THEORETICAL ATOMIC PHYSICS FOR FUSION

1992 Annual Report

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by

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The understanding of electron-ion collision processes in high temperature plasmas remains a key factor in the ultimate development of nuclear fusion as a viable energy source for the nation. Our 1990-1992 research proposal delineated 3 main areas of research in electron-ion scattering theory. In the paragraphs below we summarize our 1992 efforts in each of these research areas.

I. RESEARCH

1. Electron-Impact Excitation of Atomic Ions

a. Excitation of Ar^{7+}

Guided by our predictions¹ of relatively large cross sections for the $3s \rightarrow 3p$ transition in Na-like atomic ions, the JILA/ORNL experimental group extended their successful merged-beams measurements on the Si^{3+} ion² to the examination of the Ar^{7+} ion³. To help analyze the Ar^{7+} experimental results, we carried out a series of differential cross section calculations in both the close-coupling and distorted-wave approximations. Contrary to our earlier differential cross section results at 100 eV⁴, which showed strong forward scattering in agreement with the LAGRIPPA experiments⁵, the Ar^{7+} results at low energies showed strong backward scattering. The fact that electrons are preferentially scattered in the backward direction in the threshold region explains why the merged-beams measurements fall off so dramatically for energies beyond a few eV above threshold. In Figure 1 we show the agreement between theory and experiment for the total cross section for the $3s \rightarrow 3p$ excitation of the Ar^{7+} ion.

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Figure 1: Electron-impact excitation of Ar^{7+} . Solid curve: theory (Ref. 1); solid circles: experiment (Ref. 3)

b. Excitation of Mg-like Ions

To guide future JILA/ORNL merged-beams measurements, and to further test the viability of resonance distorted-wave theory, we started a series of total and differential cross section calculations for the Si^{2+} , Ar^{6+} , Ti^{10+} , and Fe^{14+} ions. Based on earlier calculations by the group at Belfast, we decided that Si^{2+} was the prime candidate because of very large resonance structures for the $3s^2\ 1S \rightarrow 3s3p\ 3P$ transition in the threshold region. We have reproduced the total cross section results of Baluja et al.⁶ and extended their work to the calculation of differential cross sections in the resonance region. The angular spread of scattered electrons is an important quantity to know for a proper interpretation of the merged-beams experiment.

c) Excitation of H-like Ions

The excitation of the 2s and 2p states of H-like ions with $Z \geq 26$ were calculated in a fully relativistic distorted-wave approximation⁷. The importance of including the Moller interaction for the more highly charged ions was demonstrated.

2. Electron-Impact Ionization of Atomic Ions

a. Ionization of Ti^{3+}

We completed 21-state and 26-state R-matrix calculations for the excitation-autoionization contributions to the total ionization of the Ti^{3+} ion⁸. In Fig. 2 we compare the close-coupling calculation with the crossed-beams experiment of Falk et al.⁹ When all the LS terms within an excited configuration (19 for $3p^5 3d^2$) are included in the close-coupling expansion, improved agreement with experiment is achieved over earlier theoretical efforts¹⁰. In addition, convergence of the close-coupling method was found to be difficult

Figure 2: Electron-impact ionization of Ti^{3+} . Solid curve: theory (Ref. 8); solid circles: experiment (Ref. 9)

for excitation of the 16 bound LS terms of $3p^5 3d^2$; autoionizing decays to the $3p^6 nl$ singly excited states of Ti^{3+} were found to be important to fairly high n and l .

b) Ionization of Sc^{2+}

We carried out a 21-state R-matrix calculation for the excitation-autoionization contributions to the total ionization of the Sc^{2+} ion. All 19 LS terms within the $3p^5 3d^2$ configuration are autoionizing and were included in the close-coupling expansion. In Fig. 3 we compare the close-coupling calculation with the crossed-beams experiment of the Giessen group, both unpublished. The large difference between theory and experiment is a puzzle at this time. If we use the Ti^{3+} calculations as a guide, the theoretical cross section results should decrease when further singly-excited channels are included.

c) Ionization of Li^+

We completed 11-state and 37-state R-matrix calculations of the contribution of double-excitation followed by autoionization to the electron-impact ionization of the Li^+ ion¹¹. Our atomic structure calculations were performed using the latest MCHF package of C. Fischer's group¹². In Fig. 4 we compare the 37-state close-coupling calculation with the crossed-beams experiment of Muller et al.¹³ The agreement between theory and experiment has dramatically improved over our earlier efforts¹⁴.

