MASTER

THEORETICAL STUDIES OF HIGHLY IONIZED SPECIES

Progress Report

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Abstract

Applications were continued of the relativistic random phase approximation and of the model potential method and the properties of highly stripped ionic systems were calculated. Charge transfer recombination and ionization were identified as important processes in plasmas and calculations were performed of rate coefficients for several systems at thermal energies. A theory was constructed of collision-induced fine-structure transitions involving protons and the interaction potentials for $O^{3+} - H^+$ were calculated.

A study was made of some of the processes that occur when lithium and sodium are subject to laser radiation. Some progress was made towards the development of methods for calculating the effects on atomic systems of intense electric and magnetic fields.

Introduction

We summarize progress in several distinct categories. A list of publications that have appeared or are in press since the last progress report is appended.

1. Model Potential Methods

A large portion of our effort has been directed towards constructing model potentials for the copper and zinc isoelectronic sequences. We have obtained accurate model potentials for Cu , Zn^{+1} , Ga^{+2} and Ge^{+3} . Recent spectroscopic studies by Reader et al. 1979 have made it possible to construct accurate model potentials for the more highly stripped copper-like ions Y^{+11} and Mo^{+14} . With these data we can confidently interpolate and extrapolate the model potential parameters for other members of the isoelectronic sequence. Accurate calculations of energy levels and transition probabilities for the one- and two-valence electron ions of the copper and zinc sequences are being carried out.

Most of the calculations have been completed. Some effort is needed in order to make sure that the calculations have converged to sufficient accuracy, as some problems with basis set for such systems have been encountered.

2. Applications of the Relativistic Random Phase Approximation

We have continued our applications of the relativistic random phase approximation. We have carried out a comprehensive multi-channel study of transitions in the neon

isoelectronic sequence and the zinc isoelectronic sequence. We have initiated calculations of photoionization cross sections of Mg, Mo^{+12} , Zn and Mo^{+30} and we have begun an exploration of the contributions from excitation of inner shell electrons followed by Auger ionization.

3. Charge Transfer

We have been engaged in a comprehensive study of the charge transfer of multiply-charged ionic systems at thermal energies. We have developed procedures for the explicit construction of diabatic states and we have carried out detailed calculations of the interaction potentials and of the coupling matrix elements.

We have preliminary results for several cases for temperatures up to 50,000 K. They confirm expectations that charge transfer can be very rapid but in exceptional cases may be very slow.

Table 1 contains the results of comprehensive quantal calculations. They are as yet preliminary and further computational checks are needed.

We have also used the Landau-Zener approximation to construct a larger table of rate coefficients, which will be available shortly.

We have explored the effects of charge transfer recombination and ionization processes in shock-heated plasmas and in the solar coronal plasma. The consequences can be very large.

4. Excitation of Fine Structure Levels

In collaboration with Dr. S. Green we have calculated the interaction potentials for O^{3+} and H^+ and we have nearly completed the computer code that will solve the coupled equations which describe the scattering.

5. Laser Processes

We are interested generally in processes which can be studied using laser techniques. We have examined the efficiencies of some of the processes that affect the excited levels of Li_2 and Na_2 when subjected to laser radiation and we have calculated the effective dissociative photoionization cross sections. We have also explored the mechanism of accidental photodissociation.

We have analyzed recent long-pulse-length laser experiments in sodium and lithium and we have carried out calculations which show that effective transfer of the excitation energy of the 3p (2p in Li) level to "seed" electrons via superelastic collisions leads to rapid ionization. Two-photon ionization of the 3p level and laser-induced ionizing collisions provide sufficient "seed" electrons, although photon interactions with Na_2 also provide a significant source of initial ionization.

6. Atoms in Intense Magnetic and Electric Fields

We have made some progress in developing procedures that

will permit the accurate calculation of the effects of intense fields and we have initiated efforts to incorporate model potential methods so that systems of immediate experimental interest can be studied.

Papers published or submitted 1979

- Photodissociation of Na_2^+ , by T. Uzer and A. Dalgarno, Chem. Phys. Lett. 61, 213, 1979.
- The Photodissociation of CH^+ through Absorption into Shape Resonances of the $A^1\Pi$ State, by T. Uzer and A. Dalgarno, Chem. Phys. Lett. 63, 22, 1979.
- Resonant Dissociative Photoionization of H_2 , by K. Kirby, S. Guberman, and A. Dalgarno, J. Chem. Phys. 70, 4635, 1979.
- Photodissociation of Li_2^+ Ions, by T. Uzer and A. Dalgarno, Chem. Phys. Lett. 65, 1, 1979.
- Application of the Relativistic Random-Phase Approximation to Atoms of the Neon Isoelectronic Sequence, by P. Shorer, Phys. Rev. A 20, 642, 1979.
- Diabatic Molecular State, by T. Heil and A. Dalgarno, J. Phys. B: Atom. Molec. Phys. 12, L557, 1979.
- Charge Transfer of O^{++} and Ne^{++} with H, by S.E. Butler, C.F. Bender and A. Dalgarno, Ap. J. 230, L59, 1979.
- Nonadiabatic Long Range Forces, A. Dalgarno and P. Shorer, Phys. Rev. A, October 1979.
- Silicon Lines as Spectral Diagnostics: The Effect of Charge Transfer, by S.L. Balinas and S.E. Butler, to be published in Ap. J. Letts.
- Diabatic and Resonance Molecular States, by A. Dalgarno, to be published in Physica Scripta.

Ab Initio Potential Curves and Coupling Matrix Elements for
Charge Transfer from H to N^{++} and N^{+++} , by S.E. Butler,
to be published in the Physical Review.

Radial Couplings for Charge Transfer, by S.E. Butler, to be
published in Phys. Rev.

Intercombination Line Oscillator Strengths for the Mg I
Isoelectronic Sequence, by C. Laughlin and G.A. Victor,
to be published in Ap. J. 1979.

Charge Transfer of C^+ and S^+ in Diffuse Nebulae, by S.E. Butler
and A. Dalgarno, to be published in Astron. Astrophys.

Radiative Decay of the $2^3P_0^o$ Level of Beryllium-Like Ions, by
C. Laughlin, J. Phys. B: Atom. Molec. Phys., to be
published.

Charge Transfer in Astrophysical Shocks, by S. E. Butler and
J. C. Raymond, Submitted to Ap. J.

Table 1

Rate Coefficients in $\text{cm}^3 \text{s}^{-1}$ for Charge Transfer Recombination

$X^{n+} + H \rightarrow X^{(n-1)+} + H^+$ at Temperature T(K)

C^{+2}	3.2×10^{-11}
C^{+3}	5.5×10^{-9}
N^{+2}	4.8×10^{-10}
N^{+3}	9.5×10^{-9}
O^{+2}	1.7×10^{-9}
O^{+3}	1.8×10^{-8}
Ne^{+2}	1×10^{-15}
Ne^{+3}	1.3×10^{-8}