CHARGE TRANSFER IN A 3→2-BODY, REDUCED MASS FOCK-TANI REPRESENTATION: FIRST ORDER RESULTS AND AN INTRODUCTION TO HIGHER ORDER EFFECTS

by

JOHN CARTER STRATON

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APPROVED: Marvin D. Girardeau
Dr. Marvin D. Girardeau

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Title: CHARGE TRANSFER IN A 3→2-BODY, REDUCED MASS
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Approved: Marvin D. Girardeau
Dr. Marvin D. Girardeau

The Fock-Tani (unitary) transformation of the second-quantized Hamiltonian gives a representation which treats reactants and products symmetrically, and composites exactly. Each term in the Fock-Tani potential corresponds to a specific physical process and contains terms orthogonalizing continuum states to the bound states. The difficulty in carrying out this transformation can be lessened by working in a center of mass system, giving (n-1) reduced mass particles.

After a general analysis of such systems, the Fock-Tani transformations in the 3→2-body case are carried out for the reactions

$$a^+ + (b^+c^-) \rightarrow (a^+c^-) + b^+ \qquad (1)$$

and

$$a^- + (b^+c^-) \rightarrow (a^-b^+) + c^- \quad . \qquad (2)$$

It is found that for (2) the transformation in the symmetrical reduced mass system can easily be carried out, but the Jacobi reduced mass system requires the more complicated d-matrix approach. This transformation has not yet been attempted in the full 3-body system but is likely to be as difficult as that for (1).

First order differential and total cross sections are computed for resonant charge transfer in (1) for a proton-hydrogen initial state. The Fock-Tani T-matrix for the initial-state Jacobi system is found to be identical to that for the full 3-body system. That for the symmetrical reduced mass system gives an error of order $1/m_{prot}$ in the incident wave vector.

A comparison of the Jacobi version and a previous special case Fock-Tani transformation, where the proton mass is taken as infinite, is also made. Cross sections for (1s→1s) positronium formation in positron-hydrogen collisions, calculated using the same program as for the proton-hydrogen case, are found to disagree with the previous Fock-Tani result, probably due to lack of convergence of the previous result. Cross sections for reactions (1) involving muons in hydrogenic isotopes (of interest in quantum electrodynamics and catalyzed fusion) are also calculated.

Finally, extension of the results to higher order is considered. Polarized Schrodinger wave functions for a system containing a hydrogenic atom and a fully kinetic external charge are found to first order. These would be used in the Fock-Tani matrix elements to account for some initial- and final-state effects. Calculations of distorted second-quantized states and second and third order T-matrix elements are also outlined.

VITA

NAME OF AUTHOR: John Carter Straton

PLACE OF BIRTH: Colorado Springs, Colorado

DATE OF BIRTH: August 14, 1955

GRADUATE AND UNDERGRADUATE SCHOOLS ATTENDED

University of Oregon

DEGREES AWARDED:

Doctor of Philosophy, 1986, University of Oregon
Master of Science, 1983, University of Oregon
Bachelor of Fine Arts, 1977, University of Oregon

AREAS OF SPECIAL INTEREST:

Atomic Collision Theory
Astrophysics and Cosmology
Few Body Systems

PROFESSIONAL EXPERIENCE:

Research Assistant, Department of Physics, University of Oregon, Eugene, 1984-86

Graduate Teaching Fellow, Department of Physics, University of Oregon, Eugene, 1980-1984

AWARDS AND HONORS:

National Research Council-NASA Research Associateship, Goddard Space Flight Center, 1986

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CHAPTER I

INTRODUCTION

Atomic 3-body systems provide an ideal testing ground for theories of scattering incorporating bound states because the wave functions are known. One of the most severe tests lies in the ability to account for virtual rearrangement processes in the intermediate states of any given process. A recent calculation[1] has shown that virtual positronium formation is the leading contributor to the dynamics of elastic scattering of positrons from hydrogen in its ground state at energies below the threshold for positronium formation. The problem of virtual rearrangments is difficult to handle using conventional representations which have different Hamiltonians for the different arrangements. Thus a representation that can accurately account for various arrangements simultaneously would be of great utility.

A representation (Fock-Tani) has been developed[2] which does give a Hamiltonian that treats reactants and products symmetrically and composites exactly. This representation involves a unitary transformation of the second-quantized Hamiltonian to a Hilbert space in which creation and annihilation operators corresponding to bound states satisfy elementary commutation relations and therefore are kinematically independent of the unbound states. The potentials between the latter have orthogonalization terms subtracted from them so that there is not enough energy to bind (this binding being already accounted for in the creation and annihilation operators for the composite states). An added benefit is that each term in the Fock-Tani potential corresponds to an immediately identifiable and specific physical process. All interactions are of smaller magnitude due to terms orthogonalizing continuum the states to the bound states. Therefore the Born series in Fock-Tani representation is more convergent than the Born series in Fock (or Schrodinger) representation and the reliability of first-order approximations should be improved. In fact, this has been shown for resonant charge exchange in proton-hydrogen collisions by Ojha et al.[3]

The drawback of the Fock-Tani representation is the difficulty in actually carrying out the transformation. The transformation has been done for a full 3-body system. This is useful for a variety of problems but certainly should not exhaust the potential of the Fock-Tani approach.

The first goal of this dissertation is carrying out the Fock-Tani transformation starting in center-of-mass coordinate systems in which the degrees-of-freedom have been reduced by the coordinates and momenta of one particle, a 3→2-body, reduced-mass system. If such systems give the same physical result as the full 3-body system, they would be of great utility in actualizing the Fock-Tani transformation for 4 bodies.

In Chapter II two methods for reducing an n-body Hamiltonian to (n-1) bodies are re-derived as an aid in understanding the physics of such systems. For reduced systems in which one particle is fixed at the origin, the inertial potentials arising in these accelerated systems are analyzed to determine the regions in which they may be neglected. A fortuitous result of the generation of asymptotic states for such systems is a direct relation between these symmetrical reduced-mass systems and the more conventional unsymmetrical (initial- and final-state) center-of-mass systems. This immediately gives a relation between the initial- and final-state Jacobi systems.

In Chapter III the Fock-Tani transformations for both the symmetrical and Jacobi 3→2-body systems are derived to account for arrangement channels of the reaction

$$a^{+}+(b^{+}c^{-})\rightarrow(a^{+}c^{-})+b^{+} \quad . \qquad (1.1)$$

This transformation is an almost trivial extension of that derived by Girardeau[4] for the infinite-mass special case. It is found that the Fock-Tani Hamiltonian derived in the Jacobi system gives a first-order T-matrix for charge transfer which is identical to that for the Fock-Tani Hamiltonian derived for the full 3-body system. But the Hamiltonian derived for the symmetrical reduced-mass system gives a first-order T-matrix with error (in atomic units) of order $1/m_{\text{proton}}$ in the initial state. This error, which is not negligible for impact energies of order 5 keV, is a result of the sequestering of terms of the Fock-Tani Hamiltonian into the various physical processes. The inertial potentials which would presumably correct this error do not appear in the first-order term which gives the charge transfer T-matrix.

Next, the Fock-Tani transformation for the reaction

$$a^{-}+(b^{+}c^{-})\rightarrow(a^{-}b^{+})+c^{-} \qquad (1.2)$$

is carried out in the symmetrical reduced-mass system, and is found to be much easier than that for (1.1) because both *a* and *c* are bound to the particle fixed at the origin so that the operators corresponding to the bound states of one species commute with all operators associated with the other species. The transformation for the Jacobi initial-state system must be done by the much more complicated d-matrix method. The Fock-Tani transformation for (1.2) has not yet been carried out in the full 3-body system, but is expected to be as difficult as that for (1.1). Given the small error in the T-matrix for reaction (1.1) noted for the symmetrical reduced-mass system in Fock-Tani representation, one should closely examine the initial state before using this Hamiltonian and make ad hoc corrections at the matrix element level to bring the initial state in line with what is physically expected. In any case the value of reduced-mass systems is clearly demonstrated.

In Chapter IV the T-matrix for (1.1) is analytically reduced to a tractable numerical problem and the differential and total cross sections for (abc) = {(ppe), (epe), (μpμ), (μdμ), and (μtμ)} are calculated. A comparison with the Fock-Tani result for (ppe) given in Ojha et al.[3] shows that their approximations give an error of order 10 percent. A comparison with the Fock-Tani result for (epe) given by Ficocelli Varrachio and Girardeau[5] shows that the present result does not agree with theirs. The discrepancy is attributed to a lack of convergence in their calculations. The Fock-Tani total cross sections for (μpμ) are compared with those for the first Born and distorted wave Born approximations of Ma et al.[6] and to the classical-trajectory Monte Carlo result of Ohsaki et al.[7] It is found that the Fock-Tani and distorted wave results are in excellent agreement near the peak of the cross section and in good agreement for other energies. Finally, the differential and total cross sections for (μpμ), (μdμ), and (μtμ) are compared. Differences among these isotopes are found near the energy threshold for these reactions, which is near the peak in the total cross section, but they give essentially the same cross sections at higher energies.

the same cross sections at higher energies.

Because the first-order Fock-Tani total cross section for resonant charge transfer[3] does not fit the data well at energies less than 10 keV, and because the differential cross sections at 25, 60, and 125 keV do not fit the data for large angles, one must consider higher-order effects. One would expect that polarization effects would be important at lower energies, where such effects would have more time to develop in a scattering process, and at larger angles corresponding to smaller impact parameters. In Chapter V the first-order wave function for a system containing a hydrogenic atom and a fully kinetic external charge is found. The method is easily extended to higher-order. This wave function would be used as a better approximation to the Lippmann-Schwinger in-state than the asymptotic eigenstate (a plane wave multiplied by a hydrogenic wave function) used previously.

The adiabatic limit of this wave function is found to match the adiabatic wave function of Dalgarno and Stewart.[8] The kinetic terms are found to depend directly on the magnitude of the momentum of the external particle, rather than inversely, so that these wave functions do not have the expected energy dependence. As a check on this dependence, the polarization potential is calculated from the virial theorem and compared with the non-abiabatic polarization potential found by Seaton and Steenman-Clark[9] and by Drachman.[10] Kinetic effects in the present result enter at a slightly lower order in 1/R than in previous results, k/R^5 rather than k^2/R^6, but show the same qualitative sort of energy dependence.

Chapter VI is an outline of a method for including higher-order effects within the second-quantized Fock-Tani representation. It is shown that the differential equation for distorted waves can be solved approximately, but to infinite order in the distortion, for large R. This solution is to be matched to the numerical solution for small R, resulting in a significant savings in computer time and probably reducing roundoff errors. The use of this approximate distorted state in the reduction of first-, second-, and third-order terms (in the remaining potential) of the T-matrix is discussed.

Chapter VII contains a summation of the present work and explores directions that show promise for the future.

Atomic units ($\hbar = m_e = e = 1$) are used throughout.

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CHAPTER II

THE REDUCED HAMILTONIAN

Introduction

A technique for eliminating the motion of the nucleus from the dynamics of an (n-1)-electron atom was introduced in 1930 by Hughes and Eckart.[1] The explicit derivation, given in Bethe and Salpeter,[2] involves a change of variables in the general n-body momentum operator, to the center-of-mass coordinate and the relative coordinates between the (n-1) electrons and the nucleus. This introduces cross-terms in the momenta of the electrons which are referred to as "mass polarization terms"[3] or "specific mass shift terms"[4] in the literature. These terms produce shifts in the observed spectra[4] of isotopes of atoms in addition to the normal mass shift due to replacing the electron mass by the reduced-mass. Girardeau[5] has given a derivation for arbitrary masses based on a unitary transformation.

Because the momentum cross-terms lead to inertial forces in the equations of motion for this accelerated reference frame, it seems more appropriate to refer to them as "inertial potentials," their physical meaning, rather than specific mass shift terms, their spectroscopic effect. Mass polarization refers to the dominant physical process for the ground state of 2-electron atoms[2] so this label is not general enough.

This chapter is devoted to a deeper understanding of these inertial potentials so that their inclusion or neglect may be justified on physical grounds for the scattering processes considered. A comparison is also made to the discussion for bound systems in Bethe and Salpeter. Next a general derivation of the asymptotic states is given. And finally the relations between this symmetrical reduced-mass system and the inertial reduced-mass systems (which contains no intertial potentials) are examined. These latter, unsymmetrical, Jacobi coordinates were recently found to simplify a calculation by Drachman[6] of the fine-structure splitting of the Rydberg states of helium.

The Fock-Tani transformations in Chapter 3 are greatly simplified by reducing the Hamiltonian from 3- to 2-bodies using these reduced-mass systems. A comparison of their relative merit in the Fock-Tani case will be given in the next chapter, where it will be shown that for electron capture reactions, the Fock-Tani Hamiltonian can be derived in both the symmetrical and inertial systems. Whereas the latter gives the same result as the full 3-body calculation,[7] the former gives an error of order $1/m_{\text{proton}}$ in the initial state energy and in the initial momentum wave function of the first-order T-matrix. It is shown in Chapter III that the Fock-Tani transformation divides the potential into 10 (for the inertial system) or 11 (for the symmetrical system) terms corresponding to the possible physical processes. Because it is a second-quantized representation, only one term in the potential contributes to a given process at first-order because of the coupling, or lack thereof, of the creation and annihilation operators to the initial and final states. So it is not surprising that some term that would make the correspondence between these two systems might be sequestered at first-order from the process at hand.

Finally, it is shown that the Fock-Tani transformation for the process $\mu^- + (e^-p^+) \rightarrow (\mu^-p^+) + e^-$ is greatly simlified when the symmetrical reduced-mass system is used, while the transformation for the inertial reduced-mass system still requires half the work of the full 3-body transformation.

Reducing the N-body Hamiltonian to (N-1)-bodies

Girardeau's unitary transformation method of finding the n-body symmetrical reduced-mass Hamiltonian, (2.11), is outlined first, but with a little more detail. Next, a derivation is given which is essentially equivalent to that of Bethe and Salpeter[2] except that it is for arbitrary masses.

One starts with the n-body Hamiltonian with translation invariant potential,

$$H = \sum_{a=1}^{n} \frac{p_a^2}{2m_a} + V(\vec{r}_1,\ldots,\vec{r}_n) \quad , \tag{2.1}$$

where

$$V(\vec{r}_1+\vec{a},\ldots,\vec{r}_n+\vec{a}) = V(\vec{r}_1,\ldots,\vec{r}_n) \; .$$

By using Taylor's theorem,

$$\exp(\vec{a}\cdot\vec{\nabla}_j)f(\vec{r}_1,\ldots,\vec{r}_j,\ldots) = f(\vec{r}_1,\ldots,\vec{r}_j+\vec{a},\ldots) \; ,$$

where $\vec{p}_j = -i\vec{\nabla}_j$, one can remove the Hamiltonian's dependence on the first coordinate by the unitary transformation,

$$S = \exp(-iA) \; , \qquad A = \vec{r}_1\cdot(\vec{p} - \vec{p}_1) = \vec{r}_1\cdot\sum_{b=2}^{n}\vec{p}_b, \tag{2.2}$$

in that

$$S^{-1}V(\vec{r}_1,\vec{r}_2,\ldots,\vec{r}_n)S\phi(\vec{r}_1,\ldots,\vec{r}_n) =$$

$$= V(0,\vec{r}_2,\ldots,\vec{r}_n)\phi(\vec{r}_1,\ldots,\vec{r}_n) \; . \tag{2.3}$$

This, together with the commutation relations

$$[(iA)^m,\vec{p}_a] = -m\delta_{a1}\sum_{b=2}^{n}\vec{p}_b(iA)^{m-1} \quad , \; m > 0 \; , \tag{2.4}$$

gives

$$S^{-1}HS = \sum_{a=1}^{n} \frac{p_a^2}{2\mu_a} + V(0,\vec{r}_2,\ldots,\vec{r}_n) + W(\vec{p}_1,\ldots,\vec{p}_n) \ , \tag{2.5}$$

where

$$\mu_1 = m_1 \ , \text{ and } \qquad \mu_a = \frac{m_a m_1}{m_a + m_1} \qquad \text{for } \ a > 1 \ . \tag{2.6}$$

The 2-body momentum-dependent potentials in which the remaining particles move,

$$W(\vec{p}_1,\ldots,\vec{p}_n) = -\sum_{a=2}^{n} \frac{\vec{p}_1 \cdot \vec{p}_a}{m_1} + \sum_{2 \le a < b \le n}^{n} \frac{\vec{p}_a \cdot \vec{p}_b}{m_1} \ , \tag{2.7}$$

arise from the accelerated coordinate system in which the first particle is at rest, and give rise to inertial forces in the equations of motion.

Energy and total-momentum eigenstates of the original Hamiltonian, Ψ such that

$$H\Psi = E\Psi \qquad \text{and} \qquad \vec{p}\Psi = \vec{q}\Psi \ , \tag{2.8}$$

can be written in the general form

$$\Psi = (2\pi)^{-3/2} \exp[i\vec{q}\cdot\vec{f}(\vec{r}_1,\ldots,\vec{r}_n)]u(\vec{r}_1,\ldots,\vec{r}_n) \ , \tag{2.9}$$

where u is an eigenfunction of total momentum zero, and is therefore translation invariant, and $\vec{f}$ is a weighted average.

The conventional choice is $\vec{f} = \vec{R}_{cm}$. The corresponding eigenfunctions, with the same eigenvalues, in the transformed representation are

$$\Phi = S^{-1}\Psi =$$

$$= (2\pi)^{-3/2}\exp\{i[\vec{q}\cdot\vec{r}_1 + \vec{q}\cdot\vec{f}(0,\vec{r}_2,\ldots,\vec{r}_n)]\}u(0,\vec{r}_2,\ldots,\vec{r}_n) , \tag{2.10}$$

which are products of eigenstates of $\vec{p}_1$ by states depending only on $\vec{r}_2,\ldots\vec{r}_n$. As noted by Girardeau (for $\vec{f} = \vec{r}_1$),[5] this is what one would expect since $S^{-1}HS$ commutes with $\vec{p}_1$. The momentum operator of the first particle in the transformed system therefore takes on the meaning of the total momentum operator of the original system.

Starting with the center-of-mass system, in which $\vec{q}=0$, the corresponding Φ states are eigenstates of the (n-1)-body reduced Hamiltonian obtained by setting $\vec{p}_1 = 0$,

$$H_{red} = \sum_{a=2}^{n} \frac{p_a^2}{2\mu_a} + V(0,\vec{r}_2,\ldots,\vec{r}_n) + \sum_{2\le a<b\le n} \frac{\vec{p}_a\cdot\vec{p}_b}{m_1} . \tag{2.11}$$

Now to a re-derivation of (2.11) from a coordinate transformation approach is given that is equivalent to the derivation of Bethe and Salpeter,[2] but generalized to arbitrary masses.

