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Differential and Integral Cross Sections for Electron Impact Excitation of Lithium

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The differential and integral cross sections for electron impact excitation of lithium from the ground state $1s^22s$ to excited states $1s^22p$, $1s^23l$ ($l = s, p, d$) and $1s^24l$ ($l = s, p, d, f$)at incident energies ranging from 5 eV to 25 eV are calculated by using a full relativistic distorted wave method. The target state wavefunctions are calculated by using the Grasp92 code. The continuum orbitals are computed in the distorted-wave approximation, in which the direct and exchange potentials among all the electrons are included. A part of the cross sections are compared with the available experimental data and with the previous theoretical values. It is found that, for the integral cross sections, the present calculations are in good agreement with the time-independent distorted wave method calculation, for differential cross sections, our results agree with the experimental data very well.

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Atomic lithium is the simplest multielectron open-shell atomic system, and is also the more concerned atomic system in experiment and theory. Cross section information on inelastic collisions of lithium in its ground and excited states with electrons is not only of fundamental interest, but also of considerable practical importance for diagnostics of magnetically confined fusion plasmas by means of Li beam spectroscopy.[1,2] So far, experimental and theoretical cross section data for collisional processes of Li atoms in the ground state and excited states with electrons are of particular interest in the past two decades. For example, on the experimental side, Williams *et al.* performed an electron-impact spectrometer experiment to measure the differential cross sections for the individual excitations from the ground state $1s^22s$ to the excited states $1s^22p$ and $1s^23s$ and the total cross sections for excitation from the ground state $1s^22s$ to the excited states $1s^23p+1s^23d$ and $1s^24p + 1s^24d + 1s^24f$.[3] Vuskovic *et al.* measured the differential cross sections of the excited states $1s^22p\ ^2P$ from the ground state of lithium also using the electron-impact spectrometer experiment technique at 10, 20, 60, 100, 150, 200 eV.[4] On the theoretical side, Burke *et al.* studied the elastic electron scattering by lithium atoms and evaluated the $2s \to 2p$ excitation cross sections using the close-coupling approximation.[5] Moores *et al.* studied the electron impact excitation processes of lithium in five-state ($2s$, $2p$, $3s$, $3p$, $3d$) close-coupling approximation.[6] Bray *et al.* reported the differential and total cross sections of lithium from the ground state using the coupled-channel optical (CCO) approximation.[7] Schweinzer *et al.* reported lots of cross sections from the ground state $1s^22s$ of Li to the higher $n = 2$, 3, 4 states by convergent close-coupling (CCC).[8] Griffin *et al.* calculated the total cross sections for the excitation of Li from the $1s^22s$ to the excited states $1s^22p$, $1s^23l$ and $1s^24l$ using R-matrix with pseudostates (RMPS) and time-dependent close-coupling (TDCC) method.[9] Witthoeft *et al.* calculated electron-impact excitation cross sections for the $\mathrm{Li}(1s^22s) \to \mathrm{Li}(1s^2nl)$ and $\mathrm{Li}(1s^22p) \to \mathrm{Li}(1s^2nl)$ transitions at incident energies just above the ionization threshold also using the TDCC method.[10] In this Letter, we report a complete calculation of the differential and integral cross sections from the ground state $1s^22s$ to excited state $1s^22p$, $1s^23l$ and $1s^24l$ of Li by applying program REIE06[11–15] based on the widely used packages Grasp92 and Ratip.[16–18]

In our calculations, the wave function of the target states is generated by the widely used atomic structure package Grasp92[16,17] and the continuum wave function is generated by Ratip package.[18] The wave functions for both the initial and final states of the impact systems are the antisymmetric wave functions of the total $(N+1)$-electron system including the target ion plus a continuum electron, which can be written as[11–15]

$$\Psi = \frac{1}{(N+1)^{\frac{1}{2}}} \sum_{p=1}^{N+1} (-1)^{N+1-p} \sum_{M_t,m} C(J_t j M_t m; JM) \times \Phi_{\beta_t J_t}(x_p^{-1}) u_{\kappa m\varepsilon}(x_p), \quad (1)$$

where C is Clebsch–Gordon coefficient, J_t, j, and J are the angular momentum quantum numbers of the target ion, continuum electron and the impact system, respectively, $\Phi_{\beta_t J_t}$ are the target-ion wave functions, β_t represents all other quantum numbers in addition to J_t, x_p designates the space and spin coordinates for electron p and x_p^{-1} is the space and spin coordinates of all the N electrons other than p, $u_{\kappa m\varepsilon}$ is the rel-

