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20. ABSTRACT (Continue on reverse side if necessary and identify by block number)

Methods of quantum field theory will be applied to prediction of atomic collision and reaction phenomena in gases and partially ionized plasmas, and of the effects of such processes on electromagnetic absorption and emission spectra. Better understanding of such phenomena is important for (a) use of spectra as a diagnostic tool for assessing the state of a gas or plasma under nonequilibrium conditions; (b) prediction of the effect of a gaseous or plasma environment on propagation of electromagnetic radiation.

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Applications of *Quantum Field Theory* to Atomic Collisions and Spectral Lines

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Summary of renewal proposal for
contract N00014-81-K-0759

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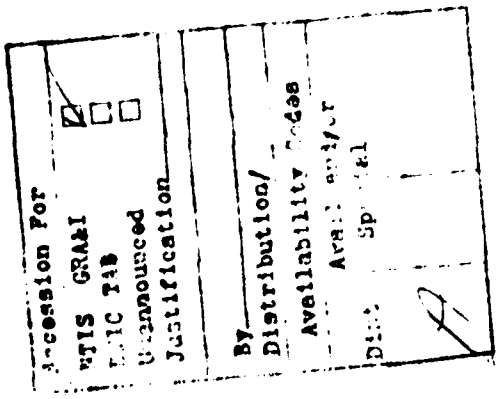

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1. Principal Investigator: Marvin D. Girardeau, Professor of Physics, University of Oregon

2. Contract Description

Methods of quantum field theory will be applied to prediction of atomic collision and reaction phenomena in gases and partially ionized plasmas, and of the effects of such processes on electromagnetic absorption and emission spectra.

During the next contract year (1 July 1982-30 June 1983), cross sections for elastic, inelastic, and reactive collisions will be calculated for simple atomic systems, with emphasis on the contribution of resonance channels.

During the same period, calculations will be carried out for predicting various environmental effects on spectral lines of simple atomic systems. Environmental influences to be investigated will include (1) high-intensity electromagnetic fields, e.g. laser environments; (2) ionic environments (free electrons, atomic ions) of the type present in plasmas in and out of thermal equilibrium; (3) other atoms (gaseous environment); (4) combinations of the above three. These results are expected to be useful in connection with (a) use of spectra as a diagnostic tool for assessing the state of a gas or plasma under nonequilibrium conditions; (b) prediction of the effect of a gaseous or

plasma environment on the propagation of electromagnetic radiation.

3. Scientific Problems

With regard to the atomic scattering calculations, emphasis will be laid on evaluation of the effect of virtual bound and resonance states on the collision cross sections. Electron-hydrogen scattering is a prototype for problems of this type. The incident electron can be temporarily captured by the proton to form an H^- ion or Feshbach resonance state, which then dissociates, with the electron re-emitted. Such virtual bound state and resonance effects can make important contributions to the calculated cross sections and are straightforward to include by using our new representation for the scattering problem.

With regard to the calculations of spectral line shifts, widths, and shapes, little has been done previously with regard to first-principles calculation of the effects of nonequilibrium environments on spectral lines. Our new "Liouvillian Green's function" approach is well-adapted to prediction of such effects.

4. Scientific and Technical Approach

The new approach which will be used for the atomic scattering calculations is that of the "Fock-Tani representation" developed by the Principal Investigator and

his co-workers*. This method is based on a canonical transformation which transforms the Fock-representation Hamiltonian of the standard quantum field theoretic approach to atomic scattering theory** so as to introduce new field operators for the various composite bound states (atoms, molecules, ···) involved in the given scattering process, and new terms in the interaction Hamiltonian which depend explicitly on the wave functions of these bound states. This representation is very convenient for calculating contributions of processes such as that discussed in Sec. 3 of this report. The Fock-Tani representation Hamiltonian for positron-hydrogen scattering has been recently evaluated*** by the PI and some related work on incorporation of the positronium channel into the standard field-theoretic scattering theory formalism has been carried out by E. Ficocelli Varrachio****. In the second contract year we will apply the same techniques to electron-atom scattering problems of the type discussed in Sec. 3. Dr. Ficocelli Varrachio is an Associate Professor of Chemistry and member of the Centro Studio Chimica Plasmi, CNR (Italian

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*M. D. Girardeau, Phys. Rev. Lett. 27, 1416 (1971);
M. D. Girardeau, J. Math. Phys. 16, 1901 (1975);
M. D. Girardeau and J. D. Gilbert, Physica 97A, 42 (1979).

