p\ ^2P^e_{3/2}$. Obviously the widths of these two resonances are much smaller than the experimental electron-energy distribution described by the electron temperatures $(kT_{\parallel},kT_{\perp})=(0.2$ meV, 18 meV). Therefore we can use Eq. (9) of Ref. [21] to evaluate the rate coefficients. The convoluted cross sections in the *R*-matrix *LS* coupling scheme and the perturbative results from the $1s2p(^3P)3p\ ^2P^e_{1/2,3/2}$ were added together and given in Fig. 2, where the solid line represents our theoretical calculations and the dots with error bars are the experimental measurements of Saghiri *et al.* [9]. The good agreement with experiment has been exhibited. The reason why these two resonances of the extremely small Auger widths produce results comparable with the resonances of large Auger widths can be readily understood from $\hat{\sigma}_d\propto\Gamma_a\Gamma_r/(\Gamma_a+\Gamma_r)$ (also see Gorczyca and Badnell's analysis [3]). Based on the expression, one may see that the rate coefficient $\langle v\sigma\rangle$ is determined by the smaller of Γ_a and Γ_r when $\Gamma_r\gg\Gamma_a$ or vice versa. Our perturbative calculations indicated that the radiative widths of most of the resonances in Fig. 1 have the same orders of magnitude, $\sim10^9$/s, as the states $1s2p(^3P)3p\ ^2P^e_{1/2,3/2}$. That means that although the Auger widths of the $1s2p(^3P)3p\ ^2P^e_{1/2,3/2}$ resonances are four orders of magnitude smaller than that of the $1s2s(^1S)3d\ ^2D^e$, they still can produce comparable results, as shown in the 0.1–0.2 energy region in Fig. 2. From the above analysis, we can notice that whether a resonance is significant depends not only on Γ_r and Γ_a of the resonance themselves but also on the Γ_r and Γ_a of the dominant resonances. So in the calculation of dielectronic recombination, it is not safe to assert that a very narrow resonance, which is often due to spin-orbit interaction, is negligible without any check. The relativistic effect may play an important role, even for ions with extremely low *Z*. It should be mentioned that we adopted the experimental energy level 0.167 eV [12] in our calculations. From the perturbative views, it is straightforward to include or exclude radiation damping. So we also give undamped results (dotted line) in Fig. 2. The comparison has displayed that the DR cross sections through the $1s2p(^3P)3p\ ^2P^e_{1/2,3/2}$ resonances are damped by up to a factor of 1.4. This is different from the view of Ref. [9] that this system is one of the few where damping can be omitted. Except for these two resonances, however, our *R*-matrix calculations have shown radiation damping to be indeed negligible. This may be attributed to the special magnitude of both Auger and radiation widths of the $1s2p(^3P)3p\ ^2P^e_{1/2,3/2}$ state.

All our *R*-matrix DR calculations for the metastable $1s2s\ ^3S$ state of Li^+ have been carried out in the energy region 0–3.15 eV, below the $1s2p\ ^1P$ threshold. The total cross sections, including all $^2L^\pi$ symmetries in the region, are evaluated, and are convoluted with the experimental energy distribution. The rate coefficients obtained (solid line) are depicted in Fig. 3 along with the measurements of Saghiri *et al.* [9]. The dotted line represents the results involving all states of configurations $1s2p(^1P)nl$ ($n=5-7$, all l), while the solid line is the contribution from only the configurations with $l=0-3$. Using perturbation theory we also calculated DR through all the resonance states except for $1s2p(^3P)3p\ ^2P^e_{1/2,3/2}$, such as the $1s2p(^3P)np\ ^2P^e_{1/2,3/2}$ ($n=4-7$) states, which do not occur in the *LS* coupling scheme and can only be due to the relativistic interaction. The Auger widths for these resonances are too small to contribute to the observation. That means that in the 0.2–3.15

eV energy region, the relativistic and nonrelativistic results are equivalent. From Fig. 3 it may be seen that our theoretical results, excluding the high-angular-momentum states, are much closer to the experimental ones. The comparison suggested that the sharp cutoff n_c to take the field ionization effect into account should be a rough approximation, and the initial field-ionized states should be not only n dependent but also l dependent, as pointed out by Saghiri *et al.* [9]. However, from Fig. 3 we did not notice any significant contribution from the configurations with the high angular momentum. This is markedly different from the result of Saghiri *et al* [9]. They demonstrated that DR from high-l states is twice as much as that from the $1s2p(^1P)nl$ $(l<3)$. It must be emphasized that the contribution from the $l=3$ state is small $(<18\%)$ in the energy region concerned, on the basis of our calculation. Therefore, even though the contribution from the $l=3$ state is removed in the solid line, the discrepancy, which represents the contribution from the states with high l including $l=3$, between the solid and dotted lines is still not large. It remains unexplained why the radiative optical potential method employed in Ref. [9] yields DR from the high-l states to be dominant but the present method does not. We do not think that the two different theoretical methods might give rise to this difference, because both the methods have proved to be equivalent [22]. A further exploration may be necessary. Using the perturbation theory we also evaluated DR from the high-angular-momentum states $1s2p(^1P)nl$ $(n=5-7)$, and discovered that the Auger widths for the resonances grow more and more narrow with increasing l; consequently their contributions are trivial. This result is in agreement with the *R*-matrix calculations. Above the energy ~ 2.9 eV, we can see a large discrepancy between the experiment and our calculations. This may be attributed to the radiative decay during the time of flight. The Li atoms recombined into the states with $n>n_c$ may survive field ionization if the outer electron radiates to a final state below n_c during the time of flight from the electron cooler to the analyzer [23,9].

In conclusion, we investigated dielectronic recombination for He-like lithium with very low Z in the metastable state by using the close-coupling *R*-matrix method and perturbation theory. We found that the occurrence of the experimental double peak can be surprisingly attributed to relativistic effects. It is the first discovery that the relativistic effects play a significant role in recombination of so low Z ions. The striking effect of radiation damping, by up to a factor of 1.4, on the $1s2p(^3P)3p\ ^2P^e_{1/2,3/2}$ resonances was noticed. Our calculations have shown that the contribution to DR from high-angular-momentum states is very small. This point is markedly different from Saghiri *et al.* [9].

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