AD-A129 236 APPLICATIONS OF QUANTUM FIELD THEORY TO ATOMIC 1/1
COLLISIONS AND CHEMICAL REACTIONS(U) OREGON UNIV EUGENE
M D GIRARDEAU APR 83 QFT-2 N00014-81-K-0759

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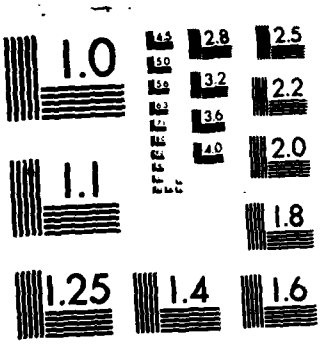

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE	READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER: QFT-2 — 2. GOVT ACCESSION NO.: AD-A129236	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle): Applications of Quantum Field Theory to Atomic Collisions and Chemical Reactions	5. TYPE OF REPORT & PERIOD COVERED: Renewal proposal summary 1 July 1983-30 June 1984
	6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s): Marvin D. Girardeau	8. CONTRACT OR GRANT NUMBER(s): N00014-81-K-0759
9. PERFORMING ORGANIZATION NAME AND ADDRESS: Department of Physics & Institutes of Chemical Physics and Theoretical Science, University of Oregon, Eugene, OR 97403	10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS: NR 394-055
11. CONTROLLING OFFICE NAME AND ADDRESS: Physics Program, Physical Sciences Division Office of Naval Research (Code 421) Arlington, VA 22217	12. REPORT DATE: April 1983
	13. NUMBER OF PAGES: 8
14. MONITORING AGENCY NAME & ADDRESS(if different from Controlling Office)	15. SECURITY CLASS. (of this report): Unclassified
	15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

16. DISTRIBUTION STATEMENT (of this Report)

Approved for public release; distribution unlimited.

17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)

18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Atomic and molecular collisions and reactions

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 and molecular collision and reaction phenomena. Emphasis will be on (a) reactive collisions such as $D^+ + H \rightarrow D + H^+$, $D^+ + H_2 \rightarrow D + H_2^+$, and $A + BC \rightarrow AB + C$; (b) theory of resonance and transition states and their influence on such reactive processes and on scattering processes such as $e + H \rightarrow e + H$; (c) electromagnetic absorption due to such transition states.

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Applications of Quantum Field Theory to Atomic Collisions and Chemical Reactions

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

Unclassified report #QFT-2 prepared for
the Physics Program (Code 421),
Office of Naval Research.

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 1983-30 June 1984), cross sections for elastic, inelastic, and reactive collisions will be calculated for simple atomic and molecular systems. Emphasis will be on (a) reactive collisions such as $D^+ + H \rightarrow D + H^+$, $D^+ + H_2 \rightarrow D + H_2^+$, and $A + BC \rightarrow AB + C$; (b) theory of resonance and transition states and their influence on reactive processes such as the above and scattering processes such as $e + H \rightarrow e + H$; (c) electromagnetic absorption due to transition states of reaction and scattering processes such as the above.

3. Scientific Problems

The most important question to be investigated during the coming year is that of the influence of resonance and transition states on scattering and reaction cross sections. The "Fock-Tani representation" approach which we have been using is particularly well suited to investigation of this

question, since resonance and transition state wave functions can easily be explicitly "built into" the interaction Hamiltonian used for calculations in this representation. Electromagnetic absorption due to transition states of chemical reactions can provide information on the structure of these states and hence on the dynamics of the reactive collision. Calculations of such (in general broad) absorption lines can easily be formulated in the same representation.

4. Scientific and Technical Approach

The general approach to be used for the proposed atomic and molecular scattering and reaction 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 Hamiltonian of the standard quantum field theoretic approach to atomic and molecular 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.

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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).

The method used during the current contract year* to formulate a field-theoretic approach to electron-hydrogen scattering and the reaction $e^+ + H \rightarrow Ps + H^+$ and for calculation of cross sections for the latter process** will be extended to calculate cross sections for the reaction $D^+ + H \rightarrow D + H^+$ by use of a canonical transformation*** which reduces the Hamiltonian to the form used in the positron-hydrogen calculation, allowing use of the computer program used in that calculation. Work will also be started on application of the same methods to the chemical reaction $D^+ + H_2 \rightarrow D + H_2^+$ and to reactions of the form $A + BC \rightarrow AC + B$. The derivation of our Fock-Tani representation Hamiltonian to be used in such calculations has already been carried out by Ficocelli Varrachio**** by generalization of the method used for the positron-hydrogen calculation by him and the P.I. during the current contract year. The work underway on the influence of resonance channels on electron-hydrogen scattering will be continued. Work underway on the general theory of resonance

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*M. D. Girardeau, "Fock-Tani representation for positron-hydrogen scattering" Phys. Rev. A 26, 217 (1982); E. Ficocelli Varrachio, Lett. Nuovo Cim. 31, 595 (1981).

