FORMULATION OF A HAMILTONIAN WITH RELATIVISTIC EFFECTS FOR HEAVY ATOMS

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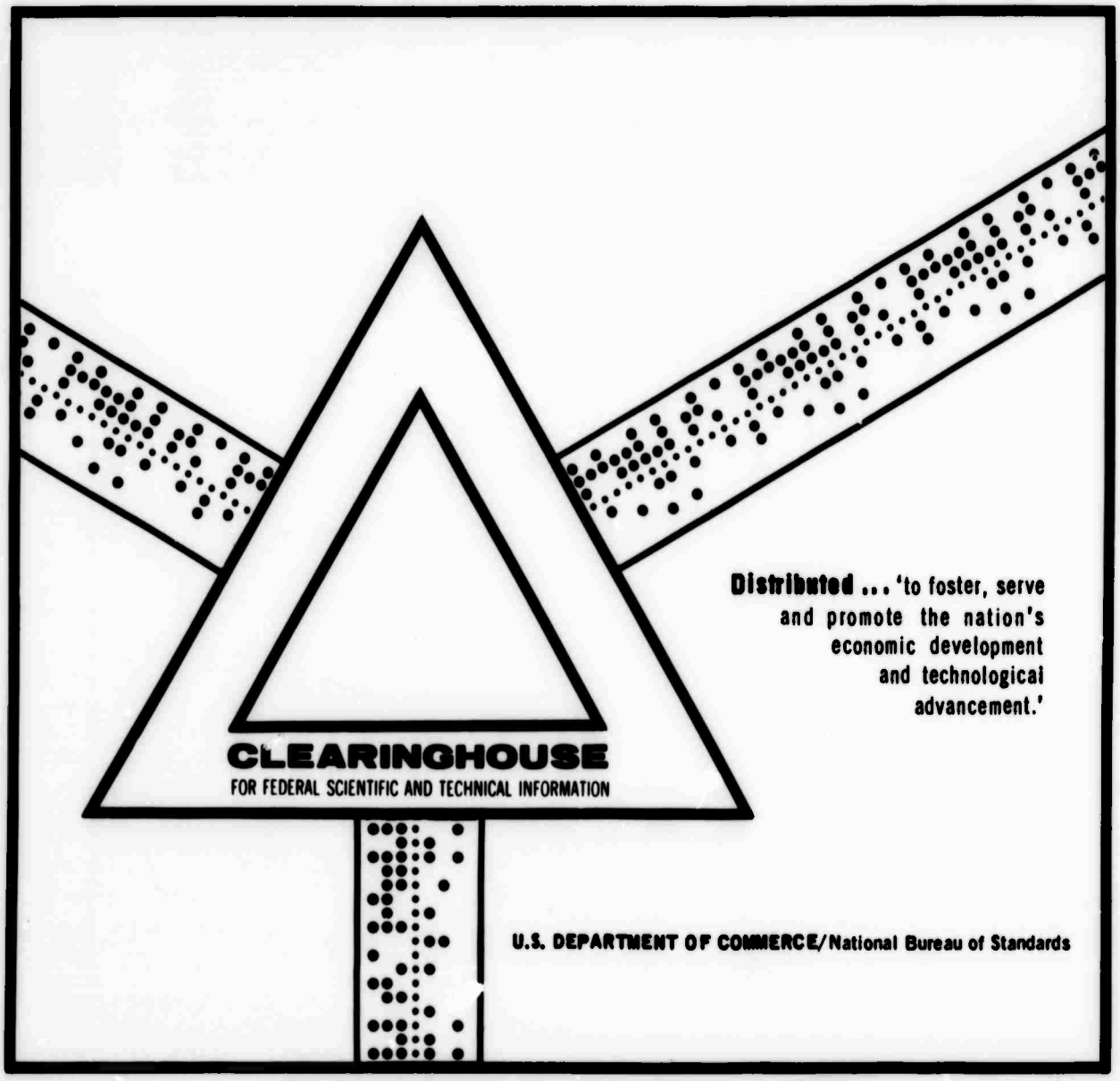

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ABSTRACT

The Atomic Physics program at the Space Sciences Laboratory has dealt with too many programs to abstract each. Instead we merely list the areas of effort and describe each briefly in the succeeding pages.