Figure 3: Electron-impact ionization of Sc^{2+} . Solid and dashed curves: close-coupling calculation; solid circles: crossed-beams experiment

Figure 4: Electron-impact ionization of Li^+ . Solid curve: theory (Ref. 11); solid circles: experiment (Ref. 13)

d) Ionization of W and W^+

The near-threshold electron-impact ionization cross sections for W and W^+ were calculated in a First-Born distorted-wave approximation¹⁵. A shape resonance was found to have a large effect on the total cross sections for 6s and 5d subshells in neutral Tungsten, but not in W^+ . The shape resonance is most clearly defined when one examines the differential cross section with ejected energy. Our original motivation for examining W is a revived interest in this highly refractory metal for use in fusion reactor divertors.

e) Ionization of Li-like, Be-like, and B-like ions

Contributions from direct ionization, excitation-autoionization, and dielectronic-capture double-autoionization were calculated for the Li-like, Be-like, and B-like ions of Fe, Kr, and Xe¹⁶. Isonuclear and isoelectronic trends for the various contributions were examined, in particular the resonance contributions. Comparisons in the Li-like ions were made with the earlier calculations by Chen and Reed¹⁷.

f) Ionization of Si^{9+} ions

Electron-impact ionization cross sections for the 2s and 2p subshells of Si^{6+} and Si^{7+} were calculated in a First-Born distorted-wave approximation. In Fig. 5 we compare theory with the crossed-beams measurements made at ORNL for the Si^{7+} ion¹⁸. The configuration-average excitation and ionization codes are now on the RISC workstation at ORNL for future use by the experimental group.

Figure 5: Electron-impact ionization of Si^{7+} . Solid curve: distorted-wave calculation; solid circles: experiment (Ref. 18)

3. Electron-Impact Recombination of Atomic Ions

a) Dielectronic-recombination of Ar^{15+} and Au^{76+}

In support of experiments at GSI-Darmstadt we calculated the dielectronic-recombination cross sections for the Li-like ions Ar^{15+} and Au^{76+} . The Ar^{15+} cross section is enhanced by electric fields at the high- n Rydberg series limit. In Fig. 6 we show the agreement between theory and experiment for Au^{76+} , for which relativistic effects are important¹⁹.

b) Dielectronic-recombination via the hyperfine transition in Bi^{82+}

In support of laser assisted experiments at GSI-Darmstadt we calculated the dielectronic and radiative recombination cross sections between the hyperfine levels of the ground state of the Bi^{82+} ion²⁰. The dielectronic recombination cross section is strongly peaked towards zero energy, but its overall magnitude is extremely small when compared to the radiative recombination background.

c) Dielectronic recombination of C^{4+} and Se^{25+}

In support of experiments at MPI-Heidelberg we calculated the dielectronic recombination cross section for the ground states of C^{4+} and Se^{25+} . The preliminary agreement between theory and experiment for Se^{25+} , over an energy range of almost 2000 eV, is excellent.

d) Dielectronic recombination of O^+

The dielectronic recombination rate coefficient for O^+ was re-examined in the light of a recent close-coupling calculation by the Belfast group²¹. Differences between the distorted-wave and close-coupling results can be largely attributed to atomic structure configuration-interaction effects²².

recombination rate ($10^{-9} \text{ cm}^3/\text{s}$)