Starting with (2.1) one changes variables to

$\vec{\rho}_a = \vec{r}_a - \vec{r}_1$, for a > 1 ,

and

$$\vec{R} = \sum_{a=1}^{n} \frac{m_a \vec{r}_a}{M} , \quad \text{where} \quad M = \sum_{a=1}^{n} m_a . \tag{2.12}$$

Then the $\vec{\nabla}_{r_a}$ transform as

$$\vec{\nabla}_{r_1} = \frac{m_1}{M}\vec{\nabla}_R - \sum_{a=2}^{n} \vec{\nabla}_{\rho_a} , \text{ and } \qquad \vec{\nabla}_{r_a} = \frac{m_a}{M}\vec{\nabla}_R + \vec{\nabla}_{\rho_a} \quad \text{for } a > 1 . \tag{2.13}$$

But a transformation of the metric of the original coordinate system to that of the new system[8] using these relations gives off-diagonal terms in the new metric which are non-zero except for those with index 1 . Because this transformation is given by inner products of pairs of partial derivatives, the only possible structure for each of these terms is the paired cross-term form of (2.7). This gives the final term of (2.11), apart from constants. The equation of motion for such a metric[9] contains inertial force terms reflecting the accelerated frame.

In a notation where $\vec{q} = -i\vec{\nabla}_R$ and $\vec{q}_a = -i\vec{\nabla}_{\rho_a}$,

$$p_1{}^2 = \frac{m_1}{M^2} q^2 - \frac{2m_1}{M} \vec{q} \cdot \sum_{a=2}^{n} \vec{q}_a \quad \text{, and} \quad p_a^2 = \frac{m_a}{M^2} q^2 + \frac{2m_a}{M} \vec{q} \cdot \vec{q}_a + q_a^2$$

for $a > 1$. (2.14)

Substituting these expressions into the momentum terms of (2.1), and setting the total momentum q equal to zero, (2.11) is reproduced if if the q's are renamed as p's.

One might sense a contradiction inherent in a zero-total-momentum coordinate system in which one particle is fixed at the origin. Can momentum be zero in such a system? In the familiar case of the transformation from a 2-body system to the reduced-mass system, one is left with a single "fictitious particle" moving in a potential centered at the origin. How can one "particle" conserve momentum? This is resolved by noting that in a relative/center-of-mass decomposition, the choice of internal (relative) coordinates is not unique.[10] Choosing internal coordinates relative to the position of one particle or a geometrical center (a choice which also results in momentum cross-terms[10]) is as reasonable as choosing them relative to the center-of-mass. Once the total momentum has been accounted for, there need not be any further restrictions on the relationships among the particles other than reducing the degrees of freedom by three through <u>some</u> choice of internal relations.

The Inertial Potentials

Considering the complication of the Hamiltonian (2.11) due to the intertial potentials, one would like to know in which regions they can be neglected. The W's arise, physically, from the passage to the rest frame of the first particle, which is being accelerated, through the V-interactions, by all other particles. It is for this reason that they are refered to as "inertial potentials" (the physical meaning) rather than "specific mass shift terms" (the spectroscopic effect) in this dissertation.

Given this physical meaning for these momentum dependent potentials, one can examine their importance for various regions. First, if all other particles are infinitely separated from the first, assuming that the V-interactions go to zero at infinite separation, all forces on particle 1 go to zero, and hence the inertial potentials should also.

Suppose particle 2 is bound to particle 1, and all others, {j}, are at infinity. Since any correlation between 2 and any j is established through the Coulomb interactions (V), which go to zero at infinite separation, the dot product of the momenta of 2 and {j}, representing their correlation or average in the time dependent formalism, should go to zero in the time independent formalism.

Suppose more than one particle is bound to the first particle, say $\{2,\ldots,\ell\}$. Again dot products of $\{2,\ldots,\ell\}$ with the other $\{\ell+1,\ldots,n\}$ would be expected to be zero if the latter are at an infinite distance from the former. And if the W arise solely from the acceleration of the first particle, one would expect the dot products among the $\{\ell+1,\ldots,n\}$, even if some are clustered together, to go to zero (in the time independent formalism) if these clusters are infinitely removed from particle 1 . If some terms in W arose partially from some additional peculiarity in the choice of coordinates, then the latter assertion might be false. But the second derivation of (2.11) clearly shows that the only peculiarity of this system is that it is the accelerated rest frame of the first particle.

Finally, the dot products of the momenta of pairs of particles bound to 1 can be zero in the time independent Hamiltonian formulation only if the probability densities of their wave functions are spherically symmetrical (so that these products would average to zero in the time dependent formalism). For Fermions, the Pauli exclusion principle additionally dictates that these products are zero only for two particles, {2,3}, bound to 1 in an s-state. The exclusion of the third and fourth bound particles, {4,5}, from the ground state is a correlation mechanism. So even if 4 and 5 reside in an s-state, the dot products of the momenta of 4 and 5 with the momenta of 2 and 3 are expected to be non-zero.

Bethe and Salpeter[2] examine the case of {2,3} bound to particle 1 in more detail. Initially ignoring any polarization effects, they examine the energy shift due to the Pauli interaction of 2 and 3. If the solution, U, of (2.11) is approximated by a sum of products of eigenfunctions belonging to the individual (non-interacting) electrons, $U = 2^{-1/2}[u(1)v(2) \pm u(2)v(1)]$, then the energy shift (in atomic units) is

$$\varepsilon_2 = \frac{m}{m_1}\int(\vec{\nabla}_1 u^*(1))v^*(2)\cdot[u(1)\vec{\nabla}_2 v(2) \pm v(1)\vec{\nabla}_2 u(2)]d\tau_1 d\tau_2 \ .$$

But the first term is zero since the expectation value of the momentum of a bound electron, in any direction, is zero.

The second term,

$$\varepsilon_2 = \pm\frac{m}{m_1}\left|\int\vec{\nabla}u^* v d\tau\right|^2 \ ,$$

is the optical transition probability for going from one occupied state to another. Since one of the electrons is in the 1s state, ε_2 is zero except for p states. This supports the reasoning, above, that if both electrons are in spherically symmetric states, this term is zero.

Turning to the correlation effect due to polarization, produced by the electrostatic repulsion of the electrons, Bethe and Salpeter note that the exact wave function would not be of the above form, but would depend on the inter-electron distance. For excited states the largest contributor would again be the $\ell = 1$ term (due to the dipole symmetry of the problem). But because of the close proximity of the electrons, the ground state polarization cannot be neglected . A recent calculation[11] of the specific mass shifts between ^{3}He and ^{4}He, agreeing well with experiment[4], shows the s, p, and d state frequency shifts in the proportion of 2200, -1100, and 0 MHz, respectively.

For scattering problems it is important to know the range of R (the projectile-target distance) for which the inertial potentials are negligible. It is shown in Chapter V that they can be neglected in calculating the first-order energy shift of a hydrogenic atom due to the presence of a free charge at $R \geq 1/(2m_1)$.

The range of projectile momenta in which the intertial potentials can be neglected might also be considered. As noted by Girardeau, these terms are suppressed by a factor of $1/m_1$ relative to the potentials V, for all values of the radius vectors. Calculations[7] for the reaction $p^+ + H(1s) \rightarrow H(1s) + p^+$ have revealed that one can generally neglect terms of this order for projectile energies ≈ 5 keV or smaller, and this is precisely the region in which polarization effects should be important.

However, despite these considerations, correlation between the projectile (s) and the atomic electron (s) is the mechanism of polarization, so neglecting these terms in a determination of polarized asymptotic states, as in Chapter V, would seem to be inconsistent. It is found that an additional coordinate transformation from this accelerated system to the inertial center-of-mass system (in which no momentum cross-terms appear) is useful for a calculation of such effects, as well as for a calculation of the asymptotic energy eigenvalue. It should be noted that if the W terms of the reduced systems are neglected, a transformation to the coordinates appearing in the asymptotic states, in order to calculate quantities of physical interest, produces cross-terms in the new momenta of the same form as the original W's rather than an inertial system. It is therefore important not to neglect these terms too early in a calculation, even when such an approximation is physically justified.

The Asymptotic States

Next is a general derivation of the asymptotic states. For the reaction of two composites with component transfer,

$$(\ell,\ell+1,\ldots,n) + (1,2,\ldots,\ell-1) \rightarrow$$
$$\rightarrow (j,j+1,\ldots,\ell,\ldots,n) + (1,2,\ldots,j-1) \ ,$$

in the original total-center-of-mass system, one can also define the centers of mass of the composites,

$$\vec{R}_s = \sum_{i=a_s}^{b_s} \frac{m_i \vec{r}_i}{M_s} \ , \qquad M_s = \sum_{i=a_s}^{b_s} m_i \ , \tag{2.15}$$

where $a_s = \ell,1,j,1$ and $b_s = n,\ell-1,n,j-i$ for composite label, s, equal to projectile-initial (pi), target-initial (ti), projectile-final (pf), and target-final (tf), respectively.

Then the zero-total-momentum eigenstates of the original Hamiltonian are

$$\Psi_i = (2\pi)^{-3/2}\exp[i\vec{k}_i\cdot(\vec{R}_{pi}- \vec{R}_{ti})u(\vec{r}_1,\ldots,\vec{r}_n) \qquad (2.16)$$

and

$$\Psi_f = (2\pi)^{-3/2}\exp[i\vec{k}_f\cdot(\vec{R}_{pf}- \vec{R}_{tf})u(\vec{r}_1,\ldots,\vec{r}_n) \ . \qquad (2.17)$$

The reaction in the reduced system is represented by

$$(\ell,\ell+1,\ldots,n) + ((1),2,\ldots,\ell-1) \rightarrow$$
$$\rightarrow (j,j+1,\ldots,\ell,\ldots,n) + ((1),2,\ldots,j-1) \ ,$$

where the notation for the ghosted particle, fixed at the origin, is (1). The corresponding reduced states are

$$\Phi_i = (2\pi)^{-3/2}\exp[i\vec{k}_i\cdot(\vec{R}_{pi}-\sum_{a=2}^{\ell-1}\frac{m_a\vec{r}_a}{M_{ti}})]u(\vec{r}_2,\ldots,\vec{r}_n) \qquad (2.18)$$

and

$$\Phi_f = (2\pi)^{-3/2}\exp[i\vec{k}_f\cdot(\vec{R}_{pf}- \sum_{a=2}^{j-1}\frac{m_a\vec{r}_a}{M_{tf}})]u(\vec{r}_2,\ldots,\vec{r}_n) \ . \qquad (2.19)$$

For the 3-body atomic charge transfer reaction $(3) + ((1),2) \rightarrow (2,3) + ((1))$, the reduced asymptotic states are

$$\Phi_i = (2\pi)^{-3/2}\exp[i\vec{k}_i\cdot(\vec{r}_3 - \frac{m_2\vec{r}_2}{m_1+m_2})]u_{n\ell m}(\vec{r}_2) \qquad (2.20)$$

and

$$\Phi_f = (2\pi)^{-3/2}\exp[i\vec{k}_f\cdot(\frac{m_2\vec{r}_2 + m_3\vec{r}_3}{m_2+m_3})]u_{n'\ell'm'}(\vec{r}_2-\vec{r}_3) \ . \qquad (2.21)$$

To check this the variables in the 3→2-body reduced Hamiltonian,

$$H_{red} = \sum_{a=2}^{3} \frac{p_a^2}{2\mu_a} + V(0,\vec{r}_2,\vec{r}_3) + \frac{\vec{p}_2\cdot\vec{p}_3}{m_1} \ , \qquad (2.22)$$

are changed to

$$\vec{R}_i = \vec{r}_3 - \frac{m_2\vec{r}_2}{m_1+m_2} \quad \text{and} \quad \vec{r}_i = \vec{r}_2 \ , \qquad (2.23)$$

or

$$\vec{R}_f = \frac{m_2\vec{r}_2 + m_3\vec{r}_3}{m_2+m_3} \quad \text{and} \quad \vec{r}_f = \vec{r}_2 - \vec{r}_3 \ . \qquad (2.24)$$

Using (2.23) and (2.24), the relations between initial- and final-state coordinates, which are not all obvious from a graph of the system, may be written down as

$$\vec{R}_f = \zeta\vec{R} + \iota\vec{r} \;, \qquad \vec{r}_f = \gamma\vec{r} - \vec{R} \;,$$

and

$$\vec{R} = \lambda\vec{R}_f - \iota\vec{r}_f \;, \qquad \vec{r} = \zeta\vec{r}_f + \vec{R}_f \;,$$

where

$$\zeta = \frac{m_3}{m_3 + m_2} \;, \qquad \eta = \frac{m_2}{m_3 + m_2} \;,$$

$$\gamma = \frac{m_1}{m_1 + m_2} \;, \qquad \lambda = \frac{m_2}{m_1 + m_2} \;,$$

and

$$\iota = \zeta\lambda + \eta \;. \tag{2.24}$$

The momentum cross-terms exactly cancel in the new coordinate system, giving initial and final Hamiltonians for coulomb potentials (easily generalizable to other types of potentials)

$$H = -\frac{\nabla_R^2}{2M} - \frac{\nabla_r^2}{2m} - \frac{Z_A}{r} + \frac{Z_A Z_P}{|\vec{R}+c(1-\nu)\vec{r}|} - \frac{Z_P}{|\vec{R}-c\nu\vec{r}|} \;, \tag{2.25}$$

where

$$R = R_i \,, \qquad r = r_i \,,$$

$$A = ((1),2) \,, \qquad P = (3) \,,$$

$$c = +1 \,, \qquad \nu = \frac{m_1}{m_1 + m_2} \,,$$

$$M = \frac{m_3(m_2 + m_1)}{m_1 + m_2 + m_3} \,, \text{ and} \qquad m = \frac{m_2 m_1}{m_1 + m_2} \,, \qquad (2.26i)$$

or

$$R = R_f \,, \qquad r = r_f \,,$$

$$A = (2,3) \,, \qquad P = ((1)) \,,$$

$$c = -1 \,, \qquad \nu = \frac{m_3}{m_3 + m_2} \,,$$

$$M = \frac{m_1(m_2 + m_3)}{m_1 + m_2 + m_3} \,, \text{ and} \qquad m = \frac{m_2 m_3}{m_3 + m_2} \,. \qquad (2.26f)$$

For later reference, the asymptotic energy eigenvalues of initial and final states (in atomic units), are

$$E = \frac{k^2}{2M} - \frac{Z_A^2}{2n^2 a_0} , \qquad (2.27)$$

where $a_0 = 1/m$.

If Girardeau's approximate eigenstates, in which m_2 is neglected, had been the starting point, there would have been an error in E of order m_2/m_1, which is negligible. However, in this approximation, conservation of energy would give a much more complicated expression for the relation between initial and final momenta than does the exact energy relation.

Equations (2.25) are just the relative initial and final Hamiltonians for the standard (Jacobi) center-of-mass system. The present derivation starts from a system in which the first particle is at the origin, so the relations defining the inter-cluster and intra-cluster coordinates, (2.23) and (2.24), do not contain the coordinates of particle 1 that appear in the standard derivation of this coordinate system (see, for example, C. J. Joachain[12]).

The Relation to Inertial Coordinates

In calculating initial and final polarized states, as in Chapter V, the inertial coordinate system is the most convenient one to work in because the arguments of the momentum and atomic wave functions of (2.18) and (2.19) are independent variables. The transformation for the 3-body case is given in (2.23) and (2.24). A discussion of the relative merit of the two types of systems and a look at the feasibility of finding transformations to inertial coordinates in the general case follows. Although transformations for n>3 will not be used in the present work, specific examples of these will be presented for completeness. As noted earlier, these relations comprise a very direct tool for finding a relation between initial- and final-state coordinates. Such relations for complex systems are not easily found by other methods.

The standard Jacobi center-of-mass Hamiltonian is in two dynamic variables, r and ρ in the notation of Joachain's (19.20), and an energy conserving delta function appears as a prefactor of the matrix elements of physical interest. Equation (2.22) is also a Hamiltonian in two dynamic variables with energy conservation accounted for.

Given the essential equivalence of both approaches, and the problems with the 3-body Lippmann-Schwinger equations noted for the Jacobi form,[14] it would be expected that the symmetric Hamiltonian, (2.22), would lead to the same problems. Indeed, the trace of the Born Kernel is infinite in this case also, due to integrals over squares of delta functions of the momenta which do not participate in a given interaction, such interactions existing between particles 2 or 3 and the origin.

One might ask what has been gained by the transformation to obtain (2.22). It is found in Chapter III that carrying out the Fock-Tani transformation for the system containing two negative charges and one positive charge is greatly facilitated by starting with the Fock version of (2.22). A more convoluted method of finding the Fock-Tani Hamiltonian[14] would have to be used if the Jacobi 3→2-body or a full 3-body Fock Hamiltonian were the starting point.

An attempt at realizing a coordinate transformation which would eliminate the momentum cross-terms from the n→(n-1)-body Hamiltonian could not succeed due to the impossiblility ofsolving $\binom{n-1}{2}$ non-linear (momentum cross-term) equations in $(n-1)^2$ unknowns (the coefficients of the old to new coordinate relations). For a specific n, the problem can be reduced somewhat by inducing that one new coordinate is the projectile-target relative coordinate and that the remaining (n-2) new coordinates are intra-cluster relative coordinates for which all coefficients of the old coordinates except for one, in each such relation, may be set to unity. Finally, pattern recognition from simpler systems gives the general form for a trial set of equations for a given n. However one must still solve non-linear equations. It is found that this approach succeeds for both 3-body sytems, (2.23) and (2.24), two 4-body systems and one 5-body system for all masses. For the special case of all projectile masses being equal, solutions exist for the remaining 4-body system, one 5-body system and one 6-body system (for which three target masses are also equal). Systems of 7-bodies and higher were not explored.