I. Construction of a Hamiltonian for the Problem of a Heavy Atom.

II. A Critical Assessment of the Polarized Orbital Method in Atomic Scattering.

III. Rotational Excitation of Polar Molecules by Electrons.

IV. Polarization of Atomic Radiation Excited by Electron Impact at Threshold.

V. Excitation of Two Atoms by a Single Photon.

VI. A Model of High Energy Charge Transfer.

VII. Positronium Formation in Positron-Helium Scattering.

VIII. Formal Problems in the Theory of Dissociative Attachment and Recombination.

I. Construction of a Hamiltonian for the Problem of a Heavy Atom

The major effort has been concerned with the derivation of a usable configuration space Hamiltonian for a heavy atom; i.e. for many electrons moving in the strong central field of a high Z point nucleus. The strong field can make the electrons move relativistically, thus the difficulty of the problem. The history and importance of the problem has been previously described so that we shall not repeat it here. The status of our progress can be described as follows:

1. We have first attacked the few body problem where an expansion in α, and $N\alpha$ is possible but not an expansion in $Z\alpha$. Here $\alpha \simeq 1/137$ is the fine structure constant, N is the number of electrons and Z the nuclear charge number. The starting point is a quantum-electrodynamic formulation. A contact transformation on the field theoretic Hamiltonian decouples the radiation field to order α. The Fock space wave function is then expanded in eigenstates of the total charge. For N = 3, it is a superposition of all possible 3 electron states, plus all possible 3 electron plus 1 positron state, etc. The equation of motion couples these amplitudes. It is found that for small N, one can isolate the amplitude of the 3 electron part of the wave function and interpret it as the 3 body wave function. In the process one gets a Hamiltonian containing one electron potentials, two electron potentials, three electron potentials, etc. The one and two body terms have essentially been found previously by Brown[1]. They contain projection operators which eliminate the difficulty pointed out many years

ago by Bethe[2] in connection with the Breit interaction. The three body term is new and complicated. For a heavy ion, iso-electronic with Lithium, the effects of this potential are not negligible.

2. The next step in our program was an attempt to extend this method to the many electron problem, i.e. $N \simeq Z$. In that case the couplings between the N electron and the (N+1) electron + 1 positron amplitudes are not negligible (they contain a factor $N\alpha$). Therefore the elimination of the N+1 electron, 1 positron amplitude introduces a complication in the resultant Hamiltonian which essentially makes it unusable. The saving feature is the fact that the way to define a positron and an electron is not obvious. In (1) an electron (positron) was defined as a positive (negative) frequency state in the Coulomb representation of the field operator. The Coulomb representation is chosen since it is the dominant potential that an electron "sees" for this case. However for the many electron case, the electron "sees" all the other electrons in addition to the nucleus. Hence the Coulomb representation is not appropriate. A different one is chosen and fixed by the condition that the couplings mentioned above which result in a complicated Hamiltonian are to be minimized.

This work is still in progress.

3. The third phase of the program starts from the field theoretic formulation to the many-body generalization of the Bethe Salpeter equation given by Schwinger[3]. This is a many time equation and calculational techniques for it are still rudimentary[4]. We therefore seek a reduction

to a Hamiltonian form of the problem. Salpeter[5] has shown that the two-body B-S equation could be reduced to a Hamiltonian form provided that the interactions were essentially instantaneous. No such reduction has been given for more than two bodies. Our program is the following, (a) we attempt to find a method for this reduction in the presence of arbitrary static two electron interactions. If this can be done, (b) we then do perturbation theory for the original equation perturbing about the Hamiltonian solution. The first order corrections to the energy will contain the difference between the real interactions and the arbitrary static interactions. We chose the static interactions to make this perturbation vanish thereby determining the optimum two body static interaction for a Hamiltonian formulation. This work is in an early stage. Partially presented at the recent "International Atomic Physics Conference" at N.Y.U., June 1968.

Personnel: M. H. Mittleman

II. A Critical Assessment of the Polarized Orbital Method in Atomic Scattering

The polarized orbital[6] method is widely and somewhat successfully used in the problem of electron atom scattering and other related problems. It is an ad hoc method containing two obvious flaws: It utilizes a discontinuous wave function, violating a fundamental requirement of quantum mechanics and determines its final equation arbitrarily. We correct both these flaws at the expense of the introduction of an arbitrary cut off function. We determine equations of motion variationally and parametrize the arbitrary function in an ad hoc manner. The numerical results for electron-hydrogen-singlet-s wave scattering are sufficiently strongly dependent upon the parameters to indicate that the polarized orbital method is not reliable as a predictive model.

