COO-1674-85

BASIC STUDIES OF ATOMIC DYNAMICS

MASTER

Progress Report

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ABSTRACT

Several lines of research, mostly interrelated, have advanced this year. The study of the prototype two-electron program has been restarted. Further applications of the Quantum Defect and Frame Transformation methods have been extensive, analyzing and interrelating spectral and collision parameters of Ar, Xe, Al and of the alkaline earths. A new method for R matrix calculations has been developed and tested for Ar. This method is being adapted to a cellular approach to molecular and crystal problems.

Technical Progress Report
on Contract No. AT(11-1)-1674
for the Period October 1, 1972 to September 30, 1973.

October 1, 1973

This year's activity can be characterized as a continuing development of earlier lines of work. New, rather unanticipated branches have been opening up within those lines, even in those we intended to phase out. The development reported under Item 5, barely begun in the previous year, is producing its first most promising pilot results with its full impact probably still far in the future. The size of the group may now be stabilizing at one postdoctoral and three students, in addition to the principal investigator.

1. Scope of the Report. This report covers the scientific activity of the following personnel:

- a) U. Fano, Principal Investigator, nearly 100% of research activity.
- b) Dan Dill, Research Associate from October 1, 1972 to June 30, 1973, supported by this project.
Tu-nan Chang, Research Associate, September 10 to September 30, 1973, supported by this project.
- c) Graduate Students:
C.M. Lee supported for 12 months.
C.D. Lin supported 12 months by NSF Contract NSF GH-33636-MRL and its successor ARPA DAHC-15-73-G-18.
C. Theodosiou supported for 12 months.
- d) K.T. Lu, a former student, has been visiting for 12 months, supported partially as a temporary consultant.

2. Two-electron Problem. The study of the joint motion of two electrons in a Coulomb field, regarded as a main target of this project since its start, has been pressed again since March 1973. C.D. Lin has had a remarkable initial success in interpreting the physical characteristics of the approximate eigenchannels of He double excitation singled out numerically by Macek in 1967-8. We are thus on the track for classifying quasi-constants of the motion for this basic three-body system, and hence for developing effective procedures for calculating its levels and its transition probabilities. A preliminary discussion of the correlation problems in this system has been presented at the Belgrade Conference (C00-1674-78).

3. Channel Interactions and Spectroscopy. Fruitful applications of the frame transformation principle, and of the related Quantum Defect Theory, have continued throughout this year even as we were trying to phase them out. They appear terminated or effectively transplanted at this time. Offshoots of this program are reported in following sections.

The analysis of the perturbed discrete and continuous spectrum of Ar mentioned last year has been successfully completed by Lee and Lu (COO-1674-77) and has brought the method initiated by Lu for Xe to a much higher level of maturity. More elementary applications of the same approach have been made to the analysis of the Al absorption spectrum by C.D. Lin (COO-1674-82) and the analysis of alkaline earth spectra and of their isoelectronic sequences by Lu (COO-1674-84). These applications resolve long standing puzzles in spectroscopic problems of astrophysical interest and should serve to attract further applications by spectroscopists. This work should be continued by Dr. Lu at his forthcoming location at Imperial College, London.

Lin's work on strong effects of channel interaction on cross sections near the threshold of weak channels, mentioned in the previous report, has been brought to successful conclusion (COO-1674-75). Its results have been duplicated by more extensive independent calculations by Amusia's group in Leningrad, but Lin's treatment displays more clearly the analytical structure of the phenomena. Synchrotron light experiments by a British group have confirmed the surprising prediction of a dip in the cross section for photoionization of 3s electrons of Ar shortly above its threshold. Lin has also explained qualitatively the remarkable variations of the double excitation cross sections of He.

Application of the frame transformation principle to the electron-vibration coupling in H_2 — first sketched here in 1970 — has been pressed forward by Dr. Dill to successful numerical calculation of the channel coupling matrix. The input to the calculation consists of Born-Oppenheimer quantum defects drawn from experimental values of neutral H_2 electronic levels and of H_2^+ ion vibrational wave functions. The output should determine the nature and magnitude of the observed major perturbations of vibrational levels as well as the decay probabilities of both autoionizing and pre-

dissociating levels. Preliminary results have been presented at the Belgrade Conference (COO-1674-79). Applications of Dill's results to the accurate theoretical determination of vibrational levels have been carried out successfully by Dr. C. Jungen at Orsay. Applications to autoionization and predissociation will presumably be made by Dr. Dill at his new location at Boston University.

4. Angular Distributions of Reaction Products. Reference is made to the 1972 Report for general remarks on this class of problems.

Dill has extended his earlier work to obtain a detailed prediction of the angular distribution of photoelectrons from autoionizing levels of Xe and of other species (COO-1674-74). This distribution shows sharp spectral variations which are related quantitatively to observed spectral levels and to total photoabsorption cross sections as analyzed previously by Lu and by Lee. Dill's predictions have now been verified in great detail by J. Samson at Nebraska (submitted to Phys. Rev. Letters); minor discrepancies suggest that Samson's angular distribution measurements can determine the basic parameters more accurately than the other spectral measurements previously utilized by our group. Additional results of Dill's remain unpublished.

The increasing volume and variety of experimental studies on the light emitted by collision-excited atoms has stimulated Fano to re-examine the relevant theoretical formulations, in collaboration with Professor J.H. Macek of Nebraska. There resulted a Reviews of Modern Physics article (COO-1674-73) which follows a new pedagogical approach, closely related to experimental procedures, and which may prove very timely in view of still more recent developments.