In each of the following cases, one new coordinate is the projectile-target relative coordinate which appears in the momentum wave function of (2.18) or (2.19),

$$\vec{R} = \vec{R}_p - \sum_{a=2}^{k-1} \frac{m_a \vec{r}_a}{M_t} , \qquad (2.28)$$

where k is the number of target particles. The intra-cluster relative coordinates are as follows:

For the 4-body system (3,4) + ((1),2) ,

$$\vec{\rho}_3 = \vec{r}_4 - \vec{r}_3 \qquad \text{and} \qquad \vec{\rho}_1 = \vec{r}_2 , \qquad (2.29)$$

and for (4) + ((1),2,3) ,

$$\vec{\rho}_3 = \vec{r}_2 - \vec{r}_3 \qquad \text{and} \qquad \vec{\rho}_1 = \vec{r}_3 . \qquad (2.30)$$

For the 5-body system (4,5) + ((1),2,3) ,

$$\vec{\rho}_5 = \vec{r}_4 - \vec{r}_5 , \quad \vec{\rho}_3 = \vec{r}_2 - \vec{r}_3 , \text{ and } \quad \vec{\rho}_2 = \vec{r}_2 + \vec{r}_3 . \qquad (2.31)$$

For the special cases of equal projectile masses in equation (2.25), a solution exists for the 4-body system

(2,3,4) + ((1)) ,

$$\vec{R} = (1/3)(\vec{r}_2 + \vec{r}_3 + \vec{r}_4) \quad ,$$

$$\vec{\rho}_3 = \vec{r}_2 - \vec{r}_3 \quad \text{and} \quad \vec{\rho}_4 = \vec{r}_2 + \vec{r}_3 - 2\vec{r}_4 \quad , \qquad (2.32)$$

and for the 5-body system (3,4,5) + ((1),2) ,

$$\vec{R} = (1/3)(\vec{r}_2 + \vec{r}_3 + \vec{r}_4) - \frac{m_2\vec{r}_2}{m_1 + m_2} \quad ,$$

$$\vec{\rho} = \vec{r}_2 \quad , \quad \vec{\rho}_3 = \vec{r}_2 - \vec{r}_3 \quad , \text{ and } \quad \vec{\rho}_4 = \vec{r}_2 + \vec{r}_3 - 2\vec{r}_4 \quad . \qquad (2.33)$$

For the 6-body system, with $m_5 = m_6$ and $m_2 = m_3 = m_4$, (5,6) + ((1),2,3,4)

$$\vec{R} = (1/2)(\vec{r}_5 + \vec{r}_6) - (1/4)(\vec{r}_2 + \vec{r}_3 + \vec{r}_4) \quad ,$$

$$\vec{\rho}_6 = \vec{r}_5 - \vec{r}_6 \quad , \quad \vec{\rho}_4 = \vec{r}_2 + \vec{r}_3 - \vec{r}_4 \quad , \quad \vec{\rho}_3 = \vec{r}_2 + \vec{r}_4 - \vec{r}_3 \quad , \text{ and}$$

$$\vec{\rho}_2 = \vec{r}_3 + \vec{r}_4 - \vec{r}_2 \quad . \qquad (2.34)$$

These are transformations from the accelerated, zero-total-momentum coordinate system to coordinate systems in which the effects of acceleration, the momentum-dependent cross terms (W), are absent. Hence, these new systems must be the inertial center-of-mass systems for 4-, 5- and 6-bodies. The equations are similar to transformations directly from the Hamiltonian of (2.1), in which the coordinate of the first particle is not zero. In such a transformation some of the relations for $\vec{R}$ and the $\vec{\rho}$'s would be modified by an $\vec{r}_1$ term. As with (2.24), relations (2.28) through (2.33) constitute a very direct method of finding a relationship between initial- and final-state systems in 4- and 5-body systems. Such relations would be virually impossible to discern correctly from a graph of the system.

There is a final consideration in the use of the term "(n-1)-bodies". If the ghosted particle, (1), were truly eliminated from the reduced Hamiltonian, (2.11), one would expect that if a transformation to inertial coordinates could be found from the system containing 3 projectiles and (0+1) target particle, (3,4,5) + ((1),2) , then a transformation from the system containing 1 projectile and (0+3) target particles, (5) + ((1),2,3,4), could also be found. Likewise, if a transformation to the inertial system from the system (5,6) + ((1),2,3,4) exists, then one would expect a transformation from the system (4,5,6) + ((1),2,3) . But this symmetry does not hold, implying that the n→(n-1)-body system is not a true (n-1)-body system in all its facets. A similar implication was noted previously arising from a consideration of the V-interactions in the Born Kernel.

Notes

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CHAPTER III

THE FOCK-TANI TRANSFORMATION

Introduction

Fock-Tani representation[1,2] has been shown[3] to be a very convenient one to work in for rearrangement reactions because reactants and products are treated symmetrically, and composites exactly, within a single Hamiltonian. These composites are kinematically independent from the unbound states, and interactions between the latter are reduced by orthogonalization corrections so that they can no longer support bound states. Furthermore, the physical meaning of the various terms in the Hamiltonian is transparent and their inclusion or exclusion from a specific process is automatic due to the coupling (or lack thereof) to the creation and annihilation operators of the asymptotic states. In a field-theoretic optical potential approach to elastic scattering of positrons by hydrogen, at energies above the threshold for positronium formation, Ficocelli Varracchio has shown[4] that the inclusion of Fock-Tani corrections should give a good fit to the benchmark variational calculations of Bhatia et al.[5] Finally, a first-order calculation of the cross sections for the charge transfer process $p^{+} + H \rightarrow H + p^{+}$ in Fock-Tani representation[6] matches the data[7] for energies greater than 10 KeV and for differential angles less than 1 mrad.

The cost for this convenience is the task of actually carrying out the (Fock-Tani) unitary transformation of the Fock Hamiltonian. Such a transformation has been done on the subspace of the Fock-Tani state space containing one electron and two positive particles starting with the full 3-body Fock Hamiltonian[6] and also starting with the special case of the 3→2-body Hamiltonian, (2.22), with $m_1 \to \infty$.[3] In this chapter the latter is generalized to allow for finite masses. The transformation starting from the initial-state Hamiltonian, (2.25) is done and compared to the full 3-body Hamiltonian approach.

Finally, the transformation is found for the case of one positive particle fixed at the origin and any number of negatively charged particles of two types. The proton fixed at the origin is a "ghost" particle--one only sees its coulomb field. Therefore, each bound state involves the creation operator of only one particle, which anti-commutes with that for the other (unbound) particle, so that the transformation is formally much easier than previous transformations[3,6] (although one must still keep careful track of variables). Furthermore, in this case the transformation needs no restriction on the number of negatively charged particles of either species, a restriction required for the previous cases.[3,6] This demonstrates the full power of the reduced Hamiltonian approach of Chapter II.

Fock Representation

The nonrelativistic Fock Hamiltonian for an electron with creation operator $\hat{e}^\dagger(\vec{y})$, a particle of charge Z_a with creation operator $\hat{a}^\dagger(\vec{x})$, and a particle of charge Z_b fixed at the origin is

$$\hat{H}_F = \int d\vec{x}\,\hat{a}^\dagger(\vec{x})H_a(\vec{x})\hat{a}(\vec{x}) + \int d\vec{y}\,\hat{e}^\dagger(\vec{y})H_e(\vec{y})\hat{e}(\vec{y})$$

$$+ \int d\vec{x}d\vec{y}\,\hat{a}^\dagger(\vec{x})\hat{e}^\dagger(\vec{y})\left(V_{ae}(\vec{x}\vec{y}) + W_{ae}(\vec{x}\vec{y})\right)\hat{e}(\vec{y})\hat{a}(\vec{x}) \ . \qquad (3.1)$$

The notation convention will be that $\vec{x} = (\vec{r}_a, \sigma_a)$, where σ is the spin of the particle, and $\int d\vec{x} = \sum_\sigma \int d\vec{r}_a$, except where the context determines otherwise. A similar convention is used for y. The Schrodinger operators in (3.1) are given by (2.22), with labels $\{1,2,3\} \rightarrow \{b,a,e\}$. It is assumed the charge of e is -1 but the mass is arbitrary (although labeled "e," it may be a negative muon). Also it is assumed that a and e are distiguishable. Atomic units are used throughout ($\hbar = m_{\text{electron}} = e = 1$).

$$H_a(\vec{x}) = T_a(\vec{x}) + \frac{Z_aZ_b}{x}\ , \qquad H_e(\vec{y}) = T_e(\vec{y}) - \frac{Z_b}{y}\ ,$$

$$T_a(\vec{x}) = -\frac{1}{2\mu_a}\nabla_x^2\ , \qquad T_e(\vec{y}) = -\frac{1}{2\mu_e}\nabla_y^2\ ,$$

$$V_{ae}(\vec{x}\vec{y}) = -\frac{Z_a}{|\vec{x}-\vec{y}|}\ , \text{ and} \qquad W_{ae}(\vec{x}\vec{y}) = -\frac{1}{m_b}\vec{\nabla}_x\cdot\vec{\nabla}_y\ . \tag{3.2}$$

Equation (2.6) gives

$$\mu_a = \frac{m_am_b}{m_a + m_b}\ , \text{ and} \qquad \mu_e = \frac{m_em_b}{m_e + m_b}\ . \tag{3.3}$$

First consider the case where a has positive charge. The creation operators for an electron bound to the origin and bound to particle a are, respectively,

$$\hat{E}_\nu^\dagger = \int d\vec{y}\, u_\nu^E(\vec{y})\,\hat{e}^\dagger(\vec{y}) \tag{3.4}$$

and

$$\hat{A}_\mu^\dagger = \int d\vec{x}\, d\vec{y}\, \phi_\mu^A(\vec{x}\vec{y})\,\hat{a}^\dagger(\vec{x})\,\hat{e}^\dagger(\vec{y})\ . \tag{3.5}$$

The final state wave function is

$$\phi_\mu^A = (2\pi)^{-3/2} e^{i\vec{k}\cdot(\zeta\vec{x} + \eta\vec{y})}\, u_\upsilon^A(\vec{y} - \vec{x})\ , \tag{3.6}$$

where $\mu = \{k,\upsilon\}$,

$$\zeta = \frac{m_a}{m_a + m_e} , \qquad \eta = \frac{m_e}{m_a + m_e} , \qquad (3.7)$$

and where the functions u_λ are orthonormal, free orbitals for the bound states of *A* or *E*. In Girardeau (1982)[3] it was stated that these could also be distorted orbitals, but in Chapter 5 it is shown that u^E would also have to depend on the position of the distorting particle, *a*.

The electron and *a* fields satisfy the standard anti-commutation relations

$$\{\hat{e}(y),\hat{e}^\dagger(\vec{y}\,')\}=\delta(\vec{y}-\vec{y}\,')=\delta(\vec{r}_e-\vec{r}_e\,')\delta_{\sigma\sigma'} ,$$

$$\{\hat{a}(x),\hat{a}^\dagger(\vec{x}\,')\}=\delta(\vec{x}-\vec{x}\,') , \text{ and}$$

$$\{\hat{e}(\vec{y}),\hat{e}(\vec{y}\,')\}=\{\hat{a}(\vec{x}),\hat{a}(\vec{x}\,')\}=\{\hat{e}(\vec{y}),\hat{a}(\vec{x})\}=\{\hat{e}(\vec{y}),\hat{a}^\dagger(\vec{x})\}=0 , \qquad (3.8)$$

whereas the bound state fields satisfy extremely complicated (anti-) commutation relations with the free particles and among themselves.[3] For this reason a transformation to a new representation in which all of the fields satisfy elementary (anti-) commutation relations is done.

Fock-Tani Representation

The Fock-Tani transformation involves enlarging the state space so that the Fock space ***F***, the physical space, will be isomorphic to the subspace I_0 of the enlarged space

I.

One defines operators $\hat{\varepsilon}_\nu^\dagger$ and $\hat{\alpha}_\nu^\dagger$ as representing the composite states of an electron bound to the origin and to the particle *a*, respectively. They are to be kinematically independent of the free particle states so that the commutation ([,]) and anti-commutation ({,}) relations involving the "ideal" composite states are

$$\{\hat{\varepsilon}_\mu,\hat{\varepsilon}_\nu^\dagger\}=[\hat{\alpha}_\mu,\hat{\alpha}_\nu^\dagger]=\delta_{\mu\nu} ,$$

$$\{\hat{\varepsilon}_\mu,\hat{\varepsilon}_\nu\}=\{\hat{\varepsilon}_\mu,\hat{e}^{(\dagger)}(\vec{y})\}=\{\hat{\varepsilon}_\mu,\hat{a}^{(\dagger)}(\vec{x})\}=0 \text{ , and}$$

$$[\hat{\alpha}_\mu,\hat{\alpha}_\nu]=[\hat{\alpha}_\mu,\hat{e}^{(\dagger)}(\vec{y})]=[\hat{\alpha}_\mu,\hat{a}^{(\dagger)}(\vec{x})]=[\hat{\alpha}_\mu,\hat{\varepsilon}_\nu^{(\dagger)}]=0 . \tag{3.9}$$

Initially these ideal composites have no physical content on the subspace I_0,

$$\hat{N}_\beta | > = 0 \quad \text{if} \quad | > \text{ is in } I_0 \text{ , where} \quad \hat{N}_\beta = \sum_\nu \hat{\beta}_\nu^\dagger \hat{\beta}_\nu$$

$$\text{for } \beta = \{\alpha,\varepsilon\} . \tag{3.10}$$

One then transforms the physics on the enlarged space *I* from the subspace I_0 to the subspace I_c on which these ideal[3] composite operators represent the physical composite states and the fields $\hat{a}^\dagger(\vec{x})$ and $\hat{e}^\dagger(\vec{y})$ are continuum states that will not have enough interaction energy for binding.

The Hamiltonian is transformed by means of the unitary operator[3]

$$\hat{U}=\hat{U}_A\hat{U}_E \quad , \text{ where } \hat{U}_A=\exp\left(\frac{\pi}{2}\hat{F}_\alpha\right) \quad , \hat{F}_\alpha=\sum_\nu(\hat{A}^\dagger_\nu\hat{\alpha}_\nu-\hat{\alpha}^\dagger_\nu\hat{A}_\nu) \ ,$$

$$\text{and} \qquad , \hat{U}_E=\exp\left(\frac{\pi}{2}\hat{F}_\varepsilon\right) \quad , \hat{F}_\varepsilon=\sum_\nu(\hat{E}^\dagger_\nu\hat{\varepsilon}_\nu-\hat{\varepsilon}^\dagger_\nu\hat{E}_\nu) \ . \qquad (3.11)$$

The Fock-Tani Hamiltonian is given by

$$\hat{H}=\hat{U}^{-1}\hat{H}_F\hat{U}=\hat{U}_E^{-1}(\hat{U}_A^{-1}\hat{H}_F\hat{U}_A)\hat{U}_E=\hat{H}_0+\hat{V} \ . \qquad (3.12)$$

The states are transformed as

$$|\nu\alpha)=\hat{\alpha}^\dagger_\nu|0> \equiv \hat{U}_A^{-1}\hat{A}^\dagger_\nu|0>$$

and

$$|\nu\varepsilon)=\hat{\varepsilon}^\dagger_\nu|0> \equiv \hat{U}_E^{-1}\hat{E}^\dagger_\nu|0> \ . \qquad (3.13)$$

The ordering of the U's is critical since they do not commute in general.[2] For the opposite ordering, the second equation of (3.13) is violated unless *a* and *b* are identical particles, in which case the ordering gives the post-prior discrepancy familiar in scattering theory.[8]

The mechanics of the transformation are given in detail in Gilbert[9] (who has the opposite sign for all terms due to his sign in the equivalent of (3.11)) and in Girardeau.[3] The explicit result, below, differs somewhat from Girardeau's equations (34) through (42).[10] The rightmost y's in the second and fourth matrix elements in his equation (41), which should be y' and y_2, respectively, are given correctly in (3.23) below. The α-α matrix elements (ψ-ψ in his notation) which are diagonal in label are zero. In fact those which involve two labels of the same parity are zero. Hence the corresponding energy E_μ in the unperturbed Hamiltonian, H_0, is not renormalized as in his equation (38), and the lack of terms of the same parity in *V* is indicated below by a prime on the summation sign. And finally, the momentum dependent potential, *W* of (3.2), is included below.

There are no bound state terms in *W* included in H_0 since operating with the bare terms in *W* (a given matrix element excluding the orthogonalization corrections) which are diagonal in species (whether diagonal in label or not) on the asymptotic bound states gives zero.

The free-electron/free-positron (species diagonal, of any energy label) bare matrix element containing *W* is non-zero but still is included in V rather than H_0 because, as discussed in Chapter II, this term goes to zero asymptotically. When particles *a* and *e* are both far from the proton fixed at the origin, whether moving with correlated motion or not, the acceleration of the proton (the source of *W*) goes to zero. If either particle is near the origin while the other is at infinity, the coulomb potentials between these two, which would establish correlated motion, go to zero and hence *W* should also go to zero. Finally, if both free particles are near the origin *W* could be large, but such an asymptotic state is unstable and therefore would not be found in experiment, nor could it be considered a viable Lippmann-Schwinger asymptotic state.[11]

The potentials *V* and *W* are spectators to the unitary transformation of second-quantized operators in (3.12), so *W* may be added to *V* of Girardeau's equations (21) through (26).[3] These equations are simplified using the eigenvalue relations [the latter a finite mass generalization of Girardeau's equation (26)],

$$H_e(\vec{y})u_\nu^E(\vec{y}) = E_\nu u_\nu^E(\vec{y}) \ , \tag{3.14}$$

and

$$(T_a(\vec{x}) + T_e(\vec{y}) + V_{ae}(\vec{x}\vec{y}) + W_{ae}(\vec{x}\vec{y}))\phi_\mu^A(\vec{x}\vec{y}) = E_\mu\phi_\mu^A(\vec{x}\vec{y}) \ , \tag{3.15}$$

where

$$E_\mu = \frac{k^2}{2M} + E_\upsilon \ , \qquad M = \frac{m_b(m_a+ m_e)}{m_b+ m_a+ m_e} \ , \tag{3.16}$$

and E_λ is the bound state energy of the atom of type *A* or *E*.

