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Angular Distributions for Near-threshold (*e*,2*e*) Processes for Li and Mg

Cheng Pan
University of Nebraska-Lincoln, pancheng@stanford.edu

Anthony F. Starace
University of Nebraska-Lincoln, astarace1@unl.edu

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Cheng Pan
Department of Physics and Astronomy, The University of Nebraska, Lincoln, Nebraska 68588-0111

Anthony F. Starace*
Joint Institute for Laboratory Astrophysics, University of Colorado and National Institute of Standards and Technology, Boulder, Colorado 80309-0440

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Distorted-wave calculations of the triply differential cross sections for electron-impact ionization of Li and Mg are presented for the coplanar, $\theta_{12} = \pi$ geometry in which the final-state electrons share 2 eV of excess energy equally. Our theoretical approach, described in detail elsewhere [C. Pan and A. F. Starace, Phys. Rev. A **45**, 4588 (1992)], employs a partial-wave expansion of initial- and final-state wave functions, treats direct and exchange interactions of initial- and final-state electrons with the target core, and treats the final-state interaction between the two continuum electrons by a screening potential. Li and Mg targets are found to have more complex $(e, 2e)$ angular distributions than either H or He targets, stemming in large part from significant p-wave and higher one-electron phase shifts in the former elements.

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Recently we have presented distorted-wave calculations of the triply differential cross sections for electron-impact ionization of H and the rare gases for final-state electrons departing in opposite directions ($\theta_{12} = \pi$) and sharing between 0.5 eV and 4 eV of excess energy [1, 2]. These results were shown [1, 2] to agree well with available relative experimental measurements [3–6]. In particular, they provided an interpretation of the observed target dependence of the electron angular distributions for H and He targets [4] as due to short-range effects on the s-wave phase shifts of both incident and final-state continuum electrons [1, 2]. As compared to other theoretical $(e, 2e)$ calculations for H and He at these low energies [7–9], we showed that inclusion of distortion and exchange effects in both initial and final states as well as both singlet and triplet partial waves are all essential to obtain detailed agreement with experiment [1, 2]. Furthermore, large differences in the absolute values of the triply differential cross sections predicted by different theoretical calculations [1, 2, 7, 8] were found [10]. However, recent absolute experimental measurements for electron-impact ionization of He near threshold have confirmed our values for the absolute triply differential cross sections [11, 12].

In this Brief Report we present distorted-wave calculations for triply differential $(e, 2e)$ cross sections for Li and for Mg for the $\theta_{12} = \pi$ geometry and for the two final-state electrons, each having a kinetic energy of 1 eV. Our calculations are similar to those carried out for H and for He [1, 2]. In brief, our initial and final states are expanded in partial waves; all radial one-electron wave functions are calculated treating direct and exchange interactions with the target core; in the final state, the interaction between the two continuum electrons is treated by means of a mutual screening potential [13].

These calculations are meant to serve as benchmarks for experiment and for more detailed theoretical treatments of near-threshold $(e, 2e)$ processes in the alkali metals and in the alkaline-earth metals. While these heavier targets have outer subshells that are isoelectronic to hydrogen and helium, respectively, their cross sections are in general much more difficult to describe theoretically. For example, unlike H and He targets, the alkali metals and the alkaline-earth metals have low-lying excited states that not only produce strong interchannel mixing effects but also lead to strong polarization effects. Furthermore, both the alkali metal and the alkaline-earth metals have minima in their optically allowed final-state channels that render theoretical calculations of photoionization cross sections, for example, very sensitive in general to the precise approximations employed and that also make them very sensitive functions of the photon energy. Indeed, we have calculated the near-threshold triply differential $(e, 2e)$ cross sections for all of the alkali-metal and alkaline-earth-metal elements [14] and found in general that both the absolute magnitudes and the relative cross sections are very sensitive functions of the excess energy above threshold. There were two exceptions, however: Li and Mg, whose relative cross sections were found to be nearly independent of the excess energy in the range from 0.5 to 4.0 eV above threshold. Therefore, we have chosen to present our results for these two targets in this Brief Report since their lack of sensitivity to the excess energy may indicate that our neglect of interchannel interaction and polarization effects will not prove as serious as for other alkali-metal and alkaline-earth-metal targets. Just as theoretical understanding of atomic photoionization was greatly aided by comparisons of calculations that took a detailed account of electron correlation effects with earlier Hartree-Fock level theoretical

results [15, 16], we expect that theoretical understanding of near-threshold $(e, 2e)$ triply differential cross sections will be furthered by comparisons of future experimental and theoretical results with the present distorted-wave triply differential (e,2e) results for Li and Mg.