**Gy. Csanak and H. S. Taylor, Adv. At. Mol. Phys. 7, 287 (1971).

***M. D. Girardeau, "Fock-Tani representation for positron-hydrogen scattering" Phys. Rev. A (accepted for publication).

****E. Ficocelli Varrachio, Lett. Nuovo Cim. 31, 595 (1981).

National Science Foundation) at the Unversita di Bari, Italy. He is spending the 1982 calendar year at the University of Oregon as a Visiting Associate Professor of Physics, working full time with the PI on this project. His expertise in both the quantum field theoretic approach to scattering problems and in its implementation through detailed numerical calculations* will be invaluable. Numerical calculations using the University of Oregon's DEC 1091 computer are underway and will continue during the second contract year.

The new method which will by used for the calculations of environmental effects on spectral lines will be that of "Liouvillian Green's functions"**, developed by the PI and his Postdoctoral Research Associate Charles F. Hart, who began work on this project in October 1981 and will continue during the second contract year. The method is based on operator basis expansions of the relevant Heisenberg equations of motion; for details see the references cited.

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*E. Ficocelli Varrachio, J. Chem. Phys. 66, 2026 (1977).

**M. D. Girardeau, in Lecture Notes in Physics, Vol. 142, Recent Progress in Many-Body Theories. Proceedings, Oaxtepec, Mexico, 1981, eds. J. G. Zabolitzky, M. de Llano, M. Fortes, and J. W. Clark (Springer-Verlag, Berlin, Heidelberg, New York, 1981), pp. 355 ff.; M. D. Girardeau "Liouvillian Green's functions and self energies for energy shift and decay phenomena", Phys. Rev. A (submitted); M. D. Girardeau and C. F. Hart, "Liouvillian Green's function theory of spectral line shape", Phys. Rev. A (submitted).

The method is well-adapted to calculation of the modifications of spectral lines due to nonequilibrium environments which are of frequent occurrence in practical applications (laser environments, hot and nonuniform gases and plasmas). This is not the case for standard thermal Green's functions, which are only applicable to systems in or near equilibrium. Dr. Hart's experience ranges from abstract quantum field theory* to experimental studies of spectra of electron beam excited gases** and of various laser systems***. This is an excellent background for the work of this project, which will apply quantum field theory methods to calculation of effects of laser and ionic environments on spectral lines and electromagnetic wave propagation.

5. Progress

The most important accomplishments during the past contract period were (a) evaluation of the Fock-Tani representation Hamiltonian for positron-hydrogen scattering, (b) development of a general "Liouvillian Green's function" approach for calculation of nonequilibrium environmental

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*De Witt, Hart, and Isham, invited contribution to the Schwinger Festschrift volume Physica 96A (1979); C. F. Hart, Ph.D. Dissertation, University of Texas, Austin, August 1981.

**Keto, Hart, and Kuo, J. Chem. Phys. 74, 4433, 4450 (1981).

***C. F. Hart, unpublished interdepartmental research report, Hughes Aircraft Co.

effects on spectral lines, and (c) testing the general approach (b) by detailed calculations for a two-level atom interacting with an electromagnetic radiation bath. This work is described in detail in the papers cited above as Phys. Rev. A (accepted) and Phys. Rev. A (submitted); see also part 6., below.

6. Publications

M. D. Girardeau, "Fock-Tani representation for positron-hydrogen scattering", Phys. Rev. A (submitted December 1981, accepted March 1982).

M. D. Girardeau, "Liouvillian Green's functions and self energies for energy shift and decay phenomena", Phys. Rev. A (submitted April 1982).

M. D. Girardeau and C. F. Hart, "Liouvillian Green's function theory of spectral line shape", Phys. Rev. A (submitted April 1982).

7. Extenuating Circumstances

The contract year 1 July 1981-30 June 1982 represents the start up phase of this project. ONR funds for the project were not made available to the University of Oregon until October 1981. Dr. Hart was hired as of 1 October 1981 and Prof. Ficocelli Varrachio arrived on 25 January 1982.

8. Budget Status

It is expected that there will be no unspent funds remaining in the budget on 30 June 1982, the end of the current contract period.

9. Graduate Students

No graduate students working on this project received degrees during the current contract period. One student is beginning pre-thesis work with the PI, but is currently supported by the University of Oregon Physics Department as a Teaching Assistant.

10. Other Support

This project currently has no other Federal grant or contract support. It is partially funded by the M. J. Murdock Charitable Trust through the Chemical Physics Institute, University of Oregon. This cost sharing is detailed in the budget for the current contract year and in that of the renewal proposal.