The resulting terms in the Fock-Tani Hamiltonian are

$$\hat{H}_0 = \sum_{\nu} E_{\nu}\hat{\varepsilon}_{\nu}^{\dagger}\hat{\varepsilon}_{\nu} + \mathop{\sum\!\!\!\!\!\!\int}_{\mu} E_{\mu}\hat{\alpha}_{\mu}^{\dagger}\hat{\alpha}_{\mu} + \int d\vec{y}\,\hat{e}^{\dagger}(\vec{y})\hat{T}_e(\vec{y})\hat{e}(\vec{y}) + \int d\vec{x}\,\hat{a}^{\dagger}(\vec{x})T_a(\vec{x})\hat{a}(\vec{x}) \tag{3.17}$$

and

$$\begin{aligned}
\hat{V} = {} & \int d\vec{y}d\vec{y}'\hat{e}^{\dagger}(\vec{y})(\vec{y}|V_e|\vec{y}')'\hat{e}(\vec{y}') + \int d\vec{x}\,\hat{a}^{\dagger}(\vec{x})\frac{Z_aZ_b}{x}\,\hat{a}(\vec{x}) \\
& + \mathop{\sum\!\!\!\!\!\!\int\sum\!\!\!\!\!\!\int}_{\mu\gamma}{}'\,\hat{\alpha}_{\mu}^{\dagger}(\mu|V_b|\gamma)\hat{\alpha}_{\gamma} + \mathop{\sum\!\!\!\!\!\!\int}_{\mu}\int d\vec{x}d\vec{y}\big[\hat{\alpha}_{\mu}^{\dagger}(\mu|V_b|\vec{x}\vec{y})''\hat{e}(\vec{y})\hat{a}(\vec{x}) + \text{H.c.}\big] \\
& + \mathop{\sum\!\!\!\!\!\!\int\sum}_{\mu\nu}\int d\vec{x}\big[\hat{\alpha}_{\mu}^{\dagger}(\mu|V_b|\vec{x}\nu)'\hat{\varepsilon}_{\nu}\hat{a}(\vec{x}) + \text{H.c.}\big] \\
& + \int d\vec{x}d\vec{y}d\vec{x}'d\vec{y}'\hat{a}^{\dagger}(\vec{x})\hat{e}^{\dagger}(\vec{y})(\vec{x}\vec{y}|H_{ae}|\vec{x}'\vec{y}')''\hat{e}(\vec{y}')\hat{a}(\vec{x}') \\
& + \sum_{\nu}\int d\vec{x}d\vec{y}d\vec{x}'\big[\hat{a}^{\dagger}(\vec{x})\hat{e}^{\dagger}(\vec{y})(\vec{x}\vec{y}|H_{ae}|\vec{x}'\nu)''\hat{\varepsilon}_{\nu}\hat{a}(\vec{x}') + \text{H.c.}\big] \\
& + \sum_{\nu\tau}\sum\int d\vec{x}d\vec{x}'\hat{a}^{\dagger}(\vec{x})\hat{\varepsilon}_{\nu}^{\dagger}(\vec{x}\nu|H_{ae}|\vec{x}'\tau)'\hat{\varepsilon}_{\tau}\hat{a}(\vec{x}') \; ,
\end{aligned} \tag{3.18}$$

where H.c. stands for "Hermitian conjugate" and $\sum\!\!\!\!\!\!\int$ implies a sum over discreet variables and integration over the continuous variables in the α-state label. The primed matrix elements are renormalized by orthogonalization to the α bound states. Those doubly primed are also orthogonalized to the ε bound states. In order of appearance they are

$$(\vec{y}|V_e|\vec{y}\,')' = -\frac{Z_b}{y}\delta(\vec{y}-\vec{y}\,') - \sum_\nu E_\nu u^E_\nu(\vec{y})u^{E*}_\nu(\vec{y}\,') \ , \tag{3.19}$$

$$(\mu|V_b|\gamma) = \int d\vec{x}d\vec{y}\phi^{A*}_\mu(xy)T(xy)\phi^A_\gamma(\vec{x}\vec{y}) \ , \tag{3.20}$$

$$(\mu|V_b|\vec{x}\vec{y})'' = (\mu|V_b|\vec{x}\vec{y})' - \int d\vec{y}\,'\Delta^E(\vec{y}\,',\vec{y})(\mu|V_b|\vec{x}\vec{y}\,')' \ , \tag{3.21}$$

$$(\mu|V_b|\vec{x}\nu)' = \int d\vec{y}(\mu|V_b|\vec{x}\vec{y})'u^E_\nu(\vec{y}) \ , \tag{3.22}$$

$$\begin{aligned}(\vec{x}\vec{y}|H_{ae}|\vec{x}\,'\vec{y}\,')'' = {} & (\vec{x}\vec{y}|H_{ae}|\vec{x}\,'\vec{y}\,')' - \int d\vec{y}_1\Delta^E(\vec{y},\vec{y}_1)(\vec{x}\vec{y}_1|H_{ae}|\vec{x}\,'\vec{y}\,')' \\ & - \int d\vec{y}_1(\vec{x}\vec{y}|H_{ae}|\vec{x}\,'\vec{y}_1)'\Delta^E(\vec{y}_1,\vec{y}\,') \\ & + \int d\vec{y}_1 d\vec{y}_2\Delta^E(\vec{y},\vec{y}_1)(\vec{x}\vec{y}_1|H_{ae}|\vec{x}\,'\vec{y}_2)'\Delta^E(\vec{y}_2,\vec{y}\,') \ ,\end{aligned} \tag{3.23}$$

$$\begin{aligned}(\vec{x}\vec{y}|H_{ae}|\vec{x}\,'\nu)'' = {} & \int d\vec{y}\,'(\vec{x}\vec{y}|H_{ae}|\vec{x}\,'\vec{y}\,')'\phi^E_\nu(\vec{y}\,') \\ & - \int d\vec{y}\,'d\vec{y}_1\Delta^E(\vec{y},\vec{y}_1)(\vec{x}\vec{y}_1|H_{ae}|\vec{x}\,'\vec{y}\,')'\phi^E_\nu(\vec{y}\,') \ ,\end{aligned} \tag{3.24}$$

and

$$(\vec{x}\nu|H_{ae}|\vec{x}\,'\tau)' = \int d\vec{y}d\vec{y}\,'u^{E*}_\nu(\vec{y})(\vec{x}\vec{y}|H_{ae}|\vec{x}\,'\vec{y}\,')'u^E_\tau(\vec{y}\,') \ , \tag{3.25}$$

where

$$(\mu|V_b|\vec{x}\vec{y})' = \phi_\mu^{A*}(\vec{x}\vec{y})T(xy)$$

$$- \int d\vec{x}'d\vec{y}'\phi_\mu^{A*}(\vec{x}'\vec{y}')T(x'y')\Delta^A(\vec{x}'\vec{y}',\vec{x}\vec{y}) \ , \qquad (3.26)$$

$$(\vec{x}\vec{y}|H_{ae}|\vec{x}'\vec{y}')' = [V_{ae}(\vec{x}\vec{y}) + W_{ae}(\vec{x}\vec{y})]\delta(\vec{x}-\vec{x}')\delta(\vec{y}-\vec{y}') \ ,$$

$$- \sum_\mu E_\mu \phi_\mu^A(\vec{x}\vec{y})\phi_\mu^{A*}(\vec{x}'\vec{y}') + (\vec{x}\vec{y}|V_b|\vec{x}'\vec{y}')' \ , \qquad (3.27)$$

and

$$(\vec{x}\vec{y}|V_b|\vec{x}'\vec{y}')' = -[T(xy) - T(x'y')]\Delta^A(\vec{x}\vec{y},\vec{x}'\vec{y}')$$

$$+ \int d\vec{x}_1 d\vec{y}_1 \Delta^A(\vec{x}\vec{y},\vec{x}_1\vec{y}_1)T(x_1y_1)\Delta^A(\vec{x}_1\vec{y}_1,\vec{x}'\vec{y}') \ . \qquad (3.28)$$

The potential arising from the coulomb field of the charge Z_b is

$$T(xy) = \frac{Z_a Z_b}{x} - \frac{Z_b}{y} \ , \qquad (3.29)$$

and the ε and α bound-state kernels are, respectively,

$$\Delta^E(\vec{y},\vec{y}') = \sum_\nu u_\nu^E(\vec{y})u_\nu^{E*}(\vec{y}') \qquad (3.30)$$

and

$$\Delta^A(\vec{x}\vec{y},\vec{x}'\vec{y}') = \sum_m \phi_\mu^A(\vec{x}\vec{y})\phi_m^{A*}(\vec{x}'\vec{y}') \ . \qquad (3.31)$$

Girardeau[3] has shown that the bound-state kernels are diagonal in spin indices.

Comparison to Schrodinger Representation

The initial asymptotic states for the charge transfer reaction $a^+ + (b^+e^-) \rightarrow (a^+e^-) + b^+$ are

$$|\phi_i) = (2\pi)^{-3/2}\int dx \exp(i\vec{k}_i\cdot\vec{x})\hat{a}^\dagger(\vec{x})\hat{\varepsilon}^\dagger_\rho|0> \ , \qquad (3.32)$$

with energy eigenvalue

$$E_i = \frac{k^2}{2\mu_a} + E_\rho \ , \qquad (3.33)$$

and

$$(\phi_f| = <0|\hat{\alpha}_\sigma \ , \qquad (3.34)$$

with energy eigenvalue given by (3.16). The result in (3.33) is not equal to the initial state energy eigenvalue found in Chapter II due to the mass denominator μ_a which differs from the correct value M_i by a factor of $1/m_b$. Such an error in energy is acceptable for proton masses, but an additional error in the exponents of the initial momentum wave function is found, which is not negligible for incident kinetic energies greater than 5 keV.

The first-order approximation to the T-matrix for this reaction is

$$T^{1}_{fi} = (\phi_f|\hat{V}|\phi_i) = T^{1B}_{fi} + T^{1O}_{fi} \tag{3.35}$$

where

$$T^{1B}_{fi} = (2\pi)^{-3/2}\int d\vec{x}d\vec{y}\phi^{A*}_{\sigma}(\vec{x}\vec{y})\left(\frac{Z_aZ_b}{x} - \frac{Z_b}{y}\right)u^{E}_{\rho}(\vec{y})\exp(i\vec{k}_i\cdot\vec{x}) \tag{3.36}$$

and

$$T^{1O}_{fi} = -(2\pi)^{-3/2}\int d\vec{x}d\vec{y}d\vec{x}'d\vec{y}'\phi^{A*}_{\sigma}(\vec{x}'\vec{y}')\left(\frac{Z_aZ_b}{x'} - \frac{Z_b}{y'}\right)$$

$$\times\Delta^{A}(\vec{x}'\vec{y}',\vec{x}\vec{y})u^{E}_{\rho}(\vec{y})\exp(i\vec{k}_i\cdot\vec{x}) \; . \tag{3.37}$$

Substituting (3.6) into (3.36) and changing variables to

$$\vec{r} = \vec{y} - \vec{x} \tag{3.38}$$

gives

$$T^{1B}_{fi} = (2\pi)^{-3}\int d\vec{r}d\vec{y}e^{-i\vec{C}\cdot\vec{r}}u^{A*}_{\upsilon}(r)\left(\frac{Z_aZ_b}{|\vec{y}-\vec{r}|} - \frac{Z_b}{y}\right)u^{E}_{\rho}(y)e^{i\vec{B}'\cdot\vec{y}} \; , \tag{3.39}$$

where $\sigma = \{k_f,\upsilon\}$,

$$\vec{C} = \vec{k}_i - \zeta\vec{k}_f , \qquad \vec{B}' = \vec{k}_i - \vec{k}_f \; , \tag{3.40}$$

and ζ is given by (3.7). Apart from factors of 2π, this would equal the post form of the first Born term found by Jackson and Schiff[11] [their Equations (12) and (8′)], and would also equal the result from the Fock-Tani Hamiltonian derived from the full 3-body system [Equation (4.6) of Appendix A], if $\vec{k}_i$ in $\vec{B}'$ had a coefficient $m_b/(m_b+m_e)$. The first Born result of Massey and Mohr[12] also contains this approximation in B′, but they were calculating cross sections for electron capture from hydrogen by an incident positron of energy 6.8 to 100 eV. At these energies such an error is negligible. For the incident energies of order 10 to 100 keV appearing in Jackson and Schiff's cross sections and those in Appendix B, for reasonant charge transfer in proton-hydrogen scattering, k_i is large enough that the error from such an approximation is not negligible.

It has been shown that the first-order matrix element for charge transfer of the present Fock-Tani Hamiltonian does not contain the correct initial momentum eigenstate, nor does the initial asymptotic eigenstate give the correct energy. One is led to wonder whether the Fock-Tani Hamiltonian corresponding to the specialized initial-state Schrodinger Hamiltonian, (2.25), would correct these problems.

The Initial-state Version of the Fock-Tani Hamiltonian

The Fock-Tani Hamiltonian derived from the initial state form of the Fock Hamiltonian, (2.25), is

$$\hat{H}_{Fi} = \int d\vec{R}\hat{a}^{\dagger}(\vec{R})T_a(\vec{R})\hat{a}(\vec{R}) + \int d\vec{r}\hat{e}^{\dagger}(\vec{r})H_e(\vec{r})\hat{e}(\vec{r})$$

$$+ \int d\vec{R}d\vec{r}\hat{a}^{\dagger}(\vec{R})\hat{e}^{\dagger}(\vec{r})\left(V_{ae}(\vec{R}\vec{r}) + V_{ab}(\vec{R}\vec{r})\right)\hat{e}(\vec{r})\hat{a}(\vec{R}) , \qquad (3.41)$$

where

$$H_e(\vec{r}) = T_e(\vec{r}) - \frac{Z_b}{r} ,$$

$$T_a(\vec{R}) = -\frac{1}{2M}\nabla_R^2 , \qquad T_e(\vec{r}) = -\frac{1}{2m}\nabla_r^2 ,$$

$$V_{ae}(\vec{R}\vec{r}) = -\frac{Z_a}{|\vec{R}-\gamma\vec{r}|} , \text{ and } \qquad V_{ab}(\vec{R}\vec{r}) = \frac{Z_a Z_b}{|\vec{R}+\lambda\vec{r}|} , \qquad (3.42)$$

where λ and γ are given in (3.49) below. Equation (2.26) gives

$$M = \frac{m_a(m_b + m_e)}{m_a + m_b + m_e} \quad \text{and} \qquad m = \frac{m_e m_b}{m_e + m_b} . \qquad (3.43)$$

Equation (3.41) differs physically from (3.1) in that a is a fictitious particle with a 3-body reduced mass rather than a 2-body reduced mass. Also the Schrodinger operators in the first and third terms are slightly different.

The Fock creation operators for bound species are as in (3.4) and (3.5),

$$\hat{E}^{\dagger}_{\nu} = \int d\vec{r} u^{E}_{\nu}(\vec{r})\hat{e}^{\dagger}(\vec{r}) \qquad (3.44)$$

and

$$\hat{A}^{\dagger}_{\mu} = \int d\vec{R} d\vec{r} \phi^{A}_{\mu}(\vec{R}\vec{r})\hat{a}^{\dagger}(\vec{R})\hat{e}^{\dagger}(\vec{r}) \ , \qquad (3.45)$$

except that the coordinates for the latter bound state orbital must be transformed from the natural set, $\{R_f, r_f\}$, to the set $\{R, r\}$ appearing in (3.45) using the relations given in (2.24)

$$\vec{R}_f = \zeta\vec{R} + \iota\vec{r} \ , \qquad \vec{r}_f = \gamma\vec{r} - \vec{R} \ ,$$

and

$$\vec{R} = \lambda\vec{R}_f - \iota\vec{r}_f \ , \text{ and } \qquad \vec{r} = \zeta\vec{r}_f + \vec{R}_f \ , \qquad (3.46)$$

where

$$\zeta = \frac{m_a}{m_a + m_e} \ , \qquad \eta = \frac{m_e}{m_a + m_e} \ , \qquad (3.47)$$

$$\gamma = \frac{m_b}{m_b + m_e} \ , \qquad \lambda = \frac{m_e}{m_b + m_e} \ , \text{ and} \qquad (3.49)$$

$$\iota = \zeta\lambda + \eta \ . \qquad (3.50)$$

The wave function is,

$$\phi^A_\mu(\vec{R}\vec{r}) = (2\pi)^{-3/2} e^{i\vec{k}\cdot\vec{R}_f} u^A_\upsilon(\vec{r}_f) =$$

$$= (2\pi)^{-3/2} e^{i\vec{k}\cdot(\zeta\vec{R} + \iota\vec{r})} u^A_\upsilon(\gamma\vec{r} - \vec{R}) , \qquad (3.51)$$

where $\mu = \{k,\upsilon\}$.

The electron and *a* fields satisfy the same anti-commutation relations as in (3.8),

$$\{\hat{e}(r),\hat{e}^\dagger(\vec{r}')\}=\delta(\vec{r}-\vec{r}')=\delta(\vec{r}_e-\vec{r}_e')\delta_{\sigma\sigma'} ,$$

$$\{\hat{a}(R),\hat{a}^\dagger(\vec{R}')\}=\delta(\vec{R}-\vec{R}') , \text{ and}$$

$$\{\hat{e}(\vec{r}),\hat{e}(\vec{r}')\}=\{\hat{a}(\vec{R}),\hat{a}(\vec{R}')\}=\{\hat{e}(\vec{r}),\hat{a}(\vec{R})\}=\{\hat{e}(\vec{r}),\hat{a}^\dagger(\vec{R})\}=0 . \qquad (3.52)$$

Again, the bound state fields satisfy extremely complicated (anti-) commutation relations with the free particles and among themselves.

As in (3.9) one defines ideal bound state creation operators $\hat{\varepsilon}^\dagger_\nu$ and $\hat{\alpha}^\dagger_\mu$ such that

$$\{\hat{\varepsilon}_\mu,\hat{\varepsilon}^\dagger_\nu\}=[\hat{\alpha}_\mu,\hat{\alpha}^\dagger_\nu]=\delta_{\mu\nu} \ ,$$

$$\{\hat{\varepsilon}_\mu,\hat{\varepsilon}_\nu\}=\{\hat{\varepsilon}_\mu,\hat{e}^{(\dagger)}(\vec{r})\}=\{\hat{\varepsilon}_\mu,\hat{a}^{(\dagger)}(\vec{R})\}=0 \ , \text{ and}$$

$$[\hat{\alpha}_\mu,\hat{\alpha}_\nu]=[\hat{\alpha}_\mu,\hat{e}^{(\dagger)}(\vec{r})]=[\hat{\alpha}_\mu,\hat{a}^{(\dagger)}(\vec{R})]=[\hat{\alpha}_\mu,\hat{\varepsilon}^{(\dagger)}_\nu]=0 \ . \qquad (3.53)$$

The Fock-Tani transformation is the same as (3.11) through (3.16), although (3.14) and (3.15) need to be rewritten

$$H_e(\vec{r})u^E_\nu(\vec{r}) = \mathcal{E}_\nu u^E_\nu(\vec{r}) \qquad (3.54)$$

and

$$(T_a(\vec{R}) + T_e(\vec{r}) + V_{ae}(\vec{R}\vec{r}))\phi^A_\mu(\vec{R}\vec{r}) = E_\mu\phi^A_\mu(\vec{R}\vec{r}) \ . \qquad (3.55)$$

The operators in the last expression can be expressed in $\{\vec{R}_f,\vec{r}_f\}$ to give the right-hand side.