A detailed description of our theoretical approach is presented in Ref. [2]. For the present calculations the triply differential cross section has the form

$$\sigma^{(3)} = \frac{\pi}{4k^2} \sum_{L,L'} \sum_{S} A(LS) A^*(L'S) \times \sum_{\lambda} [\lambda] P_\lambda \left(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}} \right) [L][L'] \times \begin{pmatrix} L & L' & \lambda \\ 0 & 0 & 0 \end{pmatrix}^2 . \quad (1)$$

Here $\hat{\mathbf{k}}$ is the direction of the incident electron, which has momentum $\mathbf{k}$, $\hat{\mathbf{k}}_1$ is the direction of one of the outgoing final-state electrons, and $A(LS)$ is a scattering amplitude for the LS partial wave. [$A(LS)$ is defined explicitly by Eqs. (15), (16), and either $A(13)$ for the case of Li or $A(14)$ for the case of Mg, where these equations refer to Ref. [2].] For convenience, we may rewrite the triply differential cross section in Eq. (1) in terms of a doubly differential cross section $\sigma^{(2)}$ and asymmetry parameters β_λ,

$$\sigma^{(3)} = \frac{\sigma^{(2)}}{4\pi} \left[1 + \sum_{\lambda\,(>0)} \beta_\lambda P_\lambda \left(\hat{\mathbf{k}}_1 \cdot \hat{\mathbf{k}} \right) \right] . \quad (2)$$

Here $\sigma^{(2)}$ is defined by

$$\sigma^{(2)} \equiv \int_0^{2\pi} d\phi_1 \int_{-1}^{+1} \sigma^{(3)} d(\cos\theta_1) \quad (3)$$

and the parameters β_λ may be determined by comparison of Eq. (2) with Eq. (1). Note that because of our $\theta_{12} = \pi$ geometry and the fact that $\frac{1}{2}k_1^2 = \frac{1}{2}k_2^2$, λ may take only even values, which produces a triply differential cross section that is symmetric about $\theta_{12} = \pi/2$ [17, 18].

In our calculations the target orbital wave functions were calculated in the Hartree-Fock (HF) approximation using the program of Froese-Fischer [19] and the one-electron continuum wave functions were evaluated in the frozen-core HF potential of the residual ion. For the present calculations for Li and Mg, the maximum orbital angular momentum for individual final-state continuum electrons was $\ell_{\max} = 24$. (In our calculations for H, He, the rare gases, and other alkali metals and alkaline-earth metals, maximum values of $\ell_{\max}$ ranged from 16 to 30.) The value of $\ell_{\max}$ is chosen so that all asymmetry parameters β_λ having a value greater than 0.001 converged with an uncertainty less than ± 0.001. For such a value of $\ell_{\max}$, the calculated amplitudes $A(LS)$ up to $L = \ell_{\max} - 4$ were well converged, and these amplitudes were then used to

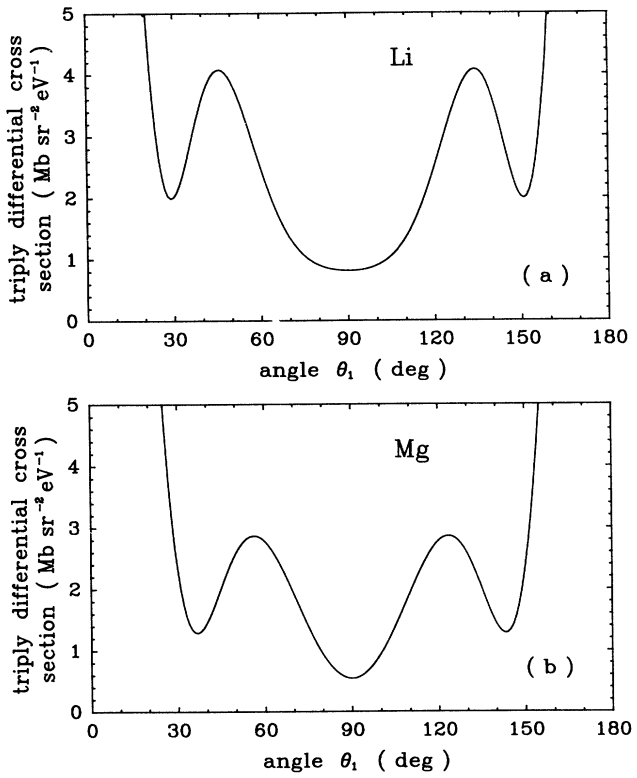

FIG. 1. Triply differential $(e, 2e)$ cross sections for final states having $\theta_{12} = \pi$ and the continuum electrons sharing 2 eV of excess energy equally: (a) Li target, (b) Mg target.