5. Theory and Calculation of Close-Coupling Eigenchannels.

The exploratory development outlined in Sect. 5 of the 1972 Report has been continued with promising results by C.M. Lee and by Fano. Lee has set up and carried out a pilot calculation of the eigenquantum defects and eigenvectors for an excited argon core in $J=1$, odd parity states. This has been done by an adaptation of variational analytical Hartree-Fock procedures which constitutes in our view a novel and substantial progress with respect to conventional R-matrix calculations. A letter-type report on this work should be prepared in the next few weeks and the main paper - constituting C.M. Lee's thesis - within a few months.

Extensive exploratory work has been done by Fano to generalize this method of calculating eigenstates of a finite-size core for application to the study of polyatomic molecules and of lattices. Relevant features are: a) that the variational method applies to any finite cell volume irrespective of its shape and of the number of its particles, b) that it can take into account particle correlations in contrast to "muffin tin" and other optical potential methods, and c) that the eigenvectors of a boundary problem calculated for any given energy of a cell form a complete system over the cell boundary. Appropriate superpositions of these eigenvectors can then be constructed to match the wave function on the boundaries of adjoining cells. A draft report embodying these concepts has been prepared last June as a basis for informal discussions with colleagues.

6. Electron Ejection into a Crystal Lattice.

Reference is made to the problem formulated in the 1972 Report, p.5, first paragraph. It is also recalled that the influence of the crystal lattice on the spectra of fast photoelectrons (Kronig structures) has been variously discussed over a 40 year period in terms of approximate diffraction theories or of multiple scattering approximations, with great controversies arising among proponents of different approaches. Fano has been seeking a unifying approach that combines the influences of two symmetries, pertaining to the atomic photoemission and to the surrounding lattice, respectively. A first essential step to the solution of this problem has been achieved by constructing a set of wavefunctions analogous to multipole waves, which propagate through the lattice surrounding any given source atom. A preliminary report on this construction has been published (COO-1674-80), but much remains to be done to exploit the results.

7. Effective Interactions and the RPA Method. The exploratory work outlined in Sect. 7 of the 1972 Report has not been pressed by our group this year until the arrival on September 10 of Dr. Tu-nan Chang who is taking responsibility for it. A subtask initiated by Dr. Starace in 1971 has been brought to conclusion by him in London and later at Nebraska and is now being published. An application of RPA methods by C.D. Lin in the course of work on Ar reported in Sect. 3 above has given rise to a methodological improvement which has been reported by him separately (COO-1674-76).

List of Reports

- COO-1674-72 Inner Shell Photoabsorption in Molecules and Crystals, abstract for Invited Talk for the International Symposium for Synchrotron Radiation Users, Daresbury Nuclear Physics Laboratory, Lancashire, England, January 5-7, 1973.
- * COO-1674-73 Impact Excitation and Polarization of the Emitted Light, U. Fano and J. H. Macek, Rev. Mod. Phys. 48, (1973).
- * COO-1674-74 Resonances in Photoelectron Angular Distributions, Dan Dill, Phys. Rev. A 7, 1976 (1973).
- * COO-1674-75 Channel Interaction and Threshold Behavior of Photoionization, C.D. Lin, Phys. Rev. A, in press.
- * COO-1674-76 A Simplified Version of the RPAE Method, C.D. Lin, Phys. Rev. A, in press.
- * COO-1674-77 Spectroscopy and Collision Theory. II. The Ar Absorption Spectrum, C.M. Lee and K.T. Lu, Phys. Rev. A, in press.
- COO-1674-78 Correlations in He**, e+He and in Related Systems, invited Progress Report at 8th International Conference on the Physics of Electronic and Atomic Collisions, Belgrade, Yugoslavia, July 16-20, 1973, to be published in the Conference's volume of invited papers.
- COO-1676-79 Quantum Defect Theory of Vibrational Autoionization in Molecules, Dan Dill, E.S. Chang, and U. Fano, Electronic and Atomic Collisions Vol II, 536 (1973), ed. by B.C. Čobić and M.V. Kurepa, presented at the 8th ICPEAC Belgrade, Yugoslavia, July 16-20, 1973.

- * COO-1674-80 Multipole Waves in Periodic Lattices, U. Fano, Phys. Rev. Letters 31, 234 (1973).
- COO-1674-81 Hydrogenic Wavefunctions in Atomic Slater Integrals, Ted Roth, (unpublished).
- * COO-1674-82 Theoretical Analysis of All Absorption Spectrum, C.D. Lin, Astrophys. J., in press.
- COO-1674-83 Foreign Trip Report (Europe).
- * COO-1674-84 Quantum Defect Analysis of the Effect of np^2 Terms on the Spectra of Alkaline Earths and of Their Isoelectronic Sequences, K.T. Lu, submitted to J. Opt. Soc. Am.
- COO-1674-85 Technical Progress Report 1973.

* Paper accepted or submitted for publication in a refereed or otherwise editorially screened printed journal.

This class includes 52 out of the 85 reports listed in the yearly Technical Reports for 6 3/4 year period January 1, 1967 - September 30, 1973.

Proposed Technical Scope

The University of Chicago

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This continuing project tries to unravel the correlations between the motions of different particles and the energy exchanges between different types of motion in electron collision and photoabsorption processes. Work to be completed in the following months deals with the correlated motion of electrons in the doubly excited states of helium, with a radically new ab initio calculation of excited states of argon and with a new cellular method for calculating energy eigenstates of crystalline and molecular aggregates of atoms.