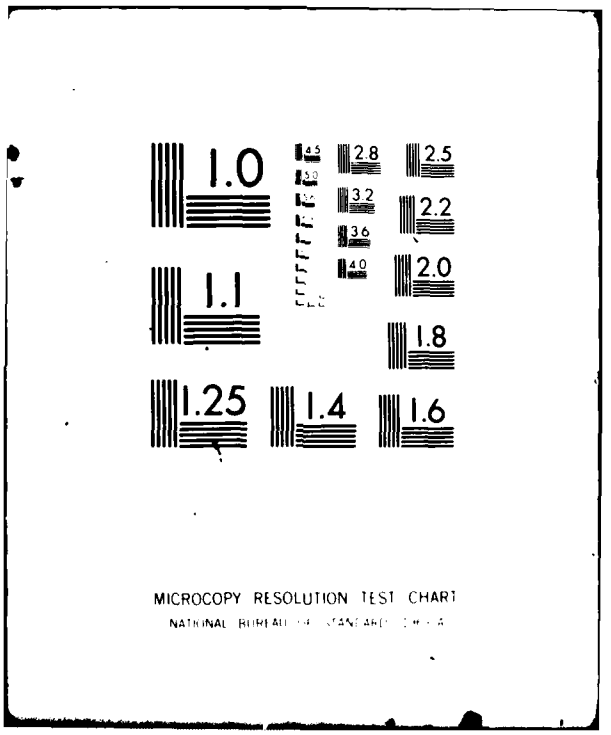
AD-A098 729 TEXAS UNIV AT AUSTIN F/G 20/8
THE STUDY OF ATOM-ATOM, ELECTRON-MOLECULE AND PHOTON MOLECULE P--ETC(U)
JUL 72 J C BROWNE N00014-67-A-0126-0017
UNCLASSIFIED NL


1.0
1.1
1.25
1.4
1.6
1.8
2.0
2.2
2.5
2.8
3.2
3.6
4.0
4.5
5.0
MICROCOPY RESOLUTION TEST CHART
NATIONAL BUREAU OF STANDARDS-1963-A

PHOTOGRAPH THIS SHEET

AD A098729

DTIC ACCESSION NUMBER

II

LEVEL

(1)

INVENTORY

THE STUDY OF ATOM-ATOM, ELECTRON-MOLECULE AND PHOTON MOLECULE PROCESSES

DOCUMENT IDENTIFICATION

N00014-75-C-0498

DISTRIBUTION STATEMENT A
Approved for public release;
Distribution Unlimited

DISTRIBUTION STATEMENT

ACCESSION FOR		
NTIS	GRA&I	☑
DTIC	TAB	☐
UNANNOUNCED		☐
JUSTIFICATION		
PER LETTER		
BY		
DISTRIBUTION /		
AVAILABILITY CODES		
DIST	AVAIL AND/OR SPECIAL	
A		

DISTRIBUTION STAMP

DTIC
ELECTE
S MAY 7 1981 D
B

DATE ACCESSIONED

81 4 27 171

DATE RECEIVED IN DTIC

PHOTOGRAPH THIS SHEET AND RETURN TO DTIC-DDA-2

DTIC FORM OCT 79 70A

DOCUMENT PROCESSING SHEET

→ 0.421

393 010

~~NR 021~~
NR 012-146
1 Cpy
10/4/72 agn

AD A098729

Semi-Annual Report

to the

Office of Naval Research

on

The Study of Atom-Atom, Electron-Molecule and Photon Molecule Processes

Contract No. N00014-67-A-0126-0017
N00014-75-C-0498

Principal Investigator

J. C. Browne
Departments of Computer Science and Physics
The University of Texas at Austin

July 31, 1972

81 4 27 171

TABLE OF CONTENTS

I. Introduction

II. Atom-Atom Scattering

III. Elastic Scattering of Fast Electrons by H_2

IV. Photon Processes

I. Introduction

The funding on this contract was initiated February 1, 1972. A post-doctoral research associate position established under this contract was filled beginning July 1, by Dr. E. Shipsey formerly of Sandia Corporation Laboratories, Albuquerque, New Mexico. During the period February 1, 1972 to July 1, 1972, the research program was carried on by graduate students and by the principal investigator.

II. Atom-Atom Scattering

The package program for the computation of matrix elements over nuclear motion operators acting on approximate eigenfunction of the fixed nuclei hamiltonian has been developed and refined. This program is now being supplied to competent investigators. In particular, Dr. T. H. Green of Sandia Laboratories is investigating the application of this package program to the computation of the coupling matrix elements for HeH+ and arrangements have been made with Dr. Ron Olson and Dr. F. T. Smith of Stanford Research Institute to work together on the computation of transition matrix elements for the scattering of He- by He. A primary focus of attention during this period has been the evaluation of the matrix elements involving the partial derivative with respect to internuclear separation, $\langle \psi_k \mid \partial/\partial R \mid \psi_l \rangle$.

The ψ_k are the set of molecular eigenfunctions

$$H_e \psi_k = E_k \psi_k \tag{1}$$

where H_e is the fixed nuclei electronic hamiltonian.