TABLE I. Parameters $\sigma^{(2)}$ (in a.u.) and β_λ determining the triply differential cross section $\sigma^{(3)}$ [cf. Eq. (2)] for $E_{ex} = 2$ eV for H, He, Li, and Mg targets. Dashed lines indicate values smaller than 0.003.

Parameter	H[a]	He[a]	Li	Mg
$\sigma^{(2)}$	3.73	0.762	34.5	35.5
β_2	3.090	1.129	1.638	1.902
β_4	2.367	1.833	0.856	1.902
β_6	0.855	0.325	1.881	2.729
β_8	0.115	0.022	2.036	1.249
β_{10}	0.008	—	0.924	0.305
β_{12}	—	—	0.216	0.046
β_{14}	—	—	0.029	0.004

[a] Ref. [2], Table III.

TABLE II. Relative amplitude and phase for electron-impact ionization scattering amplitudes $A(LS)$ for H, He, Li, and Mg targets for final-state electron kinetic energies $1/2\ k_1^2 = 1/2\ k_2^2 = 1$ eV. Only the first six partial waves for each target are shown.

Partial wave $^{2S+1}L^{\pi}$	Relative amplitude $\lvert A(LS)\rvert/\lvert A(^1S^e)\rvert$				arg $A(LS)$ (rad)			
	H	He	Li	Mg	H	He	Li	Mg
$^1S^e$	1.000[a]	1.000[a]	1.000[a]	1.000[a]	2.95	4.47	2.85	0.88
$^3P^o$	0.471	0.450	0.236	0.266	1.10	1.37	4.13	1.79
$^1D^e$	0.504	0.566	0.121	0.235	2.32	2.59	0.88	4.61
$^3F^o$	0.324	0.201	0.251	0.531	1.27	1.20	5.48	1.73
$^1G^e$	0.036	0.028	0.192	0.222	1.28	1.28	0.59	4.17
$^3H^o$	0.023	0.008	0.164	0.091	0.80	0.49	5.84	2.23

[a] The values of $\lvert A(^1S^e)\rvert$ for H, He, Li, and Mg targets are respectively 0.3430, 0.2091, 0.9003, and 0.7651.

evaluate the asymmetry parameters β_λ. Also, in our calculations the matrix elements involving two continuum radial functions were evaluated using a complex coordinate transformation beyond a radial value $r = r_0$, as discussed by Gao and Starace [20].

Our triply differential cross sections for electron impact ionization of Li and Mg for an excess energy of 2 eV are shown in Fig. 1. One sees immediately that these elements have a much more complex angular distribution than does either H or He. The parameters $\sigma^{(2)}$ and β_λ that describe these angular distributions are presented in Table I together with those for our earlier results for H and for He. One notices immediately from Table I the much larger magnitudes of the triply differential cross sections for Li and for Mg than for either H or He. Also, whereas relatively few asymmetry parameters described the triply differential cross sections for H and for He, for Li and Mg much larger numbers of β_λ parameters must be included.

The relative magnitudes and phases of the partial-wave amplitudes $A(LS)$ are presented in Table II for H, He, Li, and Mg targets for $E_{ex} = 2$ eV. As was shown for $E_{ex} = 4$ eV in Ref. [1], the relative amplitudes and phases for $L > 0$ are very similar for H and He targets; it is the phase difference for $A(^1S^e)$ which distinguishes the $(e, 2e)$ angular distributions for these two targets. In contrast, no such simple interpretation of the angular distributions for Li and Mg can be put forth. The reason for this is that, whereas for H and for He it is mainly the one-electron s-wave phase shifts that are nonzero, leading mainly to differences in the $A(^1S^e)$ phases, for Li and Mg targets the p-wave and higher one-electron phase shifts are also significant, causing the phases of the important partial-wave amplitudes $A(^{2S+1}L^{\pi})$ for $L \leq 4$ to differ significantly from one another.

In summary, we have presented distorted-wave calculations for the triply differential $(e, 2e)$ cross sections for Li and Mg targets and made comparisons of these results with those for H and for He [1, 2]. The angular distributions for Li and Mg are found to have far more structure than those for H and He. This is found to stem from significant p-wave and higher one-electron phase shifts for Li and Mg but not for H and He at the 2 eV excess energy considered.

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* Permanent address: Department of Physics and Astronomy, The University of Nebraska, Lincoln, NE 68588-0111.

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