Electron scattering from atomic gallium

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Electron scattering from atomic gallium

D. V. Fursa and I. Bray
ARC Centre for Antimatter-Matter Studies
Physics Department, Curtin University, Perth 6845, Australia
E-mail: d.fursa@curtin.edu.au

Abstract. Theoretical study of electron scattering from the $4P_{1/2}$ ground state of gallium atoms is reported. We have used relativistic convergent close-coupling method to obtain cross sections for elastic scattering and excitations of the $4P_{3/2}$, $5S_{1/2}$, $5P_{1/2,3/2}$ and $4D_{3/2,5,2}$ states for incident electron energies ranging from 0.1 to 500 eV. Comparison of our results with recent theoretical estimates that have been used in plasma modeling shows significant discrepancies for all considered transitions.

1. Introduction

Accurate electron-atom collision data is of primary importance for plasma physics modeling. Often the number of required transitions is very large and realistically can only be provided by theoretical calculations. With development of sophisticated scattering methods, such as the convergent close coupling (CCC) [1] method and R-matrix (RM) method [2, 3], accurate collision data can be obtained for a large number of scattering systems. Recent developments in the CCC [4] and RM [5] methods allow for accurate calculations of target atoms that are strongly affected by relativistic effects. Gallium is one such target, with the ground state being a P-state that is strongly affected by spin-orbit interaction resulting in fine structure splitting of 0.1 eV.

Gallium has recently attracted considerable attention in relation to the design of new mercury-free fluorescent light sources. Light emission from gallium-iodide discharge plasma has been studied by Adamson *et al* [6] and Smith *et al* [7]. In particular, Adamson *et al* [6] have presented detailed plasma physics modeling that relied on electron-atom collision data which were calculated using a rather simple technique, a combination of the similarity function method and the Born-Ochkur approximation. Given the scarcity of e-Ga collision data and very large number of transitions required it was a reasonable approach atthe time.

The purpose of this paper is to examine the accuracy of such data by comparing with the results of an advanced theoretical method. We have performed relativistic CCC (RCCC) calculations of electron scattering from gallium for incident electron energies ranging from 0.1 eV ($4P_{3/2}$ threshold) to 500 eV. Selected cross sections for elastic scattering and excitation of a number of low-lying states from the $4P_{1/2}$ ground state are presented and compared with estimates of Adamson *et al* [6].

2. Theoretical method

The RCCC method has been described by Fursa and Bray [4]. Hence we give only the most important aspects here and details specific to the e-Ga scattering system. We model the Ga atom as a quasi one-electron atom with one active electron above a frozen inert Dirac-Fock

$[Ar]3d^{10}4s^2$ core. The core orbitals are obtained from the GRASP package [9]. The set of Ga target states is obtained via diagonalization of Ga frozen-core quasi one-electron Hamiltonian in a relativistic Sturmian basis (Dirac L spinors [10]). Specifically, we have used 50 L spinors with exponential fall-offs 2.5 for $s_{1/2}$, 2.4 for $p_{1/2,3/2}$, 2.2 for $d_{3/2,5/2}$ and $f_{3/2,1/2}$ target symmetries. Similarly to the nonrelativistic CCC method [11, 12] we include phenomenological one-electron and two-electron potentials [8] in order to account more accurately for core-valence electron correlations. The resulting set of Ga target states provide an accurate representation of the Ga low-lying bound states and a finite square-integrable representation of the infinite number of high-lying bound states and the continuum. Table 1 demonstrates very good agreement of the ionization energies obtained in the RCCC structure calculations with the experimental values (NIST) [13] for the states included in the present study. Good agreement was also found the oscillator strength for the optically allowed $4P_{1/2} - 5S_{1/2}$ and $4P_{1/2} - 4D_{3/2}$ transitions, see Table 2.

The set of Ga target states is used to perform the multichannel expansion of the e-Ga scattering system total wave function and formulate a set of coupled Lippman-Schwinger equations for the T-matrix [4]. The calculations have been performed in two models. For incident electron energies above 2 eV we have performed calculations using the 75-state model that includes 11 $S_{1/2}$, 11 $P_{1/2,3/2}$, 11 $D_{3/2,5/2}$, and 10 $F_{5/2,7/2}$ states. At energies below 2 eV we have done calculations using a smaller 26-state model that includes 4 $S_{1/2}$, 4 $P_{1/2,3/2}$, 4 $D_{3/2,5/2}$, and 3 $F_{5/2,7/2}$ states.

Table 1. Ionization energies of the low-lying states of gallium. The present RCCC results compared to experiment (NIST) [13].