We represent ψ_k as

$$\psi_k = \sum_i C_i (R)\, \Phi_i \tag{2}$$

We have evaluated three different methods for the computation of these matrix elements.

$$\langle \psi_n \mid \partial/\partial R \mid \psi_m \rangle = \langle \psi_n \mid \sum_i (C_i' (R)\, \Phi_i + C_i (R)\, \Phi_i') \rangle \tag{3}$$

The prime on Φ_i and C_i indicates differentiation with respect to R.

$$\langle \psi_n \mid \partial/\partial R \mid \psi_m \rangle = (E_n - E_m)^{-1} \langle \psi_n \left| \frac{\partial H_e}{\partial R} \right| \psi_m \rangle + \frac{E'}{(E_n - E_m)} \langle \psi_n \mid \psi_m \rangle \tag{4}$$

$$\langle \psi_n \mid \partial/\partial R \mid \psi_m \rangle = (1/2R)\, (E_n - E_m) \langle \phi_n \mid \vec{r} \cdot \vec{r} \mid \phi_m \rangle$$
$$+ [R(E_n - E_m)]^{-1} \langle \psi_n \mid T \mid \psi_m \rangle + \frac{E_n - R\, E'_m}{R(E_n - E_m)} \langle \psi_n \mid \psi_m \rangle \tag{5}$$

The results will be given in detail in the Ph.D. dissertation of Larry L. Lenamon which will be issued as an ONR Technical Report on approximately October 1st. In summary it can be stated that for very accurate wavefunctions and in regions where degeneracies and crossings are not involved, eq. 4 is the most accurate result. Upon other circumstances numerical differentiation, eq. 3, must be resorted to. The Sidis[1] method, eq. 5, does not appear to be of particular value.

Considerable effort has been involved in efforts to obtain the derivative of the coefficients in an accurate and precise way.

III. Elastic Scattering of Fast Electrons by H_2

We have computed the differential elastic scattering cross-section for fast electrons from H_2 in the Born approximation. There have been no previous direct computations of this scattering cross-section. Liu[2] (private communication) has computed the elastic cross-sections by a

differencing procedure from total inelastic scattering cross-sections. An interesting situation whereby theory caused reexamination of experiment has occurred here. Professor Russell A. Bonham of Indiana University, very recently experimentally evaluated the elastic scattering cross-sections for H_2 to a very high accuracy. In a preliminary communication to the principal investigator, Professor Bonham[3] observed that his results did not agree well with our computed results. This disagreement caused a reexamination of the experimental data which lead to a correction in the experimental normalization procedure and subsequent excellent agreement between theory and experiment.

IV. Photon Processes

The study of interaction of photons with molecules alluded to in the proposal submitted in November has been continued and extended. A paper has been submitted to Physical Review containing full details of elaborate studies on the interaction of photons with hydrogen molecules. The subjects of this paper include the Rayleigh and Raman cross-sections as a function of frequency of the dynamic polarizability as a function of frequency and the straggling and stopping power cross sections (a preprint of this paper is attached). This work has demonstrated the validity of the technique proposed by Dalgarno and Epstein[4] for constructing sets of functions which yield a numerically complete resolvent operator in the dipole domain. This work has been extended to the helium molecule where an accurate value of the transition moment for the transition from the $^1\Sigma_g^+$ to the $^1\Sigma_u^+$ states are of considerable interest.

V. Papers to be Published

Preprints of the following papers are enclosed:

5.1 (with A. Lewis Ford and B. Ulrich) "The Translational Absorption of HeH" (to appear in the J. Chem. Phys., Oct. 1, 1972).

5.2 (with A. Lewis Ford) "Direct Resolvent Operator Computations on the Hydrogen Molecule Dynamic Polarizability, Rayleigh and Raman Scattering" (to appear in Phys. Rev.).

The following manuscripts are in preparation and will be submitted to the journals:

5.3 (with A. Lewis Ford and E. M. Greenawalt) "Adiabatic Corrections to the Potential Energy Curves for the Hydrogen Molecule" (to be submitted to the J. Chem. Phys.).

5.4 (with A. Lewis Ford) "The Elastic Scattering of Fast Electrons by the Hydrogen Molecule" (to be submitted to Chem. Phys. Letters).

5.5 "A Survey of Atomic and Molecular Processes" (to appear in the Proceedings of the Summer Research Conference on Theoretical Chemistry).

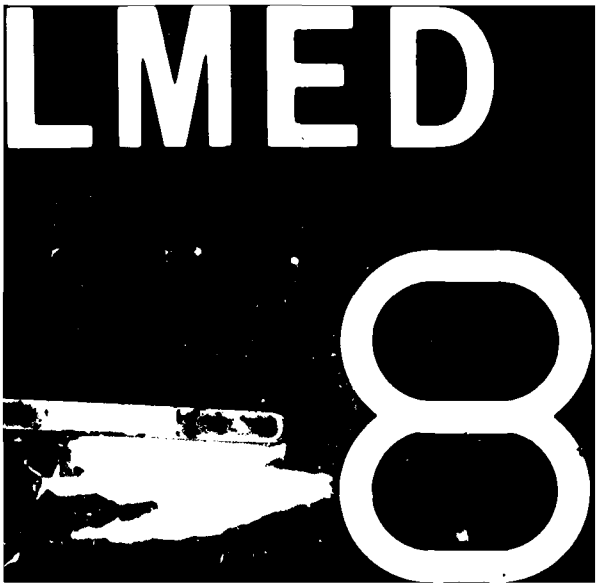
REFERENCES

1. V. Sidis, J. Chem. Phys. 55, 5838 (1971).

2. J. Liu, Private Communication.

3. R. A. Bonham and H. Wellenstein, Private Communication and preprint.

4. A. Dalgarno and S. T. Epstein, J. Chem. Phys. 50, 2837 (1969).


LMED
8