The resulting Fock-Tani Hamiltonian is given by

$$\hat{H}_0= \sum_\nu \mathcal{E}_\nu\hat{\varepsilon}^\dagger_\nu\hat{\varepsilon}_\nu + \sum_\mu E_\mu\hat{\alpha}^\dagger_\mu\hat{\alpha}_\mu + \int d\vec{r}\,\hat{e}^\dagger(\vec{r})\hat{T}_e(\vec{r})\hat{e}(\vec{r}) + \int d\vec{R}\,\hat{a}^\dagger(\vec{R})T_a(\vec{R})\hat{a}(\vec{R}) \qquad (3.56)$$

and

$$\begin{aligned}\hat{V} = {} & \int d\vec{r}d\vec{r}'\hat{e}^{\dagger}(\vec{r})(\vec{r}|V_e|\vec{r}')'\hat{e}(\vec{r}') \\ & + \mathop{\sum\!\!\!\!\!\!\int}_{\mu}\mathop{\sum\!\!\!\!\!\!\int}_{\gamma}{}'\,\hat{\alpha}_{\mu}^{\dagger}(\mu|V_b|\gamma)\hat{\alpha}_{\gamma} + \mathop{\sum\!\!\!\!\!\!\int}_{\mu}\int d\vec{R}d\vec{r}\big[\hat{\alpha}_{\mu}^{\dagger}(\mu|V_b|\vec{R}\vec{r})''\hat{e}(\vec{r})\hat{a}(\vec{R}) + \text{H.c.}\big] \\ & + \mathop{\sum\!\!\!\!\!\!\int}_{\mu}\sum_{\nu}\int d\vec{R}\big[\hat{\alpha}_{\mu}^{\dagger}(\mu|V_b|\vec{R}\nu)'\hat{\varepsilon}_{\nu}\hat{a}(\vec{R}) + \text{H.c.}\big] \\ & + \int d\vec{R}d\vec{r}d\vec{R}'d\vec{r}'\hat{a}^{\dagger}(\vec{R})\hat{e}^{\dagger}(\vec{r})(\vec{R}\vec{r}|H_{ae}|\vec{R}'\vec{r}')''\hat{e}(\vec{r}')\hat{a}(\vec{R}') \\ & + \sum_{\nu}\int d\vec{R}d\vec{r}d\vec{R}'\big[\hat{a}^{\dagger}(\vec{R})\hat{e}^{\dagger}(\vec{r})(\vec{R}\vec{r}|H_{ae}|\vec{R}'\nu)''\hat{\varepsilon}_{\nu}\hat{a}(\vec{R}') + \text{H.c.}\big] \\ & + \sum_{\nu}\sum_{\tau}\int d\vec{R}d\vec{R}'\hat{a}^{\dagger}(\vec{R})\hat{\varepsilon}_{\nu}^{\dagger}(\vec{R}\nu|H_{ae}|\vec{R}'\tau)'\hat{\varepsilon}_{\tau}\hat{a}(\vec{R}') \, . \end{aligned} \tag{3.57}$$

The matrix elements are

$$(\vec{r}|V_e|\vec{r}')' = -\frac{Z_b}{r}\delta(\vec{r}-\vec{r}') - \sum_{\nu}\mathcal{E}_{\nu}u_{\nu}^{E}(\vec{r})u_{\nu}^{E*}(\vec{r}') \, , \tag{3.58}$$

$$(\mu|V_b|\gamma) = \int d\vec{R}d\vec{r}\phi_{\mu}^{A*}(Rr)T(Rr)\phi_{\gamma}^{A}(\vec{R}\vec{r}) \, , \tag{3.59}$$

$$(\mu|V_b|\vec{R}\vec{r})'' = (\mu|V_b|\vec{R}\vec{r})' - \int d\vec{r}'\Delta^{E}(\vec{r}',\vec{r})(\mu|V_b|\vec{R}\vec{r}')' \, , \tag{3.60}$$

$$(\mu|V_b|\vec{R}\nu)' = \int d\vec{r}(\mu|V_b|\vec{R}\vec{r})'u_{\nu}^{E}(\vec{r}) \, , \tag{3.61}$$

$$
\begin{aligned}
(\vec{R}\vec{r}|H_{ae}|\vec{R}'\vec{r}')'' =& (\vec{R}\vec{r}|H_{ae}|\vec{R}'\vec{r}')' - \int d\vec{r}_1 \Delta^E(\vec{r},\vec{r}_1)(\vec{R}\vec{r}_1|H_{ae}|\vec{R}'\vec{r}')' \\
& - \int d\vec{r}_1 (\vec{R}\vec{r}|H_{ae}|\vec{R}'\vec{r}_1)' \Delta^E(\vec{r}_1,\vec{r}') \\
& + \int d\vec{r}_1 d\vec{r}_2 \Delta^E(\vec{r},\vec{r}_1)(\vec{R}\vec{r}_1|H_{ae}|\vec{R}'\vec{r}_2)' \Delta^E(\vec{r}_2,\vec{r}') \ ,
\end{aligned}
\tag{3.62}
$$

$$
\begin{aligned}
(\vec{R}\vec{r}|H_{ae}|\vec{R}'\nu)'' =& \int d\vec{r}' (\vec{R}\vec{r}|H_{ae}|\vec{R}'\vec{r}')' \phi^E_\nu(\vec{r}') \\
& - \int d\vec{r}' d\vec{r}_1 \Delta^E(\vec{r},\vec{r}_1)(\vec{R}\vec{r}_1|H_{ae}|\vec{R}'\vec{r}')' \phi^E_\nu(\vec{r}') \ ,
\end{aligned}
\tag{3.63}
$$

and

$$
(\vec{R}\nu|H_{ae}|\vec{R}'\tau)' = \int d\vec{r} d\vec{r}' u^{E*}_\nu(\vec{r})(\vec{R}\vec{r}|H_{ae}|\vec{R}'\vec{r}')' u^E_\tau(\vec{r}') \ , \tag{3.64}
$$

where

$$
\begin{aligned}
(\mu|V_b|\vec{R}\vec{r})' =& \phi^{A*}_\mu(\vec{R}\vec{r}) T(Rr) \\
& - \int d\vec{R}' d\vec{r}' \phi^{A*}_\mu(\vec{R}'\vec{r}') T(R'r') \Delta^A(\vec{R}'\vec{r}',\vec{R}\vec{r}) \ ,
\end{aligned}
\tag{3.65}
$$

$$
\begin{aligned}
(\vec{R}\vec{r}|H_{ae}|\vec{R}'\vec{r}')' =& [V_{ae}(\vec{R}\vec{r}) + V_{ab}(\vec{R}\vec{r})]\delta(\vec{R}-\vec{R}')\delta(\vec{r}-\vec{r}') \ , \\
& - \sum_\mu E_\mu \phi^A_\mu(\vec{R}\vec{r}) \phi^{A*}_\mu(\vec{R}'\vec{r}') + (\vec{R}\vec{r}|V_b|\vec{R}'\vec{r}')' \ ,
\end{aligned}
\tag{3.66}
$$

and

$$(\vec{R}\vec{r}|V_b|\vec{R}'\vec{r}')' = -[T(Rr) - T(R'r')]\Delta^A(\vec{R}\vec{r},\vec{R}'\vec{r}')$$
$$+ \int d\vec{R}_1 d\vec{r}_1 \Delta^E(\vec{R}\vec{r},\vec{R}_1\vec{r}_1) T(R_1 r_1) \Delta^A(\vec{R}_1\vec{r}_1,\vec{R}'\vec{r}') \ . \qquad (3.67)$$

The potential arising from the coulomb field of the charge Z_b is

$$T(Rr) = \frac{Z_a Z_b}{|\vec{R}+\lambda\vec{r}|} - \frac{Z_b}{r}, \qquad (3.68)$$

and the ε and α bound-state kernels are, respectively,

$$\Delta^E(\vec{r},\vec{r}') = \sum_\nu u_\nu^E(\vec{r}) u_\nu^{E*}(\vec{r}') \qquad (3.69)$$

and

$$\Delta^A(\vec{R}\vec{r},\vec{R}'\vec{r}') = \sum\!\!\!\!\!\!\int_m \phi_\mu^A(\vec{R}\vec{r}) \phi_m^{A*}(\vec{R}'\vec{r}') \ . \qquad (3.70)$$

This differs from the Fock-Tani Hamiltonian, (3.17) and (3.18), derived in the symmetrical coordinate system. The mass denominator of T_a in H_0 is changed from μ_a to M . The second term in V of (3.18) does not appear in (3.57). The physical content of this term appears in (3.66) instead, replacing the inertial potential of (3.27) (which does not appear in this inertial system).

The initial asymptotic states for the charge transfer reaction $a^+ + (b^+e^-) \rightarrow (a^+e^-) + b^+$ are

$$|\phi_i) = (2\pi)^{-3/2}\int dR \exp(i\vec{k}_i\cdot\vec{R})\hat{a}^\dagger(\vec{R})\hat{\varepsilon}_\rho^\dagger|0> , \qquad (3.71)$$

with energy eigenvalue

$$E_i = \frac{k^2}{2M} + E_\rho , \qquad (3.72)$$

and

$$(\phi_f| = <0|\hat{\alpha}_\sigma , \qquad (3.73)$$

with energy eigenvalue given by (3.16). The result in (3.72), unlike that for the non-specialized Fock-Tani version, (3.35), is equal to the initial state energy eigenvalue (2.27).

The first-order approximation to the T-matrix for this reaction is

$$T_{fi}^{1} = (\phi_f|\hat{V}|\phi_i) = T_{fi}^{1b} + T_{fi}^{1O} , \qquad (3.74)$$

where

$$T_{fi}^{1B} = (2\pi)^{-3/2}\int d\vec{R}d\vec{r}\phi^{A*}_\sigma(\vec{R}\vec{r})\left(\frac{Z_aZ_b}{|\vec{R}+\lambda\vec{r}|} - \frac{Z_b}{r}\right)u_\rho^E(\vec{r})\exp(i\vec{k}_i\cdot\vec{R}) \qquad (3.75)$$

and

$$T_{fi}^{10} = -(2\pi)^{-2/3}\int d\vec{R}d\vec{r}d\vec{R}'d\vec{r}'\phi_{\sigma}^{A*}(\vec{R}'\vec{r}')\left(\frac{Z_aZ_b}{|\vec{R}'+\lambda\vec{r}'|} - \frac{Z_b}{r}\right)$$

$$\times\Delta^{A}(\vec{R}'\vec{r}',\vec{R}\vec{r})u_{\rho}^{E}(\vec{r})\exp(i\vec{k}_{i}\cdot\vec{R}) \quad . \qquad (3.76)$$

Substituting (3.51) into (3.75) and changing variables to

$$\vec{r}' = \gamma\vec{r} - \vec{R} \qquad (3.77)$$

gives

$$T_{fi}^{1B} = (2\pi)^{-3}\int d\vec{r}'d\vec{r}e^{-i\vec{C}\cdot\vec{r}'}u_{\upsilon}^{A*}(r')\left(\frac{Z_aZ_b}{|\vec{r}-\vec{r}'|} - \frac{Z_b}{r}\right)u_{\rho}^{E}(r)e^{i\vec{B}\cdot\vec{r}} \quad , \qquad (3.78)$$

where $\sigma = \{k_f,\upsilon\}$,

$$\vec{C} = \vec{k}_i - \zeta\vec{k}_f, \qquad \vec{B} = \gamma\vec{k}_i - \vec{k}_f \quad , \qquad (3.79)$$

and ζ is given by (3.7).

Apart from a factor of 2π, this equals the post form of the first Born term found by Jackson and Schiff[11] [their Equations (12) and (8′)] and equals the result from the Fock-Tani Hamiltonian derived within the full 3-body system [Equation (4.6) in Appendix B]. Although (3.41) is the prior Fock Hamiltonian, the order of the unitary transformations in (3.12) produces the post form of the T-matrix, as in the symmetrical Fock Hamiltonian (3.1) case. Given the opposite ordering in (3.12), the prior form of the T-matrix would result from transforming either the symmetric Fock Hamiltonian, (3.1), or the initial-state Fock Hamiltonian, (3.41).

The equivalence of post and prior forms of the first order T-matrix is well known.[13] It seems reasonable that a first-order T-matrix derived from the non-specialized Schrodinger Hamiltonian, (2.22), [or Fock Hamiltonian, (3.1)] would also be equivalent to the first-order T-matrix derived from the post and prior Schrodinger Hamiltonians, (3.25) [or prior Fock Hamiltonian, (3.41), and its post equivalent]. This equivalence must be true for the exact T-matrix because of the equivalence of frames of reference. Furthermore, the T-matrices derived from the post form of the Fock-Tani Hamiltonians, produced by the ordering in (3.12), and the prior form, given by the opposite ordering in (3.12), should be equivalent provided one starts with the same Fock Hamiltonian in both cases. However, as demonstrated by the differences between (3.40) and (3.78), the Fock-Tani transformation of the various Fock Hamiltonians does not necessarily produce equivalent first-order T-matrices. In fact one can not even set up the transformation of the post Fock Hamiltonian in the present reduced-mass scheme because the crucial definition of the Fock composite state consisting of the electron bound to the origin would not be of the form of an integral over one variable, as in (3.3) and (3.44).

The Fock-Tani transformation mixes terms according to the Fock-space operators, not the Schrodinger operators, so that the inertial potential *W*, containing the effects of the accelerated coordinate system, (3.1), does not appear in many of the terms in the Fock-Tani Hamiltonian, (3.17) and (3.18), which represent the various physical processes. One would have to go to the second-order T-matrix (or higher) before the effects of *W* would be present in a given process.

It is found that this neglect in first-order is acceptable for projectile momenta not greater than the mass of the particle fixed at the origin. With this restriction in mind, the Fock-Tani transformation of a system of negatively charged particles of two kinds and a positive charge fixed at the origin will be derived.

The Fock-Tani Hamiltonian for $a^- + (b^+e^-) \rightarrow (a^-b^+) + e^-$

To illustrate of the full potential of the symmetrical 3→2-body reduced Hamiltonian, (2.22), the Fock-Tani Hamiltonian for a system consisting of one particle of positive charge (Z_b) fixed at the origin and a negatively charged particles of each of two species with creation operators $\hat{e}^\dagger(\vec{y})$ (with unit charge and reduced mass μ_e), and $\hat{a}^\dagger(\vec{x})$ (with charge $-Z_a$ and reduced-mass μ_a) is found. The Z_b will be kept general but states of more than one particle (*a* or *e*) bound to the origin will not be considered.

The Fock Hamiltonian is

$$\hat{H}_F = \int d\vec{x}\,\hat{a}^\dagger(\vec{x})H_a(\vec{x})\hat{a}(\vec{x}) + \int d\vec{y}\,\hat{e}^\dagger(\vec{y})H_e(\vec{y})\hat{e}(\vec{y})$$

$$+ \int d\vec{x}d\vec{y}\,\hat{a}^\dagger(\vec{x})\hat{e}^\dagger(\vec{y})\left(V_{ae}(\vec{x}\vec{y}) + W_{ae}(\vec{x}\vec{y})\right)\hat{e}(\vec{y})\hat{a}(\vec{x}) \ , \qquad (3.80)$$

where

$$H_a(\vec{x}) = T_a(\vec{x}) - \frac{Z_a Z_b}{x} \ , \qquad H_e(\vec{y}) = T_e(\vec{y}) - \frac{Z_b}{y} \ ,$$

$$T_a(\vec{x}) = -\frac{1}{2\mu_a}\nabla_x^2 \ , \qquad T_e(\vec{y}) = -\frac{1}{2\mu_e}\nabla_y^2 \ ,$$

$$V_{ae}(\vec{x}\vec{y}) = \frac{Z_a}{|\vec{x}-\vec{y}|} \ , \text{ and } \qquad W_{ae}(\vec{x}\vec{y}) = -\frac{1}{m_b}\vec{\nabla}_x\cdot\vec{\nabla}_y \ , \qquad (3.81)$$

and where

$$\mu_a = \frac{m_a m_b}{m_a + m_b} \quad \text{and} \quad \mu_e = \frac{m_e m_b}{m_e + m_b} \ . \qquad (3.82)$$

The number operators

$$\hat{N}_a = \int d\vec{x}\,\hat{a}^\dagger(\vec{x})\hat{a}(\vec{x}) \qquad (3.83)$$

and

$$\hat{N}_e = \int d\vec{y}\,\hat{e}^\dagger(\vec{y})\hat{a}(\vec{y}) \qquad (3.84)$$

are not necessarily equal to one.

The creation operators for particles e and a bound to the origin are, respectively,

$$\hat{E}^{\dagger}_{\nu} = \int d\vec{y}\, u^{E}_{\nu}(\vec{y})\, \hat{e}^{\dagger}(\vec{y}) \tag{3.85}$$

and

$$\hat{A}^{\dagger}_{\nu} = \int d\vec{x}\, u^{A}_{\nu}(\vec{x})\, \hat{a}^{\dagger}(\vec{x}) \tag{3.86}$$

where

$$H_{b} u^{B}_{\nu}(\vec{w}) = E_{\nu} u^{B}_{\nu}(\vec{w}) \tag{3.87}$$

for $(b,B,\vec{w}) = \{(a,A,\vec{x}) \text{ or } (e,E,\vec{y})\}$.

The e and a fields satisfy the anti-commutation relations (3.8) and the Fock bound state fields, (3.85) and (3.86), satisfy non-elementary commutation relations with the free particles.

As with (3.11) the Fock space is enlarged to include bound state operators $\hat{\varepsilon}^{\dagger}_{\nu}$ and $\hat{\alpha}^{\dagger}_{\nu}$, which satisfy the elementary (anti-) commutation relations (3.9). The Hamiltonian and the states are transformed to the subspace ε and α have physical content using

$$\hat{U} = \hat{U}_{A}\hat{U}_{E} \quad , \quad \hat{U}_{B} = \exp\left(\frac{\pi}{2}\hat{F}_{\beta}\right) \quad , \quad \hat{F}_{\beta} = \sum_{\nu}(\hat{B}^{\dagger}_{\nu}\hat{\beta}_{\nu} - \hat{\beta}^{\dagger}_{\nu}\hat{B}_{\nu}) \ , \tag{3.88}$$

where a generic notation, $B = \{A \text{ or } E\}$ and $\beta = \{\alpha \text{ or } \varepsilon\}$, is introduced for convenience. The states are transformed as in (3.13) and the transformed Hamiltonian is given by

$$\hat{H} = \hat{U}^{-1}\hat{H}_F\hat{U} = \hat{U}_E^{-1}(\hat{U}_A^{-1}\hat{H}_F\hat{U}_A)\hat{U}_E = \hat{H}_0 + \hat{V} + \hat{X} \ . \qquad (3.89)$$

In the present case the ordering of (3.89) is not important since

$$[\hat{F}_\alpha, \hat{F}_\varepsilon] = 0 \ . \qquad (3.90)$$

Because the nucleus of both bound states is fixed to the origin and, therefore, does not enter the dynamics one can bypass the lengthy "d matrix" approach to the transformation for the α bound states, given in Gilbert[8] and Girardeau,[3] in favor of their approach for the ε bound states for both species.

