000-2887-1

MASTER

THEORETICAL STUDIES OF HIGHLY IONIZED SPECIES

Progress Report

for Period March 1, 1976 - February 28, 1977

A. Dalgarno and G. A. Victor

Harvard College Observatory

November 1976

Prepared For

**The U. S. Energy Research and Development Administration
Under Contract No. EY-76-S-02-2887.*000**

DISCLAIMER

This report was prepared as an account of work sponsored by an agency of the United States Government. Neither the United States Government nor any agency Thereof, nor any of their employees, makes any warranty, express or implied, or assumes any legal liability or responsibility for the accuracy, completeness, or usefulness of any information, apparatus, product, or process disclosed, or represents that its use would not infringe privately owned rights. Reference herein to any specific commercial product, process, or service by trade name, trademark, manufacturer, or otherwise does not necessarily constitute or imply its endorsement, recommendation, or favoring by the United States Government or any agency thereof. The views and opinions of authors expressed herein do not necessarily state or reflect those of the United States Government or any agency thereof.

DISCLAIMER

Portions of this document may be illegible in electronic image products. Images are produced from the best available original document.

Abstract

A relativistic generalization of the random phase approximation has been developed that permits the non-perturbative incorporation of relativistic effects and extends the theory to allowed and forbidden transitions of all multipolarities. Calculations for $E1(2^1,^3P_1-1^1S_0)$, $M1(2^3S_1-1^1S_0)$ and $M2(2^3P_2-1^1S_0)$ transitions in the helium isoelectronic sequence for Z up to 100 have been carried out, as well as transitions between excited states for all $n=2$ levels. The method has also been applied to the beryllium isoelectronic sequence.

Model potential methods have been used to calculate $M2$ transitions from the 3P_2 metastable levels of lighter members of the beryllium and magnesium-like ions.

Also studied are: resonating states in the lithium isoelectronic sequence, two-photon processes in sodium, and radiative charge transfers of C^{+2} , C^{+3} and N^{+3} to D.

1. Introduction

We have been engaged in a wide range of activities in theoretical research in atomic and molecular physics that relate to the mission of the Division of Physical Research of the Energy Research and Development Administration. The activities can be placed into several distinct categories, which we discuss in turn.

2. Applications of the Relativistic Random Phase Approximation

The random phase approximation or equivalently time-dependent Hartree-Fock theory has been widely used in the study of allowed electric dipole transitions in atoms and molecules of low nuclear charge (cf. Amusia and Cherephov 1975, Stewart 1975, Stewart, Watson and Dalgarno 1975, 1976, Yeager, Nascimento and McKoy 1975, Watson, Stewart and Dalgarno 1976) that can be described by the L-S coupling scheme. The approximation is remarkably accurate. For large nuclear charges relativistic effects are significant and in order to treat such systems we introduced a relativistic generalization (W.R. Johnson and A. Dalgarno 1975 unpublished) of the random phase approximation that permits the non-perturbative incorporation of relativistic effects and extends the theory to allowed and forbidden transitions of all multipolarities. The method automatically provides the correct angular momentum coupling scheme.

In the initial application (Johnson, Lin and Dalgarno 1976) we calculated the $E1(2^1,^3P_1-1^1S_0)$, $M1(2^3S_1-1^1S_0)$ and $M2(2^3P_2-1^1S_0)$ transition probabilities of a few members of the helium sequence and we also calculated the transition wavelengths. A more comprehensive study for the entire helium sequence up to a nuclear charge Z of 100 was presented later (Johnson and Lin 1976).

We then showed how our relativistic version of the random phase approximation could be used to calculate transitions between excited states and we applied it to study radiative transitions from all the $n=2$ states of the helium isoelectronic sequence (Lin, Johnson and Dalgarno 1977). This paper contains the first estimates of the single photon magnetic dipole decay probabilities of the 2^1S_0 states. The paper revealed some very interesting relativistic effects on energy level positions at intermediate and large Z .

Further work involved beryllium isoelectronic sequence (Lin and Johnson 1977). The results were encouraging. It was shown that neglect of coupling to the inner shell had little effect on the outer shell transitions provided that the length formulation was used.

Inner shell excitation energies and oscillator strengths were also examined and compared with the helium isoelectronic sequence in order to demonstrate the effect of outer shell screening.

3. Model Potential Methods

Model potential methods provide a simple way of accurately predicting those properties of atomic systems which depend mainly on the outer shell valence electrons and they are particularly useful in assessing the accuracy of other approximations which do not contain a comprehensive description of the valence shell electron interactions. We have used them to calculate the probabilities of the magnetic quadrupole transitions $2^3P_2-2^1S_0$ of the beryllium isoelectronic sequence and $3^3P_2-2^1S_0$ of the magnesium isoelectronic sequence (Lin, Victor and Laughlin 1977). For beryllium-like ions, results were obtained for Be, B^+ , C^{2+} , N^{3+} and O^{4+} and for magnesium-like ions results were obtained for Mg, Al^+ , P^{3+} , S^{4+} and Cl^{5+} .

We have developed codes for the calculation of multiphoton processes and we have in particular calculated the two-photon ionization cross section of sodium.