State	RCCC	NIST
$4P_{1/2}$	6.00	6.00
$4P_{3/2}$	5.90	5.90
$5S_{1/2}$	2.89	2.93
$5P_{1/2}$	1.87	1.90
$5P_{3/2}$	1.86	1.89
$4D_{3/2}$	1.66	1.69
$4D_{5/2}$	1.66	1.69

Table 2. Oscillator strengths for transitions involving the ground state of gallium. The present RCCC results compared to experiment (NIST) [13].

Transition	RCCC	NIST
$4P_{1/2} - 5S_{1/2}$	0.12	0.123
$4P_{1/2} - 4D_{3/2}$	0.334	0.29

3. Results and discussion

Figs. 1-5 present the results of the RCCC calculations and comparison with the theoretical estimates of Adamson *et al* [6] (SFM, obtained by digitising their Fig. 17) We find very large discrepancies both in shape and magnitude for the elastic scattering cross section, Fig. 1, and for the first excited $4P_{3/2}$ state cross section, Fig. 2. For the latter cross section, the difference at the cross maximum is about a factor of six. We note that excitation of the $4P_{3/2}$ level from the ground $4P_{1/2}$ level is a transition between fine structure levels. Such a transition can be expected to be described reliably only by theoretical methods that take into account the relativistic effects sufficiently accurately.

Excitations of the $5S_{1/2}$ and $4D_{3/2}$ states are optically allowed transitions. At high energies the excitation cross section is well described by the Bethe-Born formula [14] and, therefore, is determined by the excitation energy and optical oscillator strength value. Good agreement between RCCC and experiment for Ga structure (see Tables 1 and 2) should lead to sufficient

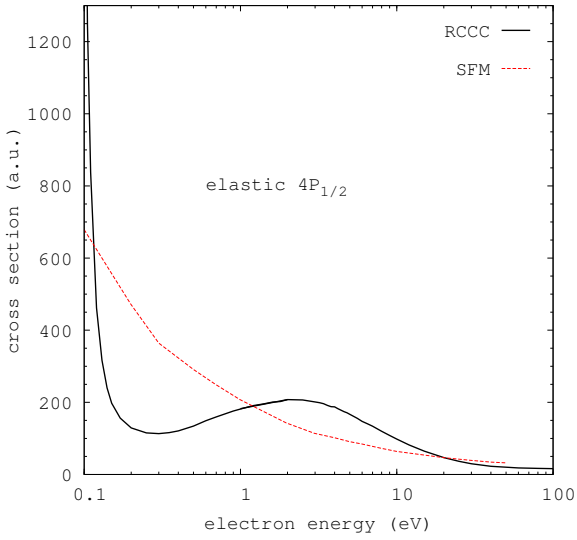

Figure 1. Cross sections for elastic electron scattering on the $4P_{1/2}$ ground state of gallium atom. Present RCCC calculations are described in the text. The theoretical estimates of Adamson *et al* [6], labelled SFM, are a combination of the similarity function method and Born-Ochkur approximation.

accuracy and reliability of the RCCC results for these transitions. The excitation of the $5S_{1/2}$ state is presented in Fig. 3. It shows that both RCCC and SFM converge to the same high-energy limit, but there is still a relatively large discrepancy in the cross section shape and its magnitude near the cross section maximum.

Cross section for the excitation of the optically allowed $4D_{3/2}$ state is much larger than the corresponding excitation cross section for the optically prohibited $4D_{3/2}$ state as follows from Fig. 4. The RCCC cross section for the fine structure combined $4D$ level agree well in the shape, but differ substantially in magnitude with the SFM results.

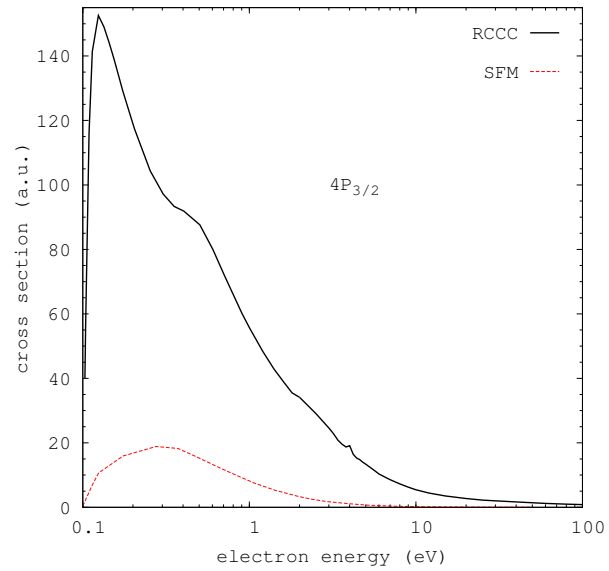

Figure 2. Cross sections for electron impact excitation of $4P_{3/2}$ state from the $4P_{1/2}$ ground state of gallium atom. The calculations as in Fig. 1.