For a generic operator $\hat{B}$ of either type (a, A, α, e, E, or ε), define the transformed operator as

$$\hat{B}(t) = e^{-t\hat{F}_\beta} \ \hat{B} \ e^{t\hat{F}_\beta} \ , \qquad (3.91)$$

where F_β is given in (3.88). This is solved using the corresponding "equation of motion,"

$$\frac{\partial \hat{B}(t)}{\partial t} = [\hat{B}(t), \hat{F}_\beta] \ . \qquad (3.92)$$

The explicit equations for the relevant operators are

$$\frac{\partial \hat{B}_\nu(t)}{\partial t} = \hat{\beta}_\nu(t) \ , \qquad (3.93)$$

$$\frac{\partial\hat{\beta}_\nu(t)}{\partial t} = -\hat{B}_\nu(t) \ , \qquad (3.94)$$

and

$$\frac{\partial\hat{b}(\vec{w},t)}{\partial t} = \sum_\tau u^B_\tau(\vec{w})\hat{b}_\tau(t) \ . \qquad (3.95)$$

Equations (3.93) and (3.94) have solutions, satisfying the initial condition $\hat{\mathcal{B}}(t) = \hat{\mathcal{B}}$,

$$\hat{\beta}_\nu(t) = \hat{\beta}_\nu \cos t - \hat{B}_\nu \sin t$$

and

$$\hat{B}_\nu(t) = \hat{\beta}_\nu \sin t + \hat{B}_\nu \cos t \ . \qquad (3.96)$$

Substituting these into (3.95), taking the indefinite integral of both sides, and setting $t=\pi/2$ gives

$$\hat{U}_A^{-1}\hat{a}(\vec{x})\hat{U}_A = \hat{a}(\vec{x}) - \int d\vec{x}'\Delta^A(\vec{x},\vec{x}')\hat{a}(\vec{x}') + \sum_\tau u^A_\tau(\vec{x})\hat{\alpha}_\tau \qquad (3.97)$$

and

$$\hat{U}_E^{-1}\hat{e}(\vec{y})\hat{U}_E = \hat{e}(\vec{y}) - \int d\vec{y}'\Delta^E(\vec{y},\vec{y}')\hat{e}(\vec{y}') + \sum_n u^E_\nu(\vec{y})\hat{\varepsilon}_\nu \ . \qquad (3.98)$$

Because of (3.8) and (3.9),

$$\hat{U}_E^{-1}\hat{a}(\vec{x})\hat{U}_E = \hat{a}(\vec{x}) \qquad \text{and} \qquad \hat{U}_A^{-1}\hat{e}(\vec{y})\hat{U}_A = \hat{e}(\vec{y}) \ . \qquad (3.99)$$

Defining the functional

$$\hat{O}[\vec{x}\vec{y}] = \hat{H}_a(\vec{x}) + \int d\vec{y}\,\hat{e}^\dagger(\vec{y})(V_{ae}(\vec{x}\vec{y}) + W_{ae}(\vec{x}\vec{y}))\hat{e}(\vec{y}) \; , \tag{3.100}$$

the first part of the transformation (3.89) is

$$\begin{aligned}
\hat{U}_A^{-1}\hat{H}_F\hat{U}_A = {} & \int d\vec{y}\,\hat{e}^\dagger(\vec{y})H_e(\vec{y})\hat{e}(\vec{y}) + \int d\vec{x}\big(\hat{a}^\dagger(\vec{x})\{\hat{O}[\vec{x}\vec{y}]\hat{a}(\vec{x}) \\
& - \int d\vec{x}'\,\hat{O}[\vec{x}\vec{y}]\Delta^A(\vec{x},\vec{x}')\hat{a}(\vec{x}') + \sum_\nu \hat{O}[\vec{x}\vec{y}]u_\nu^A(\vec{x})\hat{\alpha}_\nu\} + \text{H.c.}\big) \\
& + \int d\vec{x}\,d\vec{x}'\,d\vec{x}_1\,\hat{a}^\dagger(\vec{x}_1)\Delta^A(\vec{x}_1,\vec{x})\hat{O}[\vec{x}\vec{y}]\Delta^A(\vec{x},\vec{x}')\hat{a}(\vec{x}') \\
& - \sum_\nu\int d\vec{x}\,d\vec{x}'\{\hat{\alpha}_\nu^\dagger u_\nu^{A*}(\vec{x})\hat{O}[\vec{x}\vec{y}]\Delta^A(\vec{x},\vec{x}')\hat{a}(\vec{x}') + \text{H.c.}\} \\
& + \sum_\tau\sum_\nu\int d\vec{x}\,\hat{\alpha}_\tau^\dagger u_\tau^{A*}(\vec{x})\hat{O}[\vec{x}\vec{y}]u_\nu^A(\vec{x})\hat{\alpha}_\nu
\end{aligned} \tag{3.101}$$

Upon changing variables in the integrals and substituting (3.100) this becomes

$$\begin{aligned}\hat{U}_A^{-1}\hat{H}_F\hat{U}_A = {} & \sum_{\tau\nu}\hat{\alpha}_\tau^\dagger(\tau|H_a|\nu)\hat{\alpha} + \int d\vec{x}d\vec{x}'\hat{a}^\dagger(\vec{x})(\vec{x}|H_a|\vec{x}')'\hat{a}(\vec{x}') \\ & + \int d\vec{y}\hat{e}^\dagger(\vec{y})\Big[\sum_{\tau\nu}\hat{\alpha}_\tau^\dagger(\tau|VW|\nu\vec{y})\hat{\alpha}_\nu + \sum_\tau d\vec{x}\hat{\alpha}_\tau^\dagger(\tau|VW|\vec{x}\vec{y})'\hat{a}(\vec{x}) \\ & + H_e(\vec{y}) + \int d\vec{x}d\vec{x}'\hat{a}^\dagger(\vec{x})(\vec{x}\vec{y}|VW|\vec{x}'\vec{y}')'\hat{a}(\vec{x}')\Big]\hat{e}(\vec{y}) \ ,\end{aligned} \tag{3.102}$$

where

$$(\tau|H_a|\nu) = E_\tau\delta_{\tau\nu} \ , \tag{3.103}$$

$$(\vec{x}|H_a|\vec{x}')' = H_a\delta(\vec{x}-\vec{x}') - \sum_\nu E_\nu u_\nu^A(\vec{x})u_\nu^{A*}(\vec{x}') \ , \tag{3.104}$$

$$(\tau\vec{y}|VW|\nu\vec{y}) = \int d\vec{x}u_\tau^{A*}(\vec{x})T(\vec{x}\vec{y})u_\nu^A(\vec{x}) \ , \tag{3.105}$$

$$[\tau\vec{y}|VW|\vec{x}\vec{y})' = u_\tau^{A*}(\vec{x})T(\vec{x}\vec{y}) - \int d\vec{x}'u_\tau^{A*}(\vec{x}')T(\vec{x}'\vec{y})\Delta^A(\vec{x}',\vec{x}) \ , \tag{3.106}$$

$$\begin{aligned}(\vec{x}\vec{y}|VW|\vec{x}'\vec{y})' = {} & T(\vec{x}\vec{y})\delta(\vec{x}-\vec{x}') - [T(\vec{x}\vec{y}) + T(\vec{x}'\vec{y})]\Delta^A(\vec{x},\vec{x}') \\ & + \int d\vec{x}_1\Delta^A(\vec{x},\vec{x}_1)T(\vec{x}_1\vec{y})\Delta^A(\vec{x}_1,\vec{x}') \ ,\end{aligned} \tag{3.107}$$

and

$$T(\vec{x}\vec{y}) = V_{ae}(\vec{x}\vec{y}) + W_{ae}(\vec{x}\vec{y}) \; . \qquad (3.108)$$

Equation (3.89) has been to simplify these. It should be noted that there is no $\hat{a}^{\dagger}_{\nu}\hat{a}(\vec{x})$ term in (3.102) because

$$(\tau|H_a|\vec{x})' = u^{A*}_{\tau}(\vec{x})H_a(\vec{x}) - \int d\vec{x}' u^{A*}_{\tau}(\vec{x}')H_a(\vec{x}')\Delta^{A}(\vec{x}',\vec{x}) = 0 \; . \qquad (3.109)$$

The second transformation in (3.89) gives the final Fock-Tani Hamiltonian,

$$\hat{H}_0 = \sum_{\nu} E_{\nu}\hat{\alpha}_{\nu}\hat{\alpha}_{\nu} + \sum_{\lambda} E_{\lambda}\hat{\varepsilon}_{\lambda}\hat{\varepsilon}_{\lambda} + \int d\vec{x}\hat{a}\,(\vec{x})T_a(\vec{x})\hat{a}(\vec{x}) + \int d\vec{y}\hat{e}\,(\vec{y})T_e(\vec{y})\hat{e}(\vec{y}) \; , \qquad (3.110)$$

$$\hat{v} = \int d\vec{x}d\vec{x}'\hat{a}^\dagger(\vec{x})(\vec{x}|v_a|\vec{x}')'\hat{a}(\vec{x}') + \int d\vec{y}d\vec{y}'\hat{e}^\dagger(\vec{y})(\vec{y}|v_e|\vec{y}')'\hat{e}(\vec{y}')$$

$$+ \sum_{\tau\nu}\int d\vec{y}d\vec{y}'\hat{\alpha}_\tau^\dagger\hat{e}^\dagger(\vec{y})(\tau\vec{y}|VW|\nu\vec{y}')'\hat{e}(\vec{y}')\hat{\alpha}_\nu$$

$$+ \sum_{\eta\lambda}\int d\vec{x}d\vec{x}'\hat{a}^\dagger(\vec{x})\hat{\varepsilon}_\eta^\dagger(\vec{x}\eta|VW|\vec{x}'\lambda)'\hat{\varepsilon}_\lambda\hat{a}(\vec{x}')$$

$$+ \sum_{\tau}\int d\vec{y}d\vec{y}'d\vec{x}[\hat{\alpha}_\tau^\dagger\hat{e}^\dagger(\vec{y})(\tau\vec{y}|VW|\vec{x}\vec{y}')''\hat{e}(\vec{y}')\hat{a}(\vec{x}) + \text{H.c.}]$$

$$+ \sum_{\lambda}\int d\vec{x}d\vec{y}d\vec{x}'[\hat{a}^\dagger(\vec{x})\hat{e}^\dagger(\vec{y})(\vec{x}\vec{y}|VW|\vec{x}'\lambda)''\hat{\varepsilon}_\lambda\hat{a}(\vec{x}') + \text{H.c.}]$$

$$+ \sum_{\tau\lambda}\int d\vec{x}d\vec{y}[\hat{\alpha}_\tau^\dagger\hat{e}^\dagger(\vec{y})(\tau\vec{y}|VW|\vec{x}\lambda)''\hat{\varepsilon}_\lambda\hat{a}(\vec{x}) + \text{H.c.}]$$

$$+ \int d\vec{x}d\vec{y}d\vec{x}'d\vec{y}'\hat{a}^\dagger(\vec{x})\hat{e}^\dagger(\vec{y})(\vec{x}\vec{y}|VW|\vec{x}'\vec{y}')''\hat{e}(\vec{y}')\hat{a}(\vec{x}') \ , \qquad (3.111)$$

and

$$\hat{X} = \sum_{\tau\eta\nu\lambda}\alpha_\tau\varepsilon_\eta(\tau\eta|VW|\nu\lambda)\varepsilon_\lambda\alpha_\nu$$

$$+ \sum_{\tau\eta\lambda}\int d\vec{x}[\hat{\alpha}_\tau^\dagger\hat{\varepsilon}_\eta^\dagger(\tau\eta|VW|\vec{x}\lambda)'\hat{\varepsilon}_\lambda\hat{a}(\vec{x}) + \text{H.c.}]$$

$$+ \sum_{\tau\lambda\nu}\int d\vec{y}[\hat{\alpha}_\tau^\dagger\hat{e}^\dagger(\vec{y})(\tau\vec{y}|VW|\nu\lambda)'\varepsilon_\lambda\alpha_\nu + \text{H.c.}] \ . \qquad (3.112)$$

The terms in $\hat{X}$ involve a superposition of both *a* and *e* bound to the origin. These terms must be considered as very rough approximations to the scattering, creation, and breakup processes for the $(a^-b^+e^-)$ molecular state, respectively.

The matrix elements are

$$(\vec{x}|V_a|\vec{x}')' = \frac{Z_aZ_b}{x}\,\delta(\vec{x}-\vec{x}') - \sum_\tau E_\tau u^A_\tau(\vec{x})u^{A*}_\tau(\vec{x}') \ , \tag{3.113}$$

$$(\vec{y}|V_a|\vec{y}')' = \frac{Z_b}{y}\,\delta(\vec{y}-\vec{y}') - \sum_\lambda E_\lambda u^E_\lambda(\vec{y})u^{E*}_\lambda(\vec{y}') \ , \tag{3.114}$$

$$\begin{aligned}(\tau\vec{y}|VW|\nu\vec{y}')' &= (\tau\vec{y}|VW|\nu\vec{y}')\delta(\vec{y}-\vec{y}') \\ &\quad - [(\tau\vec{y}|VW|\nu\vec{y}') + (\tau\vec{y}'|VW|\nu\vec{y})]\Delta^E(\vec{y},\vec{y}') \\ &\quad + \int d\vec{y}_1\Delta^E(\vec{y},\vec{y}_1)(\tau\vec{y}_1|VW|\nu\vec{y}')\Delta^E(\vec{y}_1,\vec{y}') \ ,\end{aligned} \tag{3.115}$$

$$(\vec{x}\eta|VW|\vec{x}'\lambda)' = \int d\vec{y}u^{E*}_\eta(\vec{y})(\vec{x}\vec{y}|VW|\vec{x}'\vec{y})'u^E_\lambda(\vec{y}) \ , \tag{3.116}$$

$$\begin{aligned}(\tau\vec{y}|VW|\vec{x}\vec{y}')'' &= (\tau\vec{y}|VW|\vec{x}\vec{y}')'\delta(\vec{y}-\vec{y}') \\ &\quad - [(\tau\vec{y}|VW|\vec{x}\vec{y}')' + (\tau\vec{y}'|VW|\vec{x}\vec{y})']\Delta^{E}(\vec{y},\vec{y}') \\ &\quad + \int d\vec{y}_1\Delta^{E}(\vec{y},\vec{y}_1)(\tau\vec{y}_1|VW|\vec{x}\vec{y}')'\Delta^{E}(\vec{y}_1,\vec{y}') \quad , \qquad (3.117)\end{aligned}$$

$$\begin{aligned}(\vec{x}\vec{y}|VW|\vec{x}'\lambda)'' &= [(\vec{x}\vec{y}|VW|\vec{x}'\vec{y})' \\ &\quad - \int \vec{d}y\Delta^{E}(\vec{y},\vec{y}')(\vec{x}\vec{y}'|VW|\vec{x}'\vec{y})']u^{E}_{\lambda}(\vec{y}) \quad , \qquad (3.118)\end{aligned}$$

$$\begin{aligned}(\tau\vec{y}|VW|\vec{x}'\lambda)'' &= [(\tau\vec{y}|VW|\vec{x}'\vec{y})' \\ &\quad - \int \vec{d}y\Delta^{E}(\vec{y},\vec{y}')(\tau\vec{y}'|VW|\vec{x}'\vec{y})']u^{E}_{\lambda}(\vec{y}) \quad , \qquad (3.119)\end{aligned}$$

$$\begin{aligned}(\vec{x}\vec{y}|VW|\vec{x}'\vec{y}')'' &= (\vec{x}\vec{y}|VW|\vec{x}'\vec{y}')'\delta(\vec{y}-\vec{y}') \\ &\quad - [(\vec{x}\vec{y}|VW|\vec{x}'\vec{y}')' + (\vec{x}\vec{y}'|VW|\vec{x}'\vec{y})]'\Delta^{E}(\vec{y},\vec{y}') \\ &\quad + \int d\vec{y}_1\Delta^{E}(\vec{y},\vec{y}_1)(\tau\vec{y}_1|VW|\vec{x}\vec{y}')'\Delta^{E}(\vec{y}_1,\vec{y}') \quad , \qquad (3.120)\end{aligned}$$

$$(\tau\eta|VW|\nu\lambda) = \int d\vec{y}u^{E*}_{\eta}(\vec{y})(\tau\vec{y}|VW|\nu\vec{y})u^{E}_{\lambda}(\vec{y}) \quad , \qquad (3.121)$$

$$(\tau\eta|VW|\vec{x}\lambda)' = \int d\vec{y}u_{\eta}^{E*}(\vec{y})(\tau\vec{y}|VW|\vec{x}\vec{y})'u_{\lambda}^{E}(\vec{y}) \ , \tag{3.122}$$

and

$$(\tau\vec{y}|VW|\nu\lambda)' = [(\tau\vec{y}|VW|\nu\vec{y})' - \int \vec{d}y\Delta^{E}(\vec{y},\vec{y}')(\tau\vec{y}'|VW|\nu\vec{y})']u_{\lambda}^{E}(\vec{y}) \ , \tag{3.123}$$

where

$$T(\vec{x}\vec{y}) = V_{ae}(\vec{x}\vec{y}) + W_{ae}(\vec{x}\vec{y}) \ . \tag{3.124}$$

Using (3.103) through (3.107) one can show that this Fock-Tani Hamiltonian is completely symmetric if all functions, functionals, and operators associated with the α and a fields are interchanged with those associated with the ε and e fields. This symmetry is a consequence of the commutation relation (3.90).

Considering the discrepancy (of order $1/m_b$) between the initial state energy and the initial momentum eigenstate of the Fock-Tani Hamiltonian, (3.17) and (3.18), [which was derived from the symmetrical reduced-mass Fock Hamiltonian, (3.1)] and those found in Schrodinger representation[8], one is cautioned to look for such discrepancies in the present Fock-Tani Hamiltonian, (3.10) through (3.12).

The transformation for a system containing a positive charge fixed at the origin and negative charges of two types (where no 3-particle bound states have been considered) is thus done with relative ease. That the complicated method of previous calculations[2,3] can be bypassed is a direct consequence of working in the symmetrical 3→2-body reduced-mass system.

Notice also that, unlike the previous approach, the present transformation has no restriction on the number of particles of types *a* and *e*. However, there is a restriction on the asymptotic states arising from the definition of the unitary operator (3.88). All particles must be well separated. If one wanted to calculate cross sections for reactions of the present type in a plasma of negatively charged particles, for instance, the generalized unitary operator recently found by Girardeau,[13] which allows finite densities in the asymptotic states, should be used instead of (3.88).