Figure 6: Electron-impact recombination of Au^{76+} . Solid curves: theory (Ref. 19); solid circles: experiment (Ref. 19)

e) JET/Auburn Project

Our joint theoretical project with H. Summers of JET to generate accurate dielectronic recombination rate coefficients for hot, dense plasmas is well underway. Zero density $n\ell$ bundled rate coefficients for all H-like, He-like, Li-like, Be-like, B-like, C-like, N-like, O-like, F-like, Ne-like, Na-like, and Mg-like ions with atomic numbers $Z = 2, 3, 4, 5, 6, 8, 12, 18, 26,$ and 39 have been calculated. The YMP at NERSC has been kept busy.

f) Validity of the independent-processes and isolated-resonance approximations

We examined the physics behind the continued success of the independent-processes and isolated-resonance approximations in predicting the high-resolution recombination cross sections observed in the current generation of electron-ion experiments²³. First-step extensions of theory to include the effects of radiative-dielectronic recombination interference, overlapping-resonance structures, and scattering-channel coupling were shown to be relatively small for these recombination experiments.

II. ACTIVITIES

1. Personnel

Dr. Michael S. Pindzola (P.I.) is supported full time on the grant for the summer of 1992. Dr. Nigel R. Badnell is supported full time as a Research Fellow on the grant until September 15, 1992. After that date he will assume his duties as a tenure-track Assistant Professor in the Department of Physics at Auburn. Dr. Thomas W. Gorczyca will be supported full time as a Research Associate on the grant starting September 15, 1992. Panos Gavras, a 2nd year Auburn graduate student, will hopefully start his research toward a Ph.D. in atomic theory after his doctoral exams in October.

2. Conferences and Workshops

- a) Dr. Badnell visited Rollins College in Winter Park, FL in January, 1992 to consult with Dr. Donald C. Griffin
- b) Dr. Badnell visited JET in Abingdon, U.K. in March, 1992 to consult with Dr. Hugh P. Summers
- c) Drs. Pindzola and Badnell attended an "Electron-Ion Collisions" workshop in Atlanta, Georgia in April, 1992. Dr. Pindzola presented an invited paper.
- d) Following the Atlanta meeting in April, 1992, Drs. Donald C. Griffin and Keith H. Berrington visited Auburn for a weekend discussion on R-matrix methods.
- e) Drs. Thomas W. Gorczyca and Rina H. Bardfield visited Auburn in May, 1992 to interview for the now available DOE Research Associate position.
- f) Drs. Pindzola and Badnell attended the APS Division of Atomic, Molecular, and Optical Physics Meeting in Chicago, Illinois in May, 1992 to present two contributed papers.
- g) Drs. Pindzola and Badnell attended a DOE review of the atomic physics program in the Physics Division at ORNL in May, 1992.
- h) Dr. Pindzola visited the Physics Division at ORNL in June, 1992 to consult with Dr. David R. Schultz and others.

- i) Dr. Donald C. Griffin visited Auburn for a week in July, 1992.
- j) Dr. Pindzola visited the Physics Division at ORNL in August, 1992 to consult with Drs. Chris Bottcher, David R. Schultz and others.
- k) Dr. Badnell visited JET in Abingdon, UK in August, 1992 to consult with Dr. Hugh P. Summers.
- l) Dr. Pindzola plans to attend a workshop on "Atomic and Nuclear Processes in Astrophysics" in Oak Ridge, TN in September, 1992.
- m) Dr. Pindzola plans to attend a conference on "The Physics of Highly Charged Ions" in Manhattan, Kansas in September, 1992.
- n) Dr. Pindzola plans to attend an APS Southeastern Sectional Meeting in Oak Ridge, TN in November, 1992.

3. Other

Drs. Pindzola, Griffin, and Badnell wrote two review articles, one entitled "Beyond the Standard Computational Model for Dielectronic Recombination of Atomic Ions" for a NATO workshop in Ireland, the other entitled "Theoretical Calculations of Angular Distributions of Inelastically Scattered Electrons from Multiply-Charged Ions" for the conference on the Physics of Highly Charged Ions in Kansas.

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