Calculation of electron-impact ionization of Mg and Al^+

I. Bray, K. McNamara, and D. V. Fursa
Curtin Institute for Computation and Department of Physics and Astronomy, Curtin University, GPO Box U1987, Perth WA 6845, Australia
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The total electron-impact single-ionization cross sections of Mg and Al^+ have been calculated by Ludlow *et al.* [Phys. Rev. A **79**, 032715 (2009)] using the time-dependent close-coupling and R-matrix-with-pseudostates methods. The cross-section results were found to be in good agreement with each other, but substantially smaller than those reported by several experiments. We apply the convergent close-coupling method to the problem and find a much improved agreement with experiment.

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I. INTRODUCTION

Electron-impact ionization of atomic targets is of fundamental and practical interest to science and industry. The long-ranged nature of the Coulomb potential has made the formulation of the breakup problem with three charged particles in the asymptotic region particularly problematic. Only relatively recently has there been some progress in addressing these issues [1–3]. Interestingly, the lack of an adequate formulation of the ionization amplitude did not deter progress in numerically calculating the fully differential ionization cross sections. Beginning with Rescigno *et al.* [4], the electron-hydrogen fully differential ionization problem was effectively solved directly for the cross sections with the total wave function obtained from an exterior complex scaling approach, which was later broadened to define the underlying amplitudes [5]. The convergent close-coupling (CCC) method also solves the problem with the amplitudes obtained directly from the excitation of the positive-energy pseudostates [6,7]. The relationship between the various computational theories and formal theory was reviewed recently by Bray *et al.* [8].

An accurate treatment of the fully differential ionization cross sections implies an accurate treatment of the total (single) ionization cross section, which is obtained by integration over the solid angles and the energy of the outgoing electrons. However, in practice, convergence in the total ionization cross section can be achieved with much smaller calculations than those required for fully differential cross sections. For example, in the close-coupling method, convergence needs to be checked against increasing the maximum target orbital angular momentum $l_{\max}$ and the number of orbitals N_l. Being a unitary formalism, the optical theorem ensures that the total cross sections converge rapidly due to the fact that it can be obtained from the imaginary part of the elastic-scattering amplitude. Since this amplitude, and those for the lowest excited states, converges relatively rapidly with increasing $l_{\max}$, so does the total ionization cross section [9].

The CCC method for one-electron targets [10] has been very successful in obtaining very accurate electron-impact total ionization cross sections for H [11] and He^+ [12]. For quasi-one-electron targets such as lithium, the CCC method [13] has been shown to be very accurate for excitation [14], but application to single ionization of the lithiumlike isoelectronic sequence yielded mixed agreement with experiment [15]. Subsequent nonperturbative calculations are usually closer to the CCC results than experiment [16–18]. In the case of sodium, application below the core ionization threshold [9] was subsequently found to be in good agreement with experiment [19]. For sodiumlike ions, the theories show a little variation, and agreement with experiment is also somewhat mixed [20].

Following the extension of the CCC method to two-electron targets [21], application to helium total ionization [22] and fully differential ionization [23,24] has yielded outstanding agreement with experiment. Application to heliumlike ions also yielded excellent agreement [25–27]. Of particular note was the fact that the CCC theory and experiment were in agreement on even autoionization and ionization plus excitation contributions to the total single-ionization cross section [27].

Here we concern ourselves with electron-impact total single ionization of Mg and Al^+. Ludlow *et al.* [28] reported total ionization cross sections that are substantially lower than experiment. They used two independent theoretical approaches, both of which are expected to yield accurate results. It is this discrepancy that has motivated the application of the CCC method to this problem.

II. THEORY

The CCC theory for electron scattering on quasi-two-electron atoms, such as Mg and Al^+, has been given by Fursa and Bray [29]. Briefly, the $n \leqslant 2$ core orbitals are obtained from a self-consistent-field Hartree-Fock calculation for the ground state of Mg^+ and Al^{2+}. Then, the Hamiltonian of these quasi-one-electron targets is diagonalized in a Laguerre basis of size N_l and exponential falloffs λ_l, for $0 \leqslant l \leqslant l_{\max}$, to obtain $3 \leqslant n \leqslant N_l$ one-electron orbitals. Subsequently, we use $N'_l \leqslant N_l$ in generating the two-electron configurations. Small phenomenological core-polarization potentials are also included to ensure the accuracy of the one-electron energies. The Laguerre-based one-electron orbitals are then used to form two-electron configurations to diagonalize the quasi-two-electron target Hamiltonian. The configurations included in the calculations determine the quality of the resultant target structure. Here we take all $\{nl,n'l'\}$ configurations that incorporate $3s,4s,3p,4p,3d$ orbitals, and also $\{3s,n'l'\}$ and $\{3p,n'l'\}$ configurations with $n' \leqslant N'_{l'} \leqslant N_{l'}$ for $l' \leqslant l_{\max}$. The latter two sets of configurations are responsible for the generation of states corresponding to ionization leaving the ion in the $3s$ or $3p$ states. The former set is important to yield accurate ground and lowest excited target states. The $1s,2s,2p$ core orbitals are not used in any of the configurations.

