

BASIC STUDIES OF ATOMIC DYNAMICS

MASTER

Progress Report

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Technical Progress Report
on Contract No. AT(11-1)-1674
for the Period October 1, 1973 to September 30, 1974

September 30, 1974

This year's activity has been marked by major progress on the two-electron problem and by completion of the first phase of work on the direct calculation of R-Matrix eigenchannels. Other lines have also been pursued actively. The size of the group has now been reduced further by loss of the ARPA side-support of a third student; attempts to replace this support have remained unsuccessful.

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) Tu-nan Chang, Research Associate, supported for 12 months.
- c) Graduate Students:
 - C.M. Lee, supported for 6 months as a student and for 5 months as a (low salary) Research Associate.
 - C.D. Lin, supported for 8 months by ARPA DAHC-15-73-G-18 and then by this project for 1 month as a student and for 2 months as a (low salary) Research Associate.
 - C. Theodosiou supported for 12 months by this project.

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 occupied not only the whole effort of C.D. Lin, as anticipated, but also most of Fano's. The main results achieved are reported in detail in Lin's thesis (COO-1674-93) and from a more general point of view in a Heidelberg Conference report (COO-1674-96). The report outlines the task formulated in Section 1 of the 1974 Proposed Technical Program and concludes with the identification of a critical region of configuration space where transitions seem to occur from one reaction channel to another. It also interprets, confirms and generalizes the " \pm " classification and selection rule introduced by Cooper, Fano and Prats in 1963. The results obtained in this work are qualified by persistent short-

comings of the computational procedures, noted in COO-1674-98. Additional numerical and analytical work will be required to confirm and extend our present conclusions.

Lin's work has been complemented by preliminary efforts to connect his treatment of intermediate excitation processes with the Wannier-Rau-Peterkop treatment of threshold ionization. A note on this subject has been prepared (COO-1674-90). A qualitative analytical scheme is now visualized by which lower channel excitations feed into the special type of excitations that lead to ionization. This scheme might be tested initially on the related but simpler problem of generating Landau-type excitations from the ordinary excitations of an atom in a strong magnetic field. A former member of this group, Professor Starace of the University of Nebraska, is pursuing this goal.

3. R-Matrix Eigenchannel Calculation and Frame Transformation Application. (This item corresponds to items 3 and 5 of the 1973 Report and to item 3b, expanded, of the 1974 Proposal.) Completion of the pilot calculation for argon led to the publication of Lee's thesis (COO-1674-89) and of an abbreviated version by Fano and Lee (COO-1674-87). The latter set forth a rather novel approach to eigenvalue problems, whose broad implications have been noted by physicists in quite different fields. Lee moved on quickly to obtain from his results a prediction of the spin orientation of photoelectrons (COO-1674-92). This initial pilot project has raised, but dodged, a number of questions that need exploring to complete the development of the new method.

The extension of the Quantum Defect and Eigenchannel procedures to the spectroscopy of negative ions, applied years ago in limited form, has now been developed more fully by Lee in response to the detection of novel resonances in the photodetachment of Cs. He has completed the analytical work and a numerical application before leaving this project; an abstract has been submitted (COO-1674-99) and he should now prepare a full paper in his new location.

The importance — and difficulty — of turning our development of eigenchannels and Frame Transformation theory into a generally available and powerful tool have been stressed by Fano's recent interactions with many experimentalists — at meetings and during a teaching period at Freiburg. Acceptance of the methods by others is spreading but only slowly. In response to this situation the presentation of the subject is being steadily refined; an invited paper by Fano and Dill has just been presented at an IAU Spectroscopy Colloquium and is being finished up for publication.

4. Incorporation of RPA Procedures into Spectroscopy and Collision Theories and Related Problems. T.N. Chang has devoted a great deal of effort to the main subject, as planned, but has thus far failed to make substantive progress. The matter has acquired even greater importance by Amusia's demonstration, at the Belgrade 1973 Conference, of major effects of intershell interactions on absorption spectra. Fano had also detected this influence in unpublished experimental data on Ba photoionization shown to him in 1973. He stressed this point in a Comment article (COO-1674-86) which has not yet appeared. This subject has then been pursued by Chang in a series of calculations using methods — akin to RPA — previously familiar to him. Some of his results have been reported (COO-1674-94 and 97) and his efforts seem to be converging back into the main topic.