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ativistic distorted-wave Dirac spinor for a continuum electron, and κ is the relativistic quantum number.

The electron impact excitation (EIE) scattering amplitude $B_{m_{sf}}^{m_{si}}$ can be written as[12,19]

$$B_{m_{sf}}^{m_{si}} = \frac{2a_0\pi^{1/2}}{k_i} \sum_{\substack{l_i,j_i,m_i,l_f \\ m_{if},j_f,m_f}} \sum_{J,M} (i)^{l_i-l_f}(2l_i+1)^{1/2} \times \exp[i(\delta_{k_i}+\delta_{k_f})] Y_{lf}^{m_{lf}} C\left(l_i \frac{1}{2} 0 m_{s_i}; j_i m_i\right) \times C\left(l_f \frac{1}{2} m_{lf} m_{sf}; j_f m_f\right) C(J_i j_i M_i m_i; JM) \times C(J_f j_f M_f m_f; JM) R(\gamma_i, \gamma_f), \quad (2)$$

where a_0 is the Bohr radius, C's are Clebsch–Gordan coefficients, γ_i, γ_f, J and M are the quantum numbers corresponding to the total angular momentum of the complect system, target ion plus free electron, and its z component, respectively, m_{si}, l_i, j_i, m_{l_i} and m_i are the spin, orbital angular momentum, total angular momentum, and its z component quantum numbers, respectively, for the incident electron, δ_{k_i} is the phase factor for the continuum electron, κ is the relativistic quantum number, which is related to the orbital and total angular momentum l and j. $R(\gamma_i, \gamma_f)$ is the collision matrix elements, which is given by

$$R(\gamma_i, \gamma_f) = \langle \Psi_i | \sum_{p,q}^{N+1} {}_{p<q} (V_{\rm Coul} + V_{\rm Breit}) | \Psi_f \rangle, \quad (3)$$

where $V_{\rm Coul}$ is the Coulomb operator and $V_{\rm Breit}$ is the Breit operator.[17]

The differential cross sections can be written as[20,21]

$$\frac{dQ}{d\hat{k}_f} = \frac{1}{g_i} \sum_{M_i,M_j} \frac{1}{2} \sum_{m_{si},m_{sf}} |B_{m_{sf}}^{m_{si}}|^2, \quad (4)$$

where g_i is the statistical weight of the initial level of the N-electron target ion.

The relativistic distorted wave (RDW) EIE integral cross sections $\sigma_{if}(\varepsilon)$ from an initial state i to final state f can be written as[11–15,22]

$$\sigma_{if}(\varepsilon) = \int \frac{dQ}{d\hat{k}_f} d\Omega = \frac{\pi a_0^2}{k_i^2 g_i} \sum_J (2J+1) \sum_{\kappa,\kappa'} |R(\gamma_i, \gamma_f)|^2, \quad (5)$$

where k_i is the relativistic wave number of the incident electron, and κ and κ' are the relativistic quantum number of the initial and final continuum electrons, respectively.

In the calculations of the wave functions of the initial and final states, we include the $1s^2nl$ ($n = 2, 3, 4$; $l = s, p, d, f$), $1s2s^2$, $1s2p^2$, $1s2snp$ ($n = 2-4$) and $1s2sns$ ($n = 3, 4$) configurations. In the calculations of the total EIE cross sections, we include explicitly all the partial waves up to $\ell = 45$ in order to ensure the convergence in the higher incident electron energy.