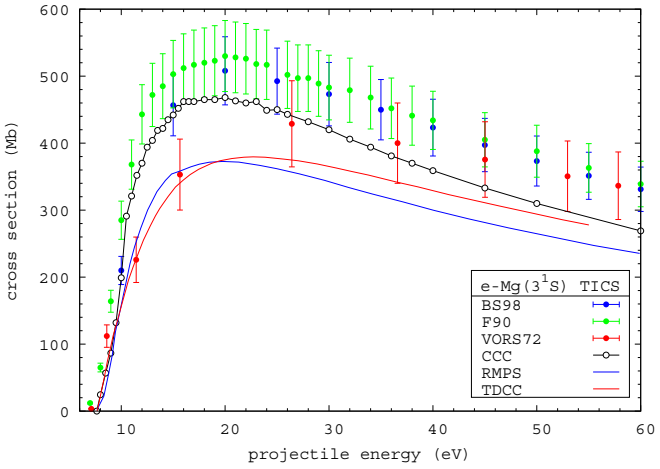

FIG. 1. (Color online) Total ionization cross sections of electron-impact single ionization of the ground state of Mg. The present calculations, denoted by CCC, have been performed at the indicated points connected by straight lines to guide the eye. The calculations labeled by RMPS and TDCC are due to Ludlow *et al.* [28]. The experimental data are due to Vainshtein *et al.* [31], Boivin and Srivastava [32], and Freund *et al.* [33].

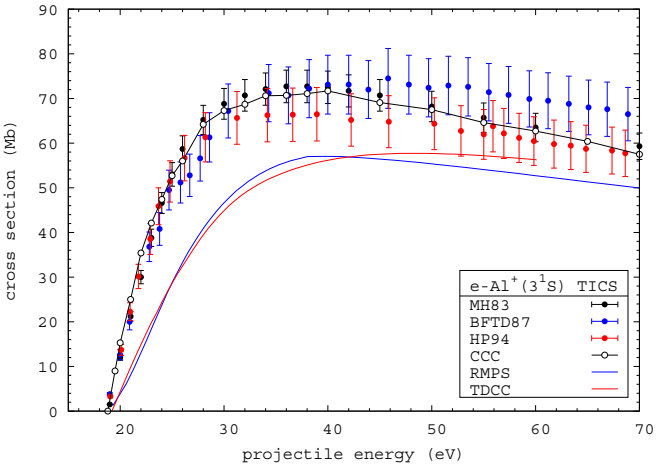

FIG. 2. (Color online) Total ionization cross sections of electron-impact single ionization of the ground state of Al^+. The present calculations, denoted by CCC, have been performed at the indicated points connected by straight lines to guide the eye. The calculations labeled by RMPS and TDCC are due to Ludlow *et al.* [28]. The experimental data are due to Montague and Harrison [34], Belic *et al.* [35], and Hayton and Peart [36].

The above approach is used for both the Mg and Al^+ targets, with $l_{max} = 3$, $N_l = 20 - l$, and $N'_l = 17 - l$. The reason that $N'_l < N_l$ is because the highest-energy orbitals are not necessary for generating either an already accurate target structure or high-energy continuum states, given the energies of interest to us here. Even so, the total number of states generated is 425, and for consistency all of them are included in the close-coupling formalism. They consist of 33 ^1S, 46 $^1P^o$, 47 $^1D^e$, 30 $^1F^o$, 15 $^1G^o$, 28 ^3S, 46 $^3P^o$, 44 $^3D^e$, 30 $^3F^o$, 14 $^3G^e$, 14 $^1P^e$, 16 $^1D^o$, 14 $^1F^e$, 17 $^3P^e$, 16 $^3D^o$, and 15 $^3F^e$ states. The most stringent test of the structure calculation is the resultant ionization energies of the ground state. In the case of Mg and Al^+, we obtain 7.654 and 18.81 eV, respectively, compared to 7.646 and 18.83 eV [30].

III. RESULTS

The electron-scattering close-coupling equations are solved separately at each considered energy of the projectile for the first 16 partial waves of the total orbital angular momentum, and then extrapolated using a Born-subtraction technique. We restrict ourselves to the same energy region as did Ludlow *et al.* [28], and we perform the CCC calculations on the dense energy mesh as indicated by the CCC points in Figs. 1 and 2. For clarity of presentation, we restrict the theoretical comparison to just the RMPS, TDCC, and CCC theories and experiment.

From Fig. 1 we see that the CCC calculation is considerably above the RMPS and TDCC results, and much closer to the experiment. Such a substantial discrepancy between these theories is most unexpected, and it is the first time that we have come across this. Since $N_l = N_0 - l$, checking convergence is readily done by just varying N_0 while keeping $N'_l = 17 - l$. We performed calculations with $N_0 = 18$, 19, and 20, with only the latter presented. All yield much the same (within $\pm 1\%$) results, with a few pseudoresonances being occasionally evident. We also reduced the size of the calculations by removing the $\{3p,n'l'\}$ configurations. This resulted in about a 5% reduction at energies above 15 eV, indicating that ionization-plus-excitation to $3p$ is a small but significant contribution. Nevertheless, it is not responsible for the majority of the difference, and we remain unable to explain it.

The same systematic trend is seen in Fig. 2 for Al^+. This time agreement of CCC with experiment is particularly outstanding. In searching for the cause of the discrepancy with TDCC and RMPS, we found that the ionization-plus-excitation contribution is even smaller. This is in line with expectations, as the $3s$ and $3p$ energies are farther apart in Al^{2+} than in Mg^+.

IV. CONCLUSION

To summarize, the CCC method was applied to the calculation of the single total ionization cross section of the quasi-two-electron targets of Mg and Al^+ by electron impact at low to intermediate energies. Convergent results to just a few percent were obtained. Unexpected substantial discrepancies with the RMPS and TDCC calculations of Ludlow *et al.* [28] have been found, which we are unable to explain. The agreement of the CCC calculations with experiment for Mg is satisfactory, and it is outstanding in the case of Al^+. We are hopeful that the discrepancies identified here will lead to a reexamination of the corresponding RMPS and TDCC calculations to find the underlying cause, and thereby establish broadly supported theoretical results for the problems considered.

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