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Annual Progress Report on Contract AT(11-1)-2276

Abstract

Progress has been made in calculation of cross-sections for dielectronic and radiative recombination when hot electrons are incident on partially stripped impurity ions. Calculations were completed for the cases of 1 keV and 10 keV electrons incident on ions of arbitrary Z with ionization state consistent with a 1 keV plasma temperature. It was found that dielectronic recombination dominates radiative recombination by a factor of 100 at 1 keV incident electron energy to a factor of 1000 at 10 keV incident electron energy. A report on this work has been submitted and accepted for publication by The Physical Review. The work is now being extended to other plasma temperatures and is being improved by more accurate calculation of the matrix elements involved.

Progress has also been made in the calculation of accurate bremsstrahlung and higher order radiative processes which also occur when hot electrons are incident on partially stripped impurity ions. Formal expressions for the matrix elements have been obtained for cross-sections in a fully relativistic partial wave analysis for bremsstrahlung radiation both with and without electron excitation of the target ion. Final evaluation now awaits the evaluation of the relativistic radial integrals involved in these matrix elements.

Two other papers were completed and prepared for publication: "Non-Adiabatic Couplings in Highly Excited States of H_2 " and "A Theoretical Study of Autoionizing States and Lifetimes of Multiply Excited Argon".

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Progress to Date

During the current contract year, five problems were worked on, of which three were completed. One has already been accepted for publication in The Physical Review; two are ready for submission to The Physical Review.

1. "Radiative Capture and Recombination in Electron-Atom Collisions" calculates radiative capture and dielectronic recombination of electrons in the 1 keV to 10 keV energy range incident on ions of any nuclear charge Z , stripped to an ionization state compatible with a 1 keV electron temperature. It has been accepted for publication in The Physical Review.

2. The problem of non-adiabatic coupling in highly excited states of H_2 , initiated three years ago, was this year completed and Manjibhai V. Patel received his doctorate for work done on this problem. The work has been written up for publication.

The problem is of concern to CTR in the area of neutral injection heating. If an H_2^+ ion captures an electron to form H_2^* in a Rydberg state with $n \geq 10$, it can be stripped on entering the plasma confining magnetic field. The theoretical work was initiated in response to puzzling differences found by Barnett et al between electron capture to Rydberg states by H^+ and H_2^+ and also by conflicts of his H_2^* results with existing theory. The apparent contradictions were removed and the work may indeed have practical consequences in that it indicates that the fraction of H_2^* suitable for plasma heating may be vastly underestimated by current measuring techniques.

3. The calculation of radial integrals involved in the matrix elements for radiative and excitative processes were completed in the non-relativistic limit. Slater functions^{12,13} were used for bound states

in a partially screened nuclear charge and free electron wave functions were calculated in a Thomas-Fermi potential appropriate to the ion under consideration.¹⁴ Codes are now in hand to do the non-relativistic radial integrals for arbitrary nuclear charge Z and electron states up to and including $n = 5$.

For purposes of a thesis, the calculations were applied to multiply excited argon, since a considerable body of literature already existed on auto-ionizing states of argon, so that meaningful comparisons could be made with other theoretical approaches and with experiment. The widespread theoretical interest in argon (and neon) stems from recent experiments in violent atomic collisions at several laboratories throughout the world, including The University of Connecticut.

4. The rigorous quantum electrodynamical formulation of radiation processes associated with electron-atom collisions was completed up to second order. Formal expressions have been obtained for the matrix elements and await completion of the relativistic radial integrals. It is anticipated that final numerical cross-sections for some processes will be obtained during the coming contract year.

5. Some time was spent by the principal investigator on single and double capture by D_2^+ in Cs vapor. This work was theoretical back-up to experiments on negative ion formation done by Barnett's group at ORNL in connection with injection heating of a plasma. This theoretical work has been completed and written up. The manuscript for the combined experiment and theory should soon be ready for submission to The Physical Review.