Starting, instead, with the initial-state Fock Hamiltonian, (3.41) with $Z_a \rightarrow -Z_a$, in defining the final bound state, the simple three-dimensional integral form of (3.86) would not be possible. The reason is that the final-state wave function written in initial coordinates would depend on both $\vec{R}_i$ and $\vec{r}_i$. Using the same method as that leading to (2.23) and (2.24),one can show that for the present arrangements

$$\vec{R}_f = (1-\lambda\tau)\vec{r}_i - \tau\vec{R}_i \qquad \text{and} \qquad \vec{r}_f = \vec{R}_i - \lambda\vec{r}_i \quad , \tag{3.125}$$

where

$$\tau = \frac{m_a}{m_a + m_b} \qquad \text{and} \qquad \lambda = \frac{m_e}{m_a + m_e} \quad . \tag{3.126}$$

Because the simple properties of the present transformation are dependent on the creation operators describing one bound species (anti-) commuting with all annihilation operators (bound state and continuum) associated with the other species, the initial state system cannot be transformed in this way. One would have to resort to the more complicated d matrix method.[2,3]

In this Chapter it has been shown that the symmetrical reduced-mass coordinate system, derived in Chapter II, greatly facilitates the process of creating a representation that fully accounts for bound states. The discrepancy of order $1/m_b$ in the initial energy and the initial asymptotic momentum eigenstate of this Fock-Tani Hamiltonian is well compensated by this facility. And it is likely that ad hoc adjustments can be made at the Schrodinger level of the T-matrix for a given processes [like those that would produce (3.79) from (3.40)] that would yield a result in conformance with the Fock-Tani Hamiltonian found by transforming the full 3-body Fock Hamiltonian.

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CHAPTER IV

EVALUATION OF THE T-MATRIX AND FIRST-ORDER RESULTS

Introduction

To test the reduced-mass Fock-Tani representation, the differential and total cross sections for the reactions $p^+ + H(1s) \rightarrow H(1s) + p^+$ and $e^+ + H(1s) \rightarrow Ps(1s) + p^+$ will be calculated, where Ps is the positronium atom, (e^+e^-). The T-matrix[1] (transition matrix) is

$$T_{fi} = (\phi_f | \hat{V} | \psi_i^+) \ , \tag{4.1}$$

where the final asymptotic state, $(\phi_f|$, is given by (3.73) and the Lippmann-Schwinger in-state[2], $|\psi_i^+)$, is given by

$$|\psi_i^+) = |\phi_i) + \hat{G}_0^+ \hat{V} |\psi_i^+) \ , \tag{4.2}$$

and $\hat{V}$ is given by (3.57). The latter equation contains the initial asymptotic state, $|\phi_i)$, given by (3.71), and

$$\hat{G}_0^+ = (E - \hat{H}_0 + i\varepsilon) \ , \tag{4.3}$$

where the limit $\varepsilon \rightarrow 0^+$ is implied and H_0 is given by (3.56).

The differential cross section for rearrangement collisions contains reduced masses for both initial and final momentum states, given by (2.26), and both center-of-mass momenta, related by (2.27). It is

$$\frac{d\sigma}{d\Omega}(\theta\phi) = (2\pi)^4 \, M_i M_f \, \frac{k_f}{k_i} \, |T_{fi}|^2 \quad . \tag{4.4}$$

The coefficient, $(2\pi)^{6-2}$ larger than Davidov's,[3] is consistent with the present $(2\pi)^{-3/2}$ momentum wave function normalization. The total cross section is

$$\sigma = \int d\Omega \frac{d\sigma}{d\Omega}(\theta\phi) \quad . \tag{4.5}$$

The First-order T-matrix

The calculations of this chapter will contain the approximation $|\psi_i^+) \approx |\phi_i)$. A formal analysis of higher-order corrections is included in Chapters VI and VII. The first-order approximation to the T-matrix, given in (3.74) through (3.79), is

$$T^1_{fi} = (\phi_f|\hat{V}|\phi_i) = T^{1B}_{fi} + T^{1O}_{fi} \quad . \tag{4.6}$$

The first term is

$$T^{1B}_{fi} = (2\pi)^{-3/2}\int d\vec{R}d\vec{r}\phi_\sigma^{A*}(\vec{R}\vec{r})\left(\frac{Z_aZ_b}{|\vec{R}+\lambda\vec{r}|} - \frac{Z_b}{r}\right)u_\rho^E(\vec{r})\exp(i\vec{k}_i\cdot\vec{R}) \tag{4.7}$$

$$= (2\pi)^{-3}\int d\vec{r}\,'d\vec{r}e^{-i\vec{C}\cdot\vec{r}\,'}u_\upsilon^{A*}(r')\left(\frac{Z_aZ_b}{|\vec{r}-\vec{r}\,'|} - \frac{Z_b}{y}\right)u_\rho^E(r)e^{i\vec{B}\cdot\vec{r}} \quad ,$$

where $\sigma = \{k_f,\upsilon\}$. (4.8)

We define

$$\vec{C} = \vec{k}_i - \zeta\vec{k}_f \quad \text{and} \quad \vec{B} = \gamma\vec{k}_i - \vec{k}_f \ , \tag{4.9}$$

where

$$\zeta = \frac{m_a}{m_a + m_e} \quad \text{and} \quad \gamma = \frac{m_b}{m_b + m_e} \ . \tag{4.10}$$

This is the post form of the first Born term found by Jackson and Schiff[5] [their equations (12) and (8′)]. The second term in (4.7) is the Brinkman-Kramers[6] (BK) term given explicitly by[5]

$$T_{fi}^{BK} = -\left(\frac{B^2}{2m_i} - E_\rho\right) u_\rho^E(B) u_\upsilon^{A*}(C) \ , \tag{4.11}$$

where m_i is given by (2.26). (Note that Jackson and Schiff set $-E = \varepsilon$.) The convention

$$f(\vec{k}) = (2\pi)^{-3/2} \int dw \ e^{-i\vec{k}\cdot\vec{w}} f(w) \tag{4.12}$$

and

$$f(\vec{w}) = (2\pi)^{-3/2} \int dw \ e^{i\vec{k}\cdot\vec{w}} f(k) \tag{4.13}$$

will be used for all Fourier transform pairs. The hydrogenic 1s momentum wave function is

$$u_{1s}(\vec{p}) = \frac{2\sqrt{2}}{\pi} P_0^{5/2} \frac{1}{(P_0^2 + p^2)^2} \ . \tag{4.14}$$

For ease of notation define

$$\alpha = P_0^E = Z_b/a_0^E \quad \text{and} \qquad \beta = P_0^A = Z_a/a_0^A , \tag{4.15}$$

where a_0 is the initial- or final-state Bohr radius given by 1/m of (2.26). With the normalization in (4.11) the 1s-1s BK term, (4.10), becomes

$$T^{BK}_{1s,1s} = - \frac{4\beta^{3/2}\alpha^{5/2}}{\pi^2(\beta^2 + B^2)(\alpha^2 + C^2)^2} . \tag{4.16}$$

The first term in (4.7), for $\rho=\upsilon=1s$, is given by Equation (II.3) of Jackson and Schiff[5], but with the expression for Δ generalized to allow $\beta \neq \alpha$ and with the alternate normalization of (4.11),

$$T^{JS1}_{1s,1s} = 4/\pi^2 \int_0^1 dx \ x(1-x)\Big(\frac{2}{\Delta^3(\Delta-q^2)^{1/2}} + \frac{1}{\Delta^2(\Delta-q^2)^{3/2}}$$

$$+ \frac{3/4}{\Delta(\Delta-q^2)^{5/2}}\Big) , \tag{4.17}$$

where

$$\Delta = \beta^2 + x(\alpha^2 - \beta^2 + C^2) + (1-x)B^2 \tag{4.18}$$

and

$$\vec{q} = x\vec{C} + (1-x)\vec{B} . \tag{4.19}$$

The orthogonalization term, the second term of (4.5), is

$$T^{10}_{fi} = -\int d\vec{R}d\vec{r}d\vec{R}'d\vec{r}'\phi^{A*}_{\sigma}(\vec{R}'\vec{r}')\left(\frac{Z_aZ_b}{|\vec{R}'+\lambda\vec{r}'|} - \frac{Z_b}{r'}\right)$$

$$\times\Delta^A(\vec{R}'\vec{r}',\vec{R}\vec{r})u^E_{\rho}(\vec{r})\exp(i\vec{k}_i\cdot\vec{R}) \quad . \qquad (4.20)$$

Now change variables to

$$\vec{R} = \gamma\vec{r}_3 - \iota\vec{r}_1 \qquad\qquad \vec{r} = \vec{r}_3 + \zeta\vec{r}_1, \qquad (4.21)$$

for both primed and unprimed variables, where

$$\gamma = \frac{m_b}{m_b + m_e} , \qquad\qquad \lambda = \frac{m_e}{m_b + m_e} , \qquad (4.22)$$

ζ and γ are given by (4.9), and

$$\iota = \zeta\lambda+\eta \quad . \qquad (4.23)$$

Then the final state wave function, (3.51), becomes simply

$$\phi^A_{\sigma}(\vec{R}\vec{r}) = (2\pi)^{-3/2}e^{i\vec{k}\cdot\vec{r}_3}\ u^A_{\upsilon}(r_1) \quad . \qquad (4.24)$$

Integration over the momentum variables in the corresponding bound-state kernel, (3.70), gives

$$\Delta^A(\vec{R}'\vec{r}',\vec{R}\vec{r}) = \delta(\vec{r}\,'_3 - \vec{r}_3)\sum_{\tau}u^A_{\tau}(\vec{r}_1{}')u^{A*}_{\tau}(\vec{r}_1) \ , \qquad (4.25)$$

so that (4.20) becomes

$$T^{1O}_{fi} = -\,(2\pi)^{-3}\sum_{\tau}\int d\vec{r}_1 d\vec{r}_3 d\vec{r}\,'_1 e^{-i\vec{C}\cdot\vec{r}_3} u^{A*}_{\upsilon}(\vec{r}\,'_1) u^{A}_{\tau}(\vec{r}\,'_1) u^{A*}_{\tau}(\vec{r}_1)$$

$$\times\left(\frac{Z_a Z_b}{|\vec{r}_3-\eta\vec{r}\,'_1|} - \frac{Z_b}{|\vec{r}_3+\zeta\vec{r}\,'_1|}\right) u^{E}_{\rho}(\vec{r}_3+\zeta\vec{r}_1) e^{-i\iota\vec{k}_i\cdot\vec{r}_1}\,, \qquad (4.26)$$

where $\vec{C}$, given in (4.8), equals $\vec{q}_1$ of Equation (4.8a) of Ojha et al.[7] (Appendix A) , and ι, given in (4.23), equals m of their Equation (4.8b). Then the identification between (4.26) and Equation (4.7) of Ojha et al. is exact. Therefore the Fock-Tani transformation of the initial-state reduced-mass Fock Hamiltonian, (3.41), is entirely equivalent to the Fock-Tani transformation of the full 3-body Hamiltonian (given by Ojha et al.). It can be shown that the Fock-Tani transformation of the symmetrical reduced-mass Fock Hamiltonian, (3.1), will have identical form except that the quantity m would differ slightly (to order $1/m_b$) from ι. For this case ι in (4.26) is replaced by η. As mentioned in Chapter III, this difference becomes noticeable at projectile energies of order 5 keV.

In calculating the cross sections for $p^+ + H \rightarrow H + p^+$, Ojha et al. note that the denominator of the first term in each of T^{1B} and T^{1O} can be approximated by r_3. Since η is small these two terms cancel. This cancellation fulfills, at first order, Wick[5]'s expectation that the internuclear potential should make a negligible contribution to the exact T-matrix.

For the reaction $e^+ + H \rightarrow Ps + p^+$, η can not be neglected because $m_a = m_e$. But because of the similarity of the form of the two terms in (4.26), the analytical reduction of the first term follows exactly the proceedure Ojha et al.[7] used for the second (see Appendix A). In fact, for the positronium case the two terms are identical in magnitude. They are of the same sign for ℓ odd, so that they add, and they differ in sign for even ℓ, so that they cancel. The generalization of their result [their Equation (5.10)] is

$$T^{10}_{\sigma\leftarrow 1s} = Z_a Z_b T^{0}_{\sigma\leftarrow 1s}(-m_e/m_a) - Z_b T^{0}_{\sigma\leftarrow 1s}(1) \ , \qquad (4.27)$$

where

$$T^{0}_{Ns,k_f\leftarrow 1s,k_i}(c) = -\frac{\zeta^3}{\sqrt{2}\pi^3}\sum_{n\ell}(2\ell+1)\int dp\,d\theta\,\sin\theta\,\frac{p^2}{|\vec{p}+\vec{q}_2|}R^{A}_{n\ell}(p)$$

$$\times\, I_{Ns,n\ell}[|c(\vec{p}+\vec{q}_2)|]\; P_\ell\left[\frac{c\vec{p}\cdot(\vec{p}+\vec{q}_2)}{p\left|c(\vec{p}+\vec{q}_2)\right|}\right]\frac{A}{(A^2-B^2)^{3/2}} \ , \qquad (4.28)$$

where ζ is given in (4.9) and all other quantities are given in Ojha et al. (or Appendix A). In their results they included only terms through n=2. It would be desirable to check the accuracy of this by including higher-order terms. For the positronium case, because the centers of mass and charge are identical, the even ℓ terms in (4.27) cancel so the 3p terms might be important.

The radial momentum wave functions R, in (4.28) are well known[8]. A general formula for the Fourier transform of the product of wave functions

$$I_{\upsilon\tau}(\vec{k}) = \int dw\, e^{-i\vec{k}\cdot\vec{w}} u_{\upsilon}^{*}(\vec{w}) u_{\tau}(\vec{w}) \tag{4.29}$$

is also be useful. For υ=1s (easily generalizable to higher s-states), a finite series solution is found by expanding u_τ in Laguerre polynomials before integrating. The resulting expression is formally given[9] in terms of Legendre polynomials. A more useful form my be had by using recursion relations[10] repeatedly. The final expression is

$$I_{1s,n\ell m}(\vec{k}) = I_{1s,n\ell}(\hat{k}) Y_{\ell m}(\hat{k}) \ , \tag{4.30}$$

where

$$I_{1s,n\ell}(\hat{k}) = (-1)^{\ell} n[\pi(n+\ell)!(n-\ell-1)!]^{1/2} \sum_{s=0}^{n-\ell-1} \frac{(-1)^{s}(2\ell+s+2)}{(n-\ell-1)!s!}$$

$$\times \frac{\omega^{s+3} b^{\ell-2}}{(\omega^{2}+b^{2})^{\ell+s+2}} \sum_{r=1}^{t} D_{\ell sr} \left(\frac{b}{\omega}\right)^{2r} \ , \tag{4.31}$$

$$\omega = (n+1)/2 \ , \qquad b = nk/2P_{0} \ , \tag{4.32}$$

$$t = \begin{cases} (s+2)/2 & \text{for } s \text{ even} \\ (s+3)/2 & \text{for } s \text{ odd} \end{cases} , \qquad (4.33)$$

$$D_{\ell sr} = \frac{C_{sr}}{(2(\ell+r)-1)!!} , \qquad (4.34)$$

$$C_{sr} = C_{s-1,r} - sC_{s-2,r-1} ,$$

$$C_{s1} = 1 , \quad \text{and} \quad C_{12} = -1 . \qquad (4.35)$$

Then

$$I_{1s,3s}(p) = \frac{864\sqrt{3\pi}[16(p/P_0)^2 + 27(p/P_0)^4]}{[16 + 9(p/P_0)^2]^4} , \qquad (4.36)$$

$$I_{1s,3p}(p) = \frac{-i\sqrt{6\pi}\ 576(p/P_0)[16 + 27(p/P_0)^2]}{[16 + 9(p/P_0)^2)^4} , \qquad (4.37)$$

and

$$I_{1s,3d}(p) = \frac{-13824\sqrt{30\pi}\ (p/P_0)^2}{5[16 + 9(p/P_0)^2]^4} . \qquad (4.38)$$

First-order Results

The general form of the first-order Fock-Tani T-matrix for the reactions $a^+ + (b^+c^-) \rightarrow (a^+c^-) + b^+$, [(4.16), (4.17), and (4.27) substituted into (4.6)] was used for a calculation of the differential and total cross sections. The integrations were none numerically using 16 point Gaussian quadrature. The upper limit of the p-integration and the number of sub-regions were varied until a consistent result was found. This program was run for (abc) = {(ppe), (epe), (μpμ), (μdμ), and (μdμ)}. The first two reactions in this set are used to check the results of previous Fock-Tani calculations.[7,11]

$p^+ + H(1s) \rightarrow H(1s) + p^+$ Results

To check the approximation made in Ojha et al.[7] in which the internuclear potential was neglected for the reaction $p^+ + H(1s) \rightarrow H(1s) + p^+$, the present program was run with and without such contributions. The latter reproduces the result of Ojha et al. to order $1/m_{prot}$. This small difference is presumed to arise from their approximating the Bohr radius by 1. The difference between the differential cross sections for exclusion or inclusion of the internuclear potential was of order 10 percent. At an

incident (C.M.) energy of 25 keV, the differential cross section of the former was found to be 12 percent larger than the latter at zero mrad and 18 percent smaller at 3 mrad. Since the experimental differential cross sections of Martin et al.[12] are for capture into all states, one should multiply the cross section for capture into n=1 by 1.2 (to account for the $1/n^3$ excited population) which moves the present (corrected) result back into good agreement with the data for angles .2 to 1. mrad at 25 keV, .2 to .8 mrad at 60 keV, and 0. to 1. mrad at 125 keV. Furthermore, the inclusion of the p-p term removes the slight oscillations found in Ojha et al. in these regions.

The present total cross section including p-p terms is 18 percent larger than when these terms are neglected. In contrast, the first-order Jackson and Schiff[5] total cross section, including the internuclear potential, is 1000 percent larger than the Brinkman-Krammers[6] result which excludes this potential. Thus the orthogonalization corrections inherent in the Fock-Tani representation, in addition to giving a first-order total cross section which agrees with experiment for a wide range of energies (greater than 10 keV), produces agreement at first order between experiment and Wick's expectation[5] that the internuclear potential should play a negligible role in exact calculations of this process. It is interesting to note that Bates[13] predicted in 1958 that accounting for orthogonalization would give such a resolution.

A check on the inclusion of the 3s, 3p, and 3d orthogonalization gives a difference of order 1 percent. At 25 keV the differential cross section including these terms was 1 percent smaller at zero mrad and 3 percent larger at 3 mrad. The total cross section including these terms was 0.3 percent smaller.

Finally, Girardeau[14] has raised the question of whether the standard neglect of proton exchange is a valid approximation. One can argue that the de Broglie wavelength for these energies and masses is so small that exchange would occur only in a direct p-p hit, giving a contribution only at 180 degrees (CM),[15] called a "knock-on" process. This is illustrated in Fig. 1 for a semi-classical analogue of electron (charge cloud) transfer between a pair of charged spheres, seen in the lab frame. For impact parameters greater than the bulk of the electron cloud the projectile is hardly deflected by the nearly neutral atom. At such distances the protons are clearly distinguishable. As the impact parameter gets smaller, the projectile is deflected further until the p-p direct hit limit, in which case the projectile (plus electron cloud) is scattered at 180 degrees. It is in the latter case that exchange becomes important because the proton wave functions may have finite overlap at closest approach. One can see from the experimental differential sections of Martin et al.[12] that the cross section is sharply peaked around zero degrees so it is plausible that the knock-on process is negligible.