To be published in Phys. Rev.

Personnel: M. H. Mittleman and J. L. Peacher

III. Rotational Excitation of Polar Molecules by Electrons

A model in which the polar molecule is replaced by a fixed point dipole is justified in a restricted energy range of the incident electron. The energy range is bounded from above by the effects of replacing the molecule by a point dipole and from below by fixing the orientation of the molecule. An effective cross section, directly related to the diffusion coefficient, is shown to be temperature independent in the model and any violation of this is shown to result from a breakdown in the approximation of fixing the orientation of the molecule. The cross sections exhibit an E^{-1} behavior. Numberical results are presented for a variety of dipole strengths and transitions.

Submitted to Phys. Rev.

Personnel: M. H. Mittleman and J. L. Peacher of Space Sciences Laboratory, and B. F. Rozsnyai of Lawrence Radiation Laboratory, Livermore.

IV. Polarization of Atomic Radiation Excited by Electron Impact at Threshold

An attempt to explain the discrepancy between theory and experiment in polarization of radiation from atoms excited by electrons near threshold has recently appeared[7]. We have shown that this explanation, which was given only at the threshold energy, can not apply to an energy where experiments have yet been done. In the process we have shown that the usual threshold laws, which are consequences only of conservation of angular momentum are not quite correct because of the neglect of spin dependent forces.

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Personnel: M. H. Mittleman of Space Sciences Laboratory, and
R. H. McFarland of Lawrence Radiation Laboratory, Livermore.

V. Excitation of Two Atoms by a Single Photon

Absorption of a photon by a pair of atoms colliding to form a quasi-molecule is considered. The effect provides an absorption line in the continuum. Ignorance of molecular wave functions and eigenvalues forces us to deal only with long range collisions of the atoms, which is in effect a restriction to low density media. For this case we estimate the magnitude and width of the absorption line for excitation of two helium atoms in the states 2^1S and 2^1P. We find the effect to be a small one for this example. However, the effect exists for many pairs of states so that the total absorption via this mechanism may not be small for all cases.

Published -- Physics Lett., 26A, 612 (1968).

Personnel: M. H. Mittleman

VI. A Model of High Energy Charge Transfer

A one dimensional model reproducing many of the features of charge transfer in atomic collisions has been solved numerically. The model consists of an attractive well with a particle in it with a second attractive well moving by. The probability of the transfer of the particle from the first to the second well has been obtained by exact numerical integration of the Schrodinger equation for a large number of values of the speed of the second well. A regularity of the phase of the numerical wave function was noted and then derived from first principles. Application of an analogous derivation to the physical problem of charge transfer between protons and hydrogen was then made with the remarkable result that the high energy cross section is reduced by roughly a factor of two. Further application of this result, as well as application of the low energy results, is contemplated.

Published -- Phys. Rev., 167, 74 (1968).

Personnel: M. H. Mittleman and J. Quong

VII. Positronium Formation in Positron-Helium Scattering

A method recently used to describe positronium formation in positron hydrogen scattering[8] is extended to this problem in anticipation of results of an experiment in progress. The calculations are complete and show a surprisingly low positronium formation cross section, consistent with the hydrogen target results.

This is being submitted as a Ph. D. thesis at the Department of Applied Science, University of California, Davis, and will be published in a condensed form.

Personnel: M. H. Mittleman, Space Sciences Laboratory, and
Margaret F. Fels, University of California, Davis.

VIII. Formal Problems in the Theory of Dissociative Attachment and Recombination

An examination of previous theories describing this process shows that they all neglect an important point which may invalidate them. The theories all deal with resonance capture in a Born-Oppenheimer approximation. The point not adequately treated is the connection of the resonance state with the physical state. We show that these curves which were assumed to join smoothly (a) join discontinuously or (b) may not join at all. We give an alternative theory which eliminates the need for the joining and introduces a non-adiabatic transition in its place. When our theory is treated phenomenologically, as it must be practically, it can give the same numerical results as the preceding theories in their phenomenological form.

Submitted for publication to Phys. Rev.

Personnel: M. H. Mittleman, Space Sciences Laboratory, and
J. C. Y. Chen, University of California at San Diego.

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