Total cross sections for the electron impact excitation of the ground state of Li are given in Table 1 at an incident electron energy of 15 eV. The results are compared with time-independent distorted-wave calculation (DW),[9,23] unitarized distorted-wave calculation (UDW),[9] time-dependent close-coupling calculation (TDCC),[9] 14-state R-matrix calculation (RM(14)),[9] 55-state R-matrix with pseudostates calculation (RMPS(55)).[9] It is clear that our results and the DW calculations are in good agreement except for $2s \to 2p$ and $2s \to 3s$ transitions. This indicates that the relativistic effect is important for $2s \to 2p$ valence-electron excitations, but the relativistic effect is very small for the other electron excitations. Moreover, the present calculation is the highest for $2s \to 2p$ transition, and is the lowest for $2s \to 4f$ in all theoretical calculation. Both the TDCC and the RMPS(55) calculations are in good agreement for all transitions. Some of the DW and the UDW calculations are in good agreement with the nonperturbative TDCC and the RMPS(55) calculations.

Table 1. Comparison of the EIE total cross sections (in 10^{-16} cm^2) at 15 eV incident electron energy ($\varepsilon_i = 15$ eV) from the ground state $1s^22s$ with other available theoretical results for lithium.

Transition	Ours	DW	UDW	TDCC	RM(14)	RMPS(55)
$2s \to 2p$	54.981	51.988	38.952	35.893	37.150	34.240
	$18.830(p_{1/2}) + 36.151(p_{3/2})$					
$2s \to 3s$	1.898	1.955	1.183	0.864	1.318	0.823
$2s \to 3p$	0.609	0.619	1.075	0.517	1.023	0.573
	$0.201(p_{1/2}) + 0.408(p_{3/2})$					
$2s \to 3d$	2.232	2.210	2.478	1.864	2.630	1.799
	$0.894(d_{3/2}) + 1.338(d_{5/2})$					
$2s \to 4s$	0.383	0.397	0.312	0.181	0.329	0.160
$2s \to 4p$	0.151	0.156	0.374	0.121	0.335	0.130
	$0.050(p_{1/2}) + 0.101(p_{3/2})$					
$2s \to 4d$	0.663	0.660	1.002	0.503	0.914	0.465
	$0.266(d_{3/2}) + 0.397(d_{5/2})$					
$2s \to 4f$	0.071	0.072	0.161	0.145	0.207	0.170
	$0.031(f_{1/2}) + 0.040(f_{3/2})$					

We show comparisons of the total cross section for the $2s \to 2p$ and $2s \to 3s$ transitions determined from the present RDW calculation, the TDCC calculation,[9] the 14-state R-matrix (RM(14)) calculation,[9] the 55-state RMPS (RMPS(55)) calculation,[9] the results from fits to the convergent close-coupling (CCC) calculations,[8] the earlier coupled-channel optical (CCO) approximation calculation,[7] the measurements (Expt.1) of Williams *et al.*[3] and the measurements (Expt.2) of Vuskovic *et al.*[4] in Fig. 1.

As can be seen from Fig. 1, both the present and the RMPS, TDCC, CCC, CCO cross sections are all in excellent agreement for the $2s \to 2p$ transition. However, our results are in excellent agreement with the experimental data. This seems to confirm the accuracy of the earlier RM, TDCC, CCC and CCO calculations for these transitions. The small difference of all the theoretical calculations indicate that the effects of the target continuum on excitation to $1s^2 2p$ are relatively small. For the $2s \to 3s$ transition, the present calculations are highest compared with the other theoretical calculations. The 14-state R-matrix calculation is closer to our results. The TDCC, RMPS and CCC cross sections are again in excellent agreement. The much larger differences in theoretical calculations indicate that the effects of the target continuum on excitation to $1s^2 3s$ become larger in the intermediate energy range.

