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THEORETICAL ATOMIC PHYSICS FOR FUSION

1993 Annual Report

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by

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The understanding of electron-ion collision processes in plasmas remains a key factor in the ultimate development of nuclear fusion as a viable energy source for the nation. Our 1993-1995 research proposal delineated several areas of research in electron-ion scattering theory. In the paragraphs below we summarize our efforts in 1993.

I. RESEARCH

A. Electron-Impact Excitation of Atomic Ions

1) Close-coupling calculations for Kr^{6+}

In collaboration with the ORNL/JILA experimental group, a joint project to study the electron-impact excitation of the $4s^2\ 1S \rightarrow 4s4p\ 3P$ intercombination transition in Kr^{6+} nears completion.¹ Near threshold the cross section is dominated by resonances. As shown in Figure 1 our preliminary 10-state close-coupling calculations, convoluted with a 0.2 eV Gaussian representing the experimental energy distribution, is in reasonable agreement with the merged-beams measurements as to the size and shape of the two resonance features. With further calculations we hope to improve the energy positions of the resonances, which appear to differ from experiment by about 0.5 eV.

2) Distorted-wave and Classical Trajectory Monte Carlo Calculations for Ar^{7+}

The $3s \rightarrow 3p$ dipole excitation cross section for Ar^{7+} was calculated using both the quantal distorted-wave and the classical trajectory Monte-Carlo methods.² Of special interest to the design of the merged-beams experiments is the strength of the backward scattering as a function of transition type and incident electron energy. A direct comparison of the quantal and classical calculations reveals the underlying dynamics common to both, as well as the limitations of the classical approach. As shown in Figure 2 for 100 eV

Fig. 1: Electron excitation $4s^2 \ ^1S \rightarrow 4s4p \ ^3P$ in Kr^{6+} . Solid curve: close-coupling; solid circles: experiment.

Fig. 2: Electron excitation $3s \rightarrow 3p$ in Ar^{7+} at 100 eV energy.
Solid curve: distorted-wave;
dashed curve: classical trajectory.

incident electron energy, both the rise and fall of the cross section through the maximum and the backward enhancement are very well reproduced by the classical trajectory Monte-Carlo method. Both methods are in excellent agreement with the experimental measurements of Huber et al.³ in the angular range from 10-30 degrees.

3) Close-coupling and Distorted-Wave Calculations for Fe^{14+}

In support of future merged-beams experiments, electron-impact excitation cross sections for the $3s^2 1s \rightarrow 3s3p \ 3,1p$ transitions in Si^{2+} and Ar^{6+} were calculated in the close-coupling method.⁴ Surprisingly, when distorted-wave calculations for the resonance structures were compared to the close-coupling results, significant differences were found due to both direct-resonant interference effects and overlapping (and interacting) resonance series. The breakdown of the isolated-resonance approximation for the $3s^2 1s \rightarrow 3s3p \ 3p$ transition in Fe^{14+} has been explored in detail.⁵ There are important implications for the description of resonant processes which are strongly radiation damped, for which the isolated-resonance approximation is widely used and the standard formulation of the close-coupling approximation is not applicable.

B. Electron-Impact Ionization of Atomic Ions

1) Close-coupling and Distorted-Wave Calculations for Kr^{4+} , Kr^{5+} , Kr^{6+} and Kr^{7+} .

In collaboration with the ORNL/JILA experimental group, a joint project to study the electron-impact ionization of low-charged ions in the Kr isonuclear sequences nears completion.⁶ As shown in Figure 3 our preliminary distorted-wave calculations for the electron ionization of Kr^{7+} are in

Fig. 3: Electron ionization of Kr^{7+} .
 Solid curve: distorted-wave for total;
 dotted curve: distorted-wave for
 direct only;
 solid circles: experiment.

reasonable agreement with the most recent crossed-beams measurements. Term-dependence and relaxation effects were found to be significant. Krypton is an important impurity for fusion research since it is introduced as a diagnostic for the central core, as a source of electrons for studies of the edge plasma, and as a radiation "coolant" for divertors.

2) Close-coupling and Distorted-Wave Calculations for Sc^{2+} .

In collaboration with the University of Giessen experimental group, a joint project to study resonance structures in the electron-impact ionization of Sc^{2+} nears completion.⁷ As shown in Figure 4 the overall agreement between theory and experiment is good. By comparing 21 and 26 state close-coupling calculations, we found that core-rearrangement autoionizing decay channels have a strong influence on the dielectronic-capture resonance structure.

3) Distorted-wave Calculations for Fe^{15+}

In collaboration with the University of Heidelberg (TSR) experimental group, a joint project to study resonance structures in the electron-impact ionization of Na-like ions has been initiated.⁸ In Figure 5 we compare preliminary experimental and theoretical results for the electron-impact ionization of Fe^{15+} . The detailed resonance structure for ionization is much more difficult to predict than the corresponding structure found in recombination.

4) Distorted-wave Calculations for Si^+ and Si^{2+}

In collaboration with the ORNL/JILA experimental group, a joint project to study the electron-impact ionization of Si^+ and Si^{2+} was completed.⁹ Excitation

Fig. 4: Electron ionization of Sc^{2+}
 Solid curve: close-coupling for total;
 dotted curve: distorted-wave for
 total;
 dashed curve: distorted-wave for
 direct only;
 solid circles: experiment.