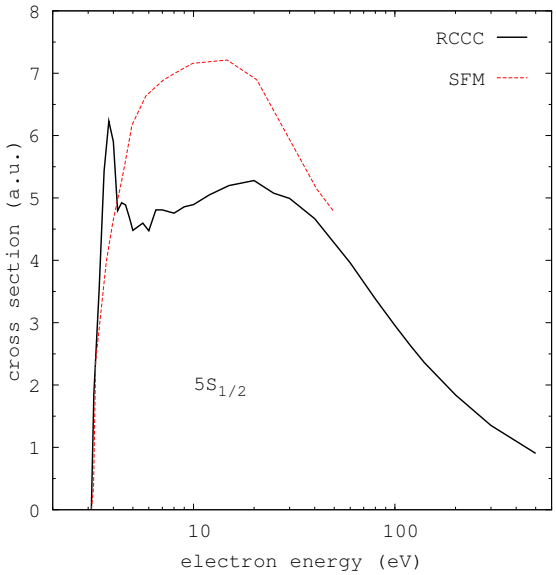

Figure 3. Same as for Fig. 2 but for excitation of $5S_{1/2}$ state.

Fig. 5 presents the RCCC results for the excitation of the optically prohibited $5P_{1/2}$ and $5P_{3/2}$ states and cross section for the fine structure combined $5P$ level. The latter cross section

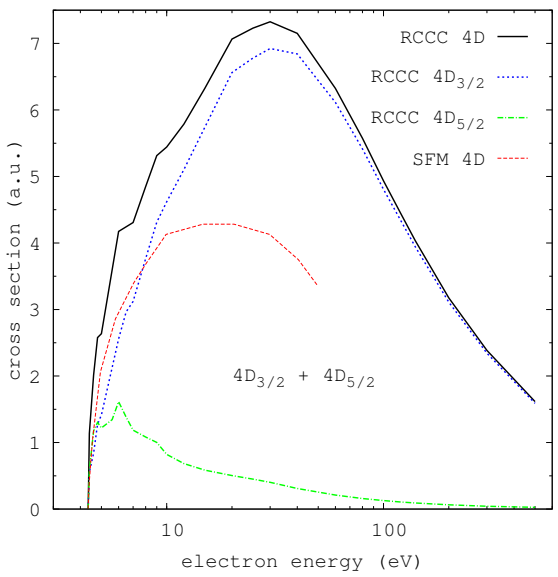

Figure 4. Same as for Fig. 2 but for excitation of $4D_{3/2}$ and $4D_{5/2}$ states. The sfm results are for combined $4D$ level.

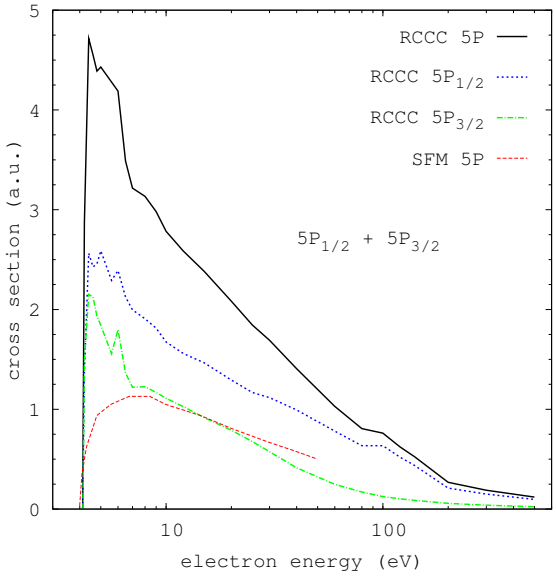

Figure 5. Same as for Fig. 2 but for excitation of $5P_{1/2}$ and $5P_{3/2}$ states. The sfm results are for combined $4D$ level.

is compared with the SFM estimate. We find very large discrepancies in the shape and magnitude for this transition.

In conclusion, we find very large discrepancies between the RCCC and SFM results for elastic scattering and optically prohibited excitations with smaller, but still significant discrepancies for the optically allowed transitions. We expect that incorporation of accurate collision data in plasma modeling calculations might lead to significantly more reliable modeling outcomes.

Acknowledgments

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