BASIC STUDIES OF ATOMIC DYNAMICS

Progress Report
for Period October 1, 1975 - September 30, 1976

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ABSTRACT

The main effort of the project has been directed this year to resumption and integration of earlier work on two-electron excitations and on R-matrix approach. Progress has been slow but encouraging; in particular it keeps opening up new vistas. Attention has been paid to the relevance of this progress to specific requirements of ERDA applications. Other tasks have been progressing satisfactorily.

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) Hubert Klar, Research Associate, supported for 12 months by the Deutsche Forschungsgemeinschaft.
- c) Research Assistants (Graduate Students) supported by this project as follows:
 - G. Strinati, 12 months.
 - C. E. Theodosiou, 12 months.
 - C. Clark, 9 months.
 - P. Persans, 6 months.
 - G. Duerksen, 2 months.

In addition it reflects continuing part-time collaboration with several former members of the project and with other associates, particularly this year with Dr. M. Inokuti of Argonne National Laboratory.

2. Post-Adiabatic Approximation. Efforts, resumed in earnest this year, to advance the problem of two-electron excitations have absorbed all of Klar's activity and most of Fano's. Most of this effort was devoted to the new goal of identifying more realistically the channels of excitation that had been previously studied by Macek and by Lin in the adiabatic approximation. This goal is also central to the more widely studied problem of atom-atom collisions. Development of an early and very promising and novel lead proceeded, however, only very slowly. Preliminary results have been submitted, and accepted in principle, as a Physical Review Letter (COO-118) but this paper is still being revised. Exploitation of this progress will require much further work.

3. Other Studies of Two-Electron Excitations. Earlier work on this topic has been reviewed by Fano in an invited American Physical Society lecture which has now been published in Physics Today (COO-117). Fano has begun an effort to extend the Macek-Lin treatment of two electrons in the field of a bare nucleus to the

far more general case of electrons in the field of an ion with a complement of electrons. An approach to this problem, which sets forth a number of its essential features, has been outlined in a preliminary report (COO-116); its publication is delayed pending investigation of some complicated aspects. More recently it has also been seen how to fit in the same framework the recently discovered phenomena of post-collision and post-autoionization interaction; a further report on this subject is being prepared.

Klar has prepared and published, since his arrival, earlier important work of his which extends the Wannier-Rau-Peterkop treatment of threshold ionization to the escape of 2 electrons with parallel spins and especially to the escape of three or more electrons (COO-115).

4. Ionization by Electron Collision. Inquiries by ERDA-CTR staff have stimulated Fano and Inokuti to prepare a critical discussion of the available alternative approaches to the calculation of ionization cross-sections. This study combined the experience from the work of this project on low-energy two-electron processes with the earlier information on higher-energy collisions which can be treated in Born approximation. The study - circulated as ANL Report 76-80 (COO-119) - concludes that none of the presently developed methods is adequate for calculating the cross sections of interest but that this goal could be reached by further moderate elaboration of recently developed concepts. The principal goal, agreed to by Professor P. G. Burke, is the extension of current R-matrix procedures to deal with the joint escape of two electrons from a core region.

5. Properties of Highly Stripped Ions. The CTR-related task, described in Item 3b of the 1975 Report, has absorbed considerable effort by Theodosiou and by two junior students in the first half of this year. Extensive calculations have been performed and analyzed on the properties of all ions with atomic number up to 37 in all their charge states. Shortage of senior manpower and of priority have prevented preparation of reports on this subject. The computing and much of the other effort for this task are centered at ANL-RER (Inokuti's group) with consultation and junior manpower contributions from this project. However neither group has felt encouraged to raise the priority of this task.

6. Angular Distribution of Collision Products. Theodosiou's calculations of secondary electrons ejected from sodium by electron collisions (Item 4 of 1975 Report) is just being concluded with results far more significant than anticipated. The results are:

- a) Electrons ejected directly from the outer shell with energies as low as 25-30 eV are strikingly peaked in angle (as though they were free).
- b) This peaking prevents very significant interference with autoionization electrons ejected in other directions.
- c) Therefore this interference could not account for Mehlhorn's experimental results that had motivated our study; our own result has led now to newer experiments which failed to reproduce the earlier finding but agree instead with theory very well.
- d) Above all, Theodosiou's calculations have now been conducted by ab initio methods to a unhopd-for degree of detail; they are in full agreement with current experimental data and provide many additional predictions for future experimental tests. Preparation of a final report is expected in the next few weeks.

7. Application of Atomic Points of View to Crystalline and Molecular Phenomena. The work of Strinati introduced as Item 5 of the 1975 Report, has continued through this year with appreciable participation by Fano. The report prepared last year (COO-108) has since been published in the J. of Math. Physics. Attention has centered this year on the full and appropriate exploitation of the diverse symmetry elements that are present in a crystal lattice or also in polyatomic molecules. The importance has emerged of identifying and evaluating properties of Bloch states averaged over an energy surface in the Brillouin zone. Progress has been slow, but encouraging. A paper on molecular applications remains incomplete. We still aim at bringing Strinati's thesis work to completion in the next year, at which time a fuller report will be in order.

8. Interaction of Electrons with Polar Molecules. The quantum defect and frame transformation methods for analyzing electron-molecule interactions, developed here years ago, have not yet been applied to polar molecules because of difficulties due to the long tail of their interaction. This long tail difficulty has also been plaguing the extensive applications of close coupling calculations to purely atomic problems, in Britain and elsewhere. This circumstance, and the reported relevance of electron-polar molecule interaction in MHD applications, have raised the priority of this problem to the point of assigning a new student, Charles Clark, to it.

Since January 1976 Clark has developed the frame transformation treatment of this problem for its shorter range portion. He is now in the midst of dealing with the long range aspect, with promising prospects.

9. Line Profiles and Threshold Intensities. It had been suggested by us years ago that observation of the profiles of autoionization lines of absorption spectra could serve to predict the threshold intensity of photoionization into the channel to which those lines belong. Discrepancies in the application of this method convinced Fano recently that its underlying concept is in error. The process of locating the error led to a reformulation of the older theory of line profiles and to a study of its relationship to the quantum defect approaches to the same problem. This progress is being reported by Fano in a paper (COO-120) to be submitted to the Physical Review.

List of Reports

- COO-1674-114 Fine Structure for D and F States of Helium Iso-electronic Sequence, Phys. Rev. A 14, 11 (1976). T.N. Chang and R. T. Poe.
- COO-1674-115 Threshold Multiple Ionization of Atoms. Energy Dependence for Double and Triple Escape, J. Phys.B 9, 1699 (1976).
- COO-1674-116 Extending Quantum Defect Theory to Multiple Excitations, preliminary manuscript. U. Fano
- COO-1674-117 Dynamics of Electron Excitation by Collision, Physics Today, September issue 1976.
- COO-1674-118 Post-Adiabatic Analysis of Collisions, Phys. Rev. Lett. H. Klar and U. Fano.
- COO-1674-119 On the Theory of Ionization by Electron Collisions, Argonne National Laboratory Report ANL-76-80 (1976), U. Fano and M. Inokuti.
- COO-1674-120 Autoionization Profiles and Threshold Intensities: Erratum and Addenda, to be submitted to Phys. Rev.
- COO-1674-121 Technical Progress Report 1976.