Fig. 5: Electron ionization of Fe^{15+}
 Top graph: experiment;
 bottom graph: distorted-wave.

tation-autoionization measurably enhances the cross sections of both ions. Not only is silicon found as an impurity in fusion devices, but it is very important as an astrophysically abundant element.

C. Electron-Impact Recombination of Atomic Ions

1. Field-Enhanced Distorted-Wave Calculation for C^{3+}

In collaboration with H.P. Summers at JET we carried out quantal calculations for the dielectronic recombination of C^{3+} in an electric field.¹⁰ We have used these results in a collisional-radiative model for a carbon-seeded hydrogen plasma. We find that the plasma microfield increases the effective dielectronic recombination rate coefficient for C^{3+} by only 40% at 10^9 particles/cm³, for example, compared to the near factor of 3 enhancement predicted by Reisenfeld et al.¹¹ The calculations formed part of a larger project to generate accurate dielectronic recombination rate coefficients for most impurities found in hot, dense plasmas.

2) Relativistic Distorted-Wave Calculations for U^{89+} .

In collaboration with the GSI (ESR) experimental group, a joint project to study the near-threshold dielectronic recombination resonances in U^{89+} nears completion.¹² Besides radiative recombination, the dielectronic recombination resonances $1s^2 2p\ 3/2\ 5l_j$ with $j = 5/2, 7/2$, and $9/2$ are clearly resolved experimentally and found at the energy positions and with relative magnitudes as expected from our Dirac-Fock calculations.

3) Relativistic Distorted-wave Calculations for U^{90+} .

Within the framework of standard electroweak gauge theory, parity-violation effects on the Auger emission from atomic ions was examined. The

Auger decay of the $2s^2$ $J = 0$ levels in U^{90+} was analyzed. In QED, the polarization-asymmetry parameter is identically zero. It is found that neutral-current mixing of the $2s^2$ $J = 0$ and $2s2p$ $J = 0$ levels yields a polarization asymmetry of 10^{-7} .

II. ACTIVITIES

A. Personnel

Dr. Michael S. Pindzola (P.I.) is supported full-time on the grant for the summer of 1993. Dr. Thomas W. Gorczyca is supported full-time as a Research Fellow on the grant for the calendar year 1993.

B. Conferences and Workshops

- 1) Dr. N.R. Badnell visited Auburn University in January 1993 to consult with Dr. M.S. Pindzola.
- 2) Drs. M.S. Pindzola, N.R. Badnell, and T.W. Gorczyca visited Rollins College in January 1993 to consult with Dr. D.C. Griffin.
- 3) Dr. M.S. Pindzola visited ORNL in March 1993 to consult with Drs. F.W. Meyer and D.R. Schultz.
- 4) Dr. T.W. Gorczyca attended the APS Meeting of the Division of Atomic, Molecular and Optical Physics in May 1993 in Reno, Nevada. Dr. Gorczyca presented two contributed papers.
- 5) Dr. M.S. Pindzola attended the APS Meeting of the Division of Computational Physics in June 1993 in Albuquerque, New Mexico. Dr. Pindzola presented an invited paper.
- 6) Dr. M.S. Pindzola visited LANL in June 1993 to present a theoretical physics colloquium.
- 7) Dr. M.S. Pindzola visited ORNL in June and July 1993 to consult with Drs. F.W. Meyer, D.R. Schultz, and D.C. Griffin.
- 8) Dr. M.S. Pindzola attended the 18th ICPFAC in July 1993 in Aarhus, Denmark. Dr. Pindzola presented an invited paper.
- 9) Dr. M.S. Pindzola visited JET in July 1993 to consult with Drs. H.P. Summers, N.R. Badnell, and D.C. Griffin.

- 10) Dr. T.W. Gorczyca visited Rollins College in August 1993 to consult with Dr. D.C. Griffin.
- 11) Dr. M.S. Pindzola visited ORNL in August 1993 to consult with Drs. F.W. Meyer and D.R. Schultz.
- 12) Drs. N.R. Badnell and D.C. Griffin plan to visit Auburn University in September 1993 to consult with Dr. M.S. Pindzola.
- 13) Dr. M.S. Pindzola plans to attend the APS Meeting on Atomic Processes in Plasmas in September 1993 in San Antonio, Texas. Dr. Pindzola will present a contributed paper.
- 14) Dr. M.S. Pindzola plans to visit ORNL in both October and November 1993 to consult with Drs. F.W. Meyer and D.R. Schultz.

C. Computing

From indirect cost recovery funds, Dr. M.S. Pindzola purchased 2 Sun Sparc Classic Workstations (16 MB internal, 424 MB external) in January 1993. From a special DOE funded equipment grant, Dr. M.S. Pindzola purchased 1 Sun Sparc 10/52 Workstation (128 MB internal, 1 GB external) and 2 additional Sun Sparc Classic Workstations in June 1993. One of the Sun Sparc Classic Workstations was delivered to Dr. D.C. Griffin at Rollins College in August 1993. Even though the bulk of our computational work remains on the CRAY supercomputers at NERSC, we plan to farm some of our work to the Sparc 10/52 and Sparc Classic workstations in the coming years.

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T.W. Gorczyca, M.S. Pindzola, N.R. Badnell, and D.C. Griffin, to be submitted to Phys. Rev. A, see draft in Appendix C.
7. "Dielectronic Capture Processes in the Electron-Impact Ionization of Sc^{2+} "
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