5. Cellular Methods for Molecules and Crystals. This promising topic has not been pursued for lack of manpower, as Fano's efforts were absorbed by the two-electron problem. He could only give a status report at the Hamburg Vacuum UV Conference (COO-1674-91).

6. Other problems. Two topics, which have been peripheral to this project, keep drawing our attention because of their relevance to external work. One of these is the theory of angular distributions, stimulated by the expansion of experimental activities. No concrete results have been obtained by us this year, but — in the wake of the Fano-Macek paper of 1973 — Fano will participate in a

symposium (COO-1674-95). The other topic is the systematic variation of atomic properties throughout the periodic system. Dehmer's past work on this subject by the PAM method has been continued this year by Theodosiou, with particular reference to the evaluation of relativistic effects. A comprehensive report on this work has been nearly ready for several months. The experience gathered in this field underlies the new plan which is being forwarded to the AEC by a separate memo.

List of Reports

- COO-1674-86 Quasi-Resonant Coupling of Atomic Shells. Amusia's Report at the VIII I.C.P.E.A.C., Comments on Atomic and Molecular Physics, 1974 (in press).
- COO-1674-87 Variational Calculation of R. Matrices. Application to Ar Photoabsorption, U. Fano and C.M. Lee, Phys. Rev. Letters 31, 1573 (1973).
- COO-1674-88 Comment on the Singlet-Triplet Splitting of He_I-Like Spectra, T. N. Chang, J. Phys. B 7, No.4, L108 (1974).
- COO-1674-89 Spectroscopy and Collision Theory III. Atomic Eigenchannel Calculation by a Hartree-Fock-Roothaan Method, (Thesis) C. M. Lee, Phys. Rev. A 10, 584 (1974).
- COO-1674-90 Excitation of Atoms to States of High Orbital Momentum, U. Fano, 1974 (in press).
- COO-1674-91 Toward a Theory of Inner Shell Photoabsorption in Crystals, U. Fano, Extended Abstracts, IV Intl. Conf. on Vacuum UV Rad. Phys., Hamburg, Germany, 1974, paper 171.
- COO-1674-92 Spin Polarization and Angular Distribution of Photoelectrons in Autoionization Resonances, C.M. Lee, submitted to Phys. Rev., 1974.
- COO-1674-93 Correlations of Excited Electrons. I. The Study of Channels, (Thesis) C.D. Lin, submitted to Phys. Rev., 1974.
- COO-1674-94 Theoretical Calculation of Multiple Photoionization of Neon, T.N. Chang, 1974 Annual Meeting of DEAP, Am. Phys. Soc., Dec. 2-4, 1974.
- COO-1674-95 Macroscopic Point of View and Technique, U. Fano, abstract for Invited Talk at the 6th Annual Meeting of DEAP, APS, Dec. 2-4, 1974.
- COO-1674-96 Correlations of Excited Electrons, U. Fano and C.D. Lin, presented by invitation at the 4th Intl. Conf. on Atomic Physics, Heidelberg, Germany, July 22-26, 1974 (to be published).

- COO-1674-97 Influence of Electronic Correlation Effects on the Photoionization of Sodium and Potassium, T. N. Chang, (submitted to J. Phys. B), 1974.
- COO-1674-98 Description of Elastic Electron-Hydrogen Scattering in Hyperspherical Coordinates, C. D. Lin, abstract for the 6th Annual DEAP meeting, Dec.2-4, 1974.
- COO-1674-99 Multichannel Photodetachment Theory, C.M. Lee and U. Fano, abstract for the 6th Annual DEAP meeting, Dec.2-4, 1974.
- COO-1674-100 Technical Progress Report 1974.

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ABSTRACT

This year's activity has been marked by major progress on the two-electron problem and by completion of initial development and testing of a novel method for calculating R matrices directly in their diagonal form. The two-electron system appears to pass from one channel to another in the critical region of configuration space (electrons equidistant from the center and on opposite sides) which was identified by Wannier as controlling ionization at threshold. This result may have very great significance. The same may hold for the R-matrix work. Continuing experience with methods developed in earlier years confirms their usefulness but also shows that much refinement and pedagogical work is needed to secure their impact. Other activities have progressed more slowly.