**E. Ficocelli Varrachio and M. D. Girardeau, "Ideal space treatment of the $e^+ + H \rightarrow p + Ps$ process", J. Phys. B 16, 1097 (1983).

***T. D. Lee, F. E. Low, and D. Pines, Phys. Rev. 90, 297 (1953); M. Girardeau, Phys. Fluids. 4, 279 (1961).

****E. Ficocelli Varrachio, "Field theory of chemical reactions. I: Ideal space representation of $A + BC \rightarrow AC + B$ processes" (to be published; preprint, Centro di Studio Chimica Plasmi, C.N.R., Universita di Bari, Italy).

states will be extended to transition states of chemical reactions. Work will be begun on the theory of electromagnetic absorption due to such transition states.

5. Progress

The mostimportant accomplishments duringthe current contract year were (a) calculation of cross sections for the reaction $e^+ + H \rightarrow p + Ps$ by a computer program which evaluates "orthogonalized wave Born approximation" matrix elements typical of our Fock-Tani representation approach; (b) completion of our series of papers on the Liouvillian Green's function approach to the prediction of spectral line shapes, including environmental effects; (c) derivation of a nonlinear integrodifferential eigenvalue equation for the wave functions and complex energies (energy, inverse lifetime) of resonance and transition states of the sort important in calculations of atomic and molecular scattering and chemical reaction cross sections, and numerical solution of this equation for a model potential (double-delta barrier) as a demonstration of the feasibility of this approach to the calculation of resonance wave functions. This work is described in the papers and lectures listed in sections 6 and 7 below.

6. Publications

M. D. Girardeau, "Fock-Tani representation for positron-hydrogen scattering", Phys. Rev. A 26, 217 (1982).

M. D. Girardeau, "Liouvillian Green's functions and self energies for energy shift and decay phenomena", Phys. Rev. A (scheduled for publication January 1983; publication delayed because of insufficiency of page charge funding).

M. D. Girardeau and C. F. Hart, "Liouvillian Green's function theory of spectral line shape", Phys. Rev. A (scheduled for publication January 1983; publication delayed for above reason).

M. D. Girardeau and C. F. Hart, "Liouvillian Green's function approach to nonequilibrium environmental effects on spectral lines", Proceedings of the 6th International Conference on Spectral Line Shapes, Boulder, July 1982 (to be published).

E. Ficocelli Varrachio and M. D. Girardeau, "Ideal space treatment of the $e^+ + H \rightarrow p + Ps$ process", J. Phys. B 16, 1097 (1983).

E. Ficocelli Varrachio, "Field theory of the e^+-H three-body system", Ann. Phys. 145, 131 (1983).

C. F. Hart, "Improved Heisenberg equations-of-motion approach for nonequilibrium decay phenomena", Phys. Rev. A (submitted).

7. Meetings

M. D. Girardeau and C. F. Hart, "Liouvillian Green's function approach to nonequilibrium effects on spectral lines", contributed paper, 6th International Conference on Spectral Line Shapes, Boulder, 12-17 July 1982.

M. D. Girardeau, "Variational principle for decaying states", contributed paper to be presented at DEAP meeting of the American Physical Society, Boulder, 23-25 May 1983.

M. D. Girardeau will be an invited lecturer at the NATO Advanced Study Institute on Quantum Electrodynamics and Quantum Optics, Boulder, 27 May-8 June 1983.

8. Budget Status

It is expected that there will be no unspent funds remaining in the budget on 30 June 1983, 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, Mr. Sungho Kim, is in the initial phases of Ph. D. thesis research under the supervision of the P.I., having been

appointed as a Graduate Research Assistant commencing 1 January 1983. He will participate in the proposed research on calculation of resonance and transition-state wave functions.

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. The Murdock funds are now totally expended and commited, so support from that source will not be available for the renewal.


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