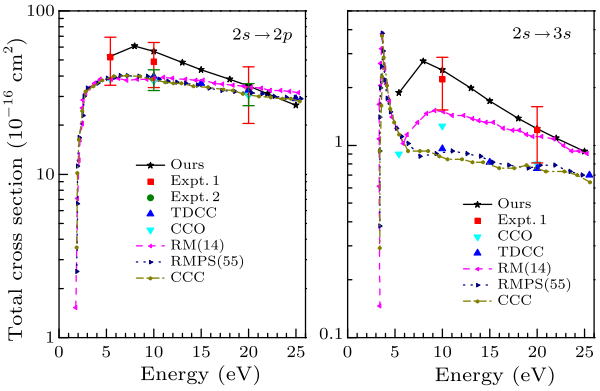

Fig. 1. Total electron-impact excitation cross sections for the $2s \to 2p$ and $2s \to 3s$ transitions in Li.

Figure 2 shows the differential cross sections for the $2s \to 2p$ and $2s \to 3s$ transitions at 10 eV, compared with the experiments (Expt.1) of Williams *et al.*,[3] the experiments (Expt.2) of Vuskovic *et al.*[4] as well as the close-coupling approximation (13CC) calculations of Burke *et al.*[5] and Moores *et al.*,[6] the coupled-channel optical approximation (13CCO) calculations of Bray *et al.*[7] and the close-coupling approximation (CC) calculations of Issa *et al.*[24] For the $2s \to 2p$ excitation, we see excellent agreement of the present calculations with the measurements of Vuskovic *et al.*[4] The 13CCO and 13CC calculations are in good agreement, but lie slightly high in ours and the experimental points in the angular range 40–140°. Again, the very small difference between the experimental and all theoretical results indicate that continuum states $1s^2 2p$ have little effect on the differential cross sections at this energy. For the $2s \to 3s$ excitation, our results also agree very well in shape with the experimental data of Williams *et al.*[3] The 13CCO results are closer to the results of 13CC, but is also above the experimental data.

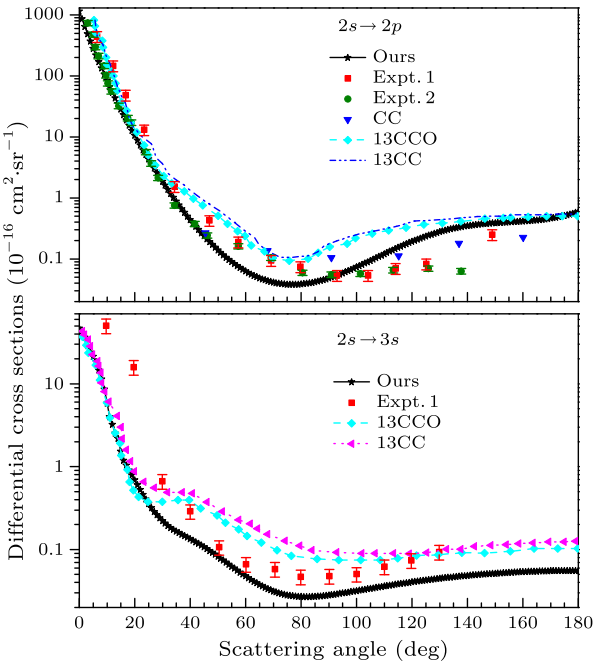

Fig. 2. Comparison of the differential cross sections for the $2s \to 2p$ and $2s \to 3s$ transitions at 10 eV incident electron energy ($\varepsilon_i = 10$ eV) in Li.

In conclusion, we have performed a full relativistic distorted wave calculation of electron impact excitation from the ground state $1s^2 2s$ to excited state $1s^2 2p$, $1s^2 3l$ and $1s^2 4l$ in neutral Li. The total and differential cross sections in the different incident electron energy have been calculated by applying a newly developed program REIE06. Comparison of the present calculations with earlier experimental measurements and theoretical calculations, it is found that the excellent agreement obtained between the present and experiment. Moreover, we find that the effects of the target continuum on electron impact excitation are relatively small for the $2s \to 2p$ excitation, but grow for the $2s \to 3s$ excitation. These conclusions are also found by Griffin *et al.*[9]

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