4. Resonating States

Resonating states are metastable bound states embedded in a continuum and they determine the contribution of autoionization to ionization and of dielectronic recombination to recombination. A simple Z-expansion theory was developed earlier (Drake and Dalgarno 1971) and applied to the $2s2p^1, ^3P$ resonances of the helium sequence. We apply it now to the resonance states

of the lithium isoelectronic sequence and explore the contribution of the satellite lines to the emission spectrum of recombining plasma. The satellite lines may be important diagnostic tools (Gabriel 1972, Bhalja, Gabriel and Presnyakov 1975). We have carried out configuration-interaction calculations of the non-relativistic eigenfunctions and eigenvalues of the $1s2p^2\ ^2P$ and $1s2p^2\ ^2D$ states of the lithium isoelectronic sequence. Our preliminary results for the lifetimes of the $1s2p^2\ ^2P$ states disagree with measurement.

5. Charge Transfer

Charge transfer processes are complicated and the cross sections are sensitive to the details of the interacting species. It may be possible to work out general formulas that illustrate the dependence on the nuclear charge in a given isoelectronic sequence and we have attempted to do so. We have obtained preliminary results for charge transfer of completely stripped ions and deuterium atoms at low velocities. Our results are different both quantitatively and qualitatively from those of Olsen and Salop (1976).

We have determined the adiabatic potential energy curves for $N^{++} + D \rightarrow N^+ + D^+$ by elaborate configuration-interaction calculations. We have completed calculations for CIII, CIV and NIII radiative charge transfers to D at low velocities and have computed the thermal rate coefficients.

References

- M. Ya. Anusia and N.A. Cherephov 1975 Case studies in atomic physics 5, 47.
- C.P. Bhalla, A.H. Gabriel and L.P. Presnyakov 1975 M.N.R.A.S. 172, 350.
- G.W.F. Drake and A. Dalgarno 1971 Proc. Roy. Soc. A
- A.H. Gabriel 1972 M.N.R.A.S. 160, 99.
- W.R. Johnson and C.D. Lin 1976 Phys. Rev. A 14, 565.
- W.R. Johnson, C.D. Lin and A. Dalgarno 1976 J. Phys. B 9, L303.
- C.D. Lin and W.R. Johnson 1977 Phys. Rev. A in press.
- C.D. Lin, W.R. Johnson and A. Dalgarno 1977 Phys. Rev. A in press.
- C.D. Lin, G.A. Victor and C. Laughlin 1977 Ap. J. in press.
- A. Salop and R.E. Olsen 1976 Phys. Rev. A 13, 1312.
- R.F. Stewart 1975 J. Phys. B, 8, 1.
- R.F. Stewart, D.K. Watson and A. Dalgarno 1975 J. Chem. Phys. 63, 3222.
- R.F. Stewart, D.K. Watson and A. Dalgarno 1976 J. Chem. Phys. 65, 2104.
- D.K. Watson, R.F. Stewart and A. Dalgarno 1976 J. Chem. Phys. 64, 4995.

Personnel

That the development and applications of the relativistic random phase approximation made such rapid progress was due in large measure to the presence of Professor W.R. Johnson of the University of Notre Dame who was on leave of absence at Harvard University for the academic year 1975-1976 and of Dr. C.D. Lin who was a postdoctoral fellow at Harvard.

Dr. C. Bottcher and Dr. C. Laughlin spent the summer of 1976 at Harvard working on electron-dipole scattering, charge transfer and model potential methods.

Professor Dalgarno's effort is 15% and Dr. Victor's effort is 25%. We expect this level of effort to be maintained during the remainder of the contract period.

Conference Activities

The work on the relativistic random phase approximation was reported by Professor W.R. Johnson at the 1976 Washington meeting of the American Physical Society and in two papers contributed at the Atomic Physics conference held in July 1976 at Berkeley, California. Professor A. Dalgarno and Dr. G. A. Victor attended the ERDA Workshop held in Washington in April where Professor Dalgarno described the work on transition probabilities and on radiative charge transfer. Dr. G. A. Victor presented an invited paper, "Theoretical Studies of Stripped Ions," at the American Physical Society April Washington meeting in 1976. Professor Dalgarno has been invited to present the keynote address on atomic physics processes in both astrophysical and laboratory plasmas at the Topical Conference on Atomic Processes in High Temperature Plasmas to be held in February 1977 at Knoxville, Tennessee.

Papers Published or Submitted

- W.R. Johnson and C.D. Lin 1976 Relativistic Random Phase Approximation Applied to Atoms of the He Isoelectronic Sequence, Phys. Rev. A 14, 565.
- W.R. Johnson, C.D. Lin and A. Dalgarno 1976 Allowed and Forbidden Transitions of Helium-Like Ions, J. Phys. B: Atom. Molec. Phys. 9, 303.
- C.D. Lin and W.R. Johnson 1976 Oscillator Strengths for the Beryllium Isoelectronic Sequence, submitted to Phys. Rev. A.
- C.D. Lin, G.A. Victor and C. Laughlin, Magnetic Quadrupole Transitions of the Beryllium and Magnesium Isoelectronic Sequences, submitted to Astrophys. J.
- C.D. Lin, W.R. Johnson and A. Dalgarno, Radiative Decays of the $n=2$ States of He-Like Ions, submitted to Phys. Rev. A.