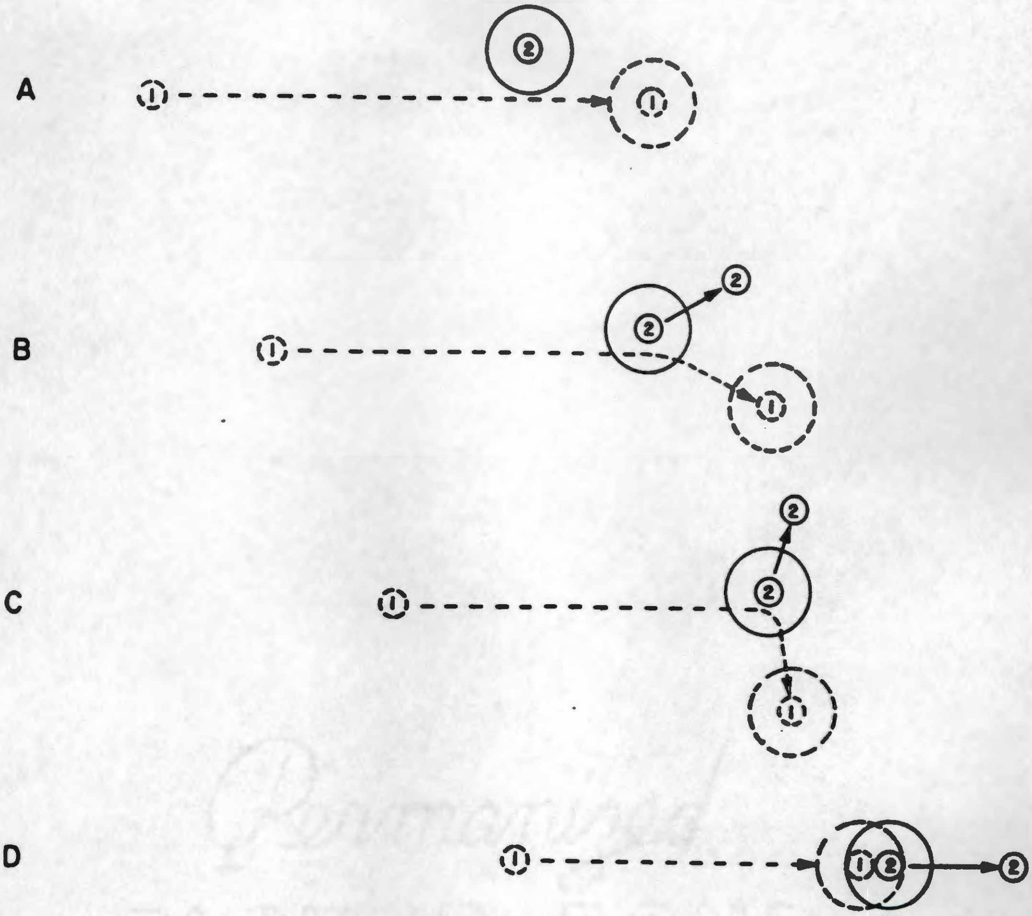

FIGURE 1. Electron (charge cloud) transfer between a pair of charged distinguishable spheres in the Lab frame.

However the statement, "exchange effects in electron transfer occur only when the projectile is scattered at 180 degrees," contains a contradiction. Girardeau[14] questions how one could know that it is the projectile (plus electron cloud) that is scattered back at 180 degrees, and not the target proton (plus electron cloud) or a mixture, if the two protons are indistinguishable. Exchange may have a small cross section, but so does electron transfer.

Support for this concern and a prediction comes from considering what an experimentalist observes in the zero degree direction. If she sees a hydrogen atom traveling with the same momentum as the incoming proton, the cross section should contain interference between contributions from electron transfer to a proton with large impact parameter (distinguishable as proton 1), elastic scattering of the target (plus electron) in the forward direction, and a term identical to that for elastic scattering but with the target and projectile exchanged, a rather novel method of electron transfer. This is illustrated in Fig. 2.

If Fig. 2 accurately reflects the quantum process then one would expect a discontinuity in the slope of the experimental data very near the forward direction due to exchange contributions to elastic scattering, in addition to a smoother change due to direct elastic scattering contibutions . The reason for an abrupt transition is that there should be no exchange for "moderately small" angles

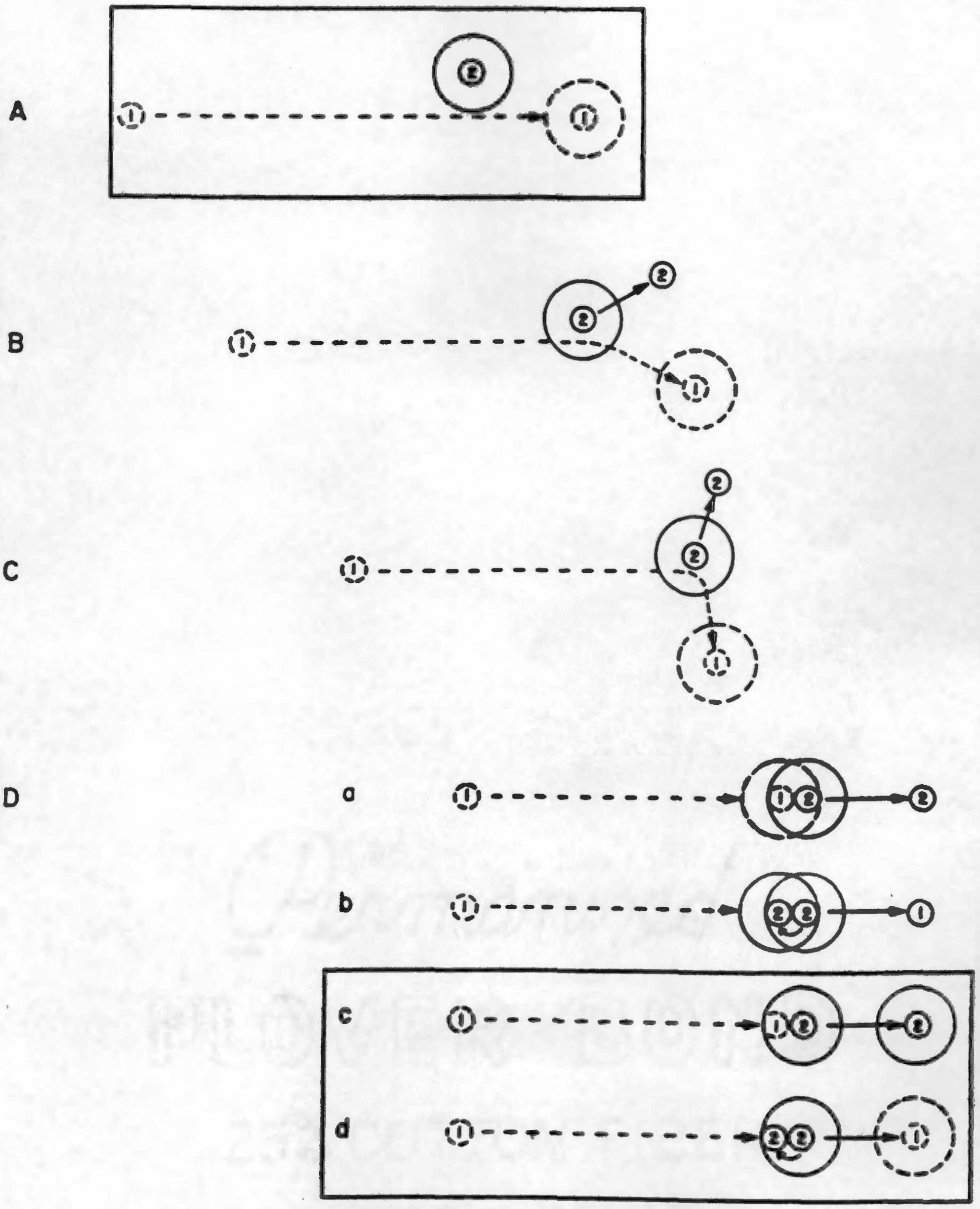

FIGURE 2. Charge transfer including exchange in the lab frame. The three boxed processes produce a fast hydrogen atom moving in the forward direction.

because small angle scattering corresponds to large impact parameters. As the angle gets smaller the associated impact parameter gets larger so exchange is even less important. As long as the impact parameter is nonzero one would expect that the protons could recoil to avoid overlap of their wave functions (presumed to be well bounded) through the Coulomb interaction. But once the impact parameter is "precisely zero" exchange effects should "turn on" due to proton wave function overlap at a turning point and through the possibility of tunneling. Of course the terms "moderately small" and "precisely zero" are not well defined in quantum mechanics. One should look for such slope changes in the data at small angles to better define these intuitive quantities. It is possible that the large impact parameter scattering contribution could be large enough to mask the direct elastic scattering, and the latter could be large enough to mask the exchange elastic scattering contribution. However, interference effects (in the square of the T-matrix) might appear in the cross section even if the magnitude of the latter is very small.

On the other hand, a theory which neglects direct and exchange elastic scattering but is perfect in every other respect would match the data at (experimentally defined) moderately small angles but not at very small angles. The theory would have no change in slope near $\theta=0$, sudden or otherwise.

Figure 4 of Ojha et al.[7] (Appendix A) shows the experimental differential cross section of Martin et al.[12] and what appear to be the best current theories for this reaction at small angles, the Fock-Tani result and the two-state atomic expansion (TSAE) of Lin, first published in Martin et al. (Also Fig. 5 of Ojha et al. shows excellent agreement with the experimental total cross section of McClure[16] for energies greater than about 10 keV and the TSAE of McCarroll[17] match at even lower energies.) Additionally, Fig. 3, below, is a reproduction of the figures in Martin et al., include the continuum distorted wave (CDW) and coupled-state (MS) theories. What is most striking about these graphs is the universality of the divergence between these theories and experiment for very small angles at 25 keV and 60 keV. The theoretical curves for all but the CDW are within the error bars at 125 keV so that no conclusion can be drawn for that energy. Figure 4 is a linear-linear plot of the result of Ojha et al., the TSAE ,and the present Fock-Tani result (including the internuclear potential and the 3s, 3p and 3d orthogonalization terms) for forward angles at 25 and 60 keV.

The theoretical results are nearly linear in this region (although the result of Ojha et al. shows small oscillations which are removed with the additions of the present Fock-Tani calculation). The experimental points are

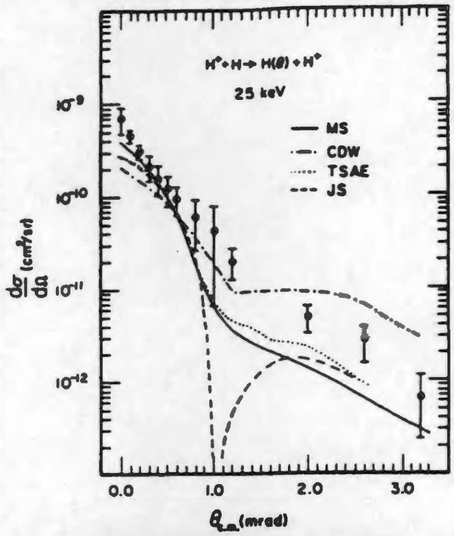

FIG. 1. Differential cross sections for electron capture in collisions between 25-keV incident protons and hydrogen atoms. Closed circles are the experimental results with error bars of one standard deviation. The solid line is the result of the MS calculation; the dot-dash-dot line is the result of the CDW calculation; the dotted line is the result of the TSAE calculation; and the dashed line is the result of a Jackson-Schiff calculation.

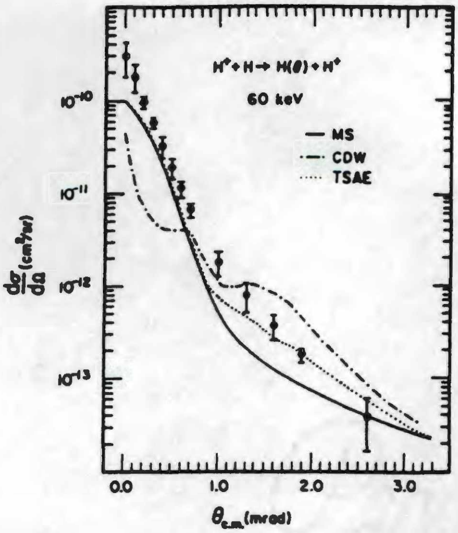

FIG. 2. Differential cross sections for electron capture in collisions between 60-keV incident protons and hydrogen atoms. For the legend see Fig. 1.

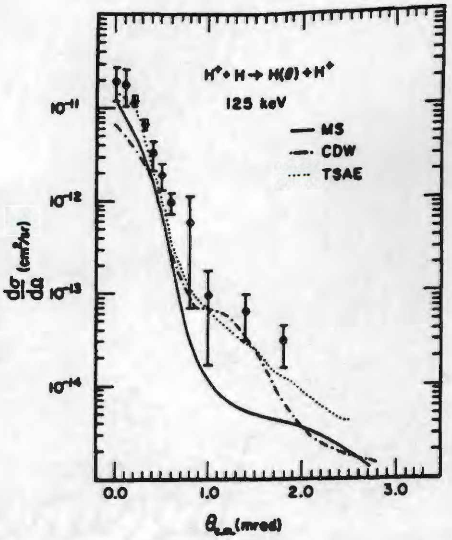

FIG. 3. Differential cross sections for electron capture in collisions between 125-keV incident protons and hydrogen atoms. For the legend see Fig. 1.

FIGURE 3. Figures from Martin et al.[12]

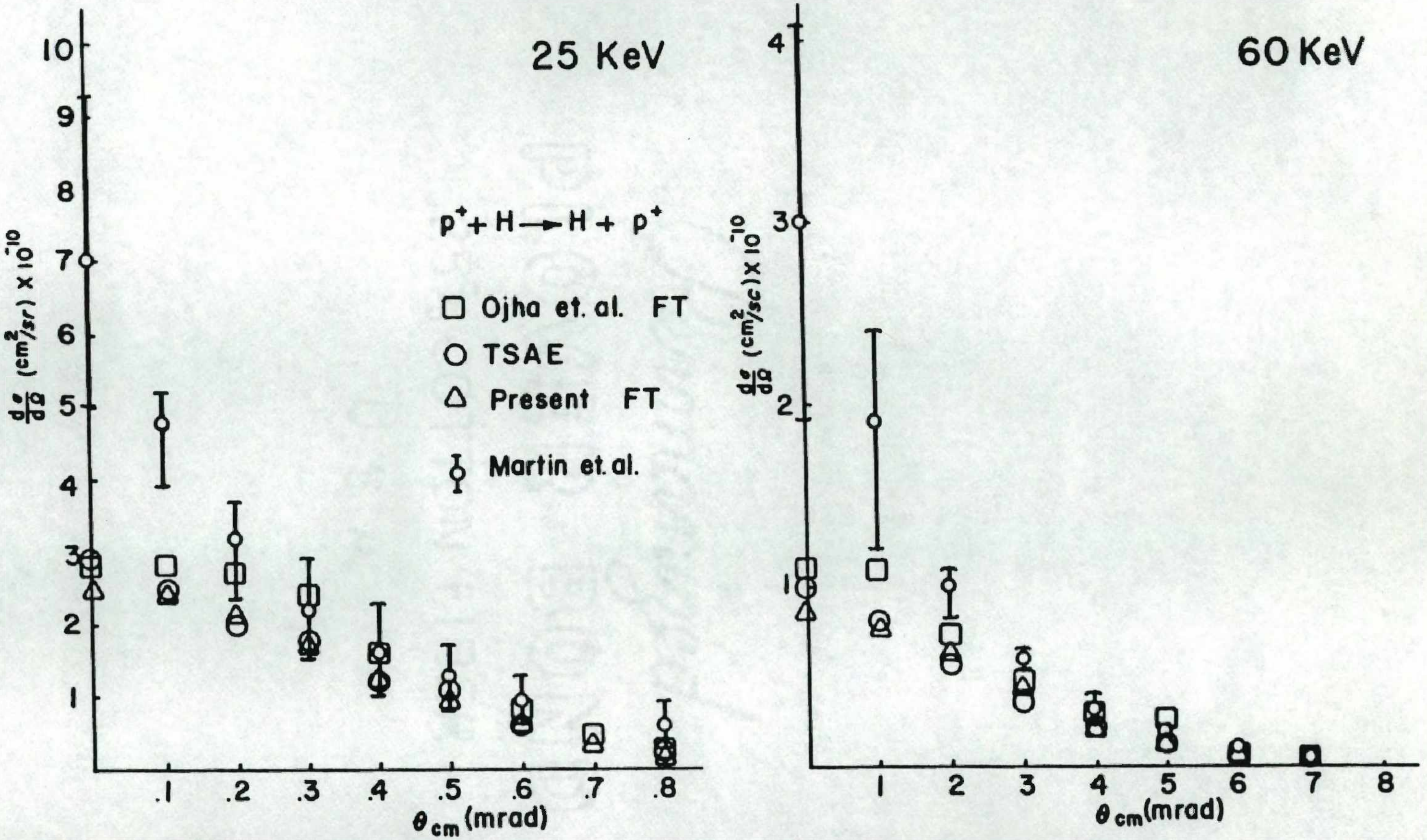

FIGURE 4. Forward scattering at 25 and 60 keV for resonant charge transfer. The experimental points are from Martin et al.[12] The theoretical points are open circles for the TSAE given in Martin et al., boxes for the Fock-Tani result of Ojha et al.,[7] and triangles for the present Fock-Tani result which includs the internuclear potential.

upwardly curving and perhaps showing signs of a sharper slope discontinuity, depending on one's bias. The divergence of experimental and theoretical curves in forward scattering is marked enough to warrant a more critical examination of the theories even if this divergence is not due to exchange.

$e^+ + H(1s) \rightarrow Ps(1s) + p^+$ Results

Consider the reaction $e^+ + H(1s) \rightarrow Ps(1s) + p^+$. The differential cross sections at energies of 10.2, 20, 50, and 100 eV are given in Figures 5, 6, 7, and 8, respectively. Figure 9 shows the forward scattering cross section over this range of eneries. A comparison is made between the present first-order Fock-Tani result (FT), that of Ficocelli Varracchio and Girardeau (EFV),[11] the first Born approximation (FBA), and the distorted wave approximation (DWA) of Mandal et al.[18]

The present result and that of Ficocelli Varracchio and Girardeau do not agree. The results given in Ojha et al.[7] for the reaction $p^+ + H(1s) \rightarrow H(1s) + p^+$ were calculated by three independent methods. In addition to the method outlined in Ojha et al., the quantity λ, of (4.22), can be set to zero for energies less than 5 keV. This simplified (4.26) so that Dr. Ojha was able to integrate analytically for τ from 1s to 3d. In the third method, I wrote a program based on (4.30) and the $\lambda=0$ approximation, which gave numerical results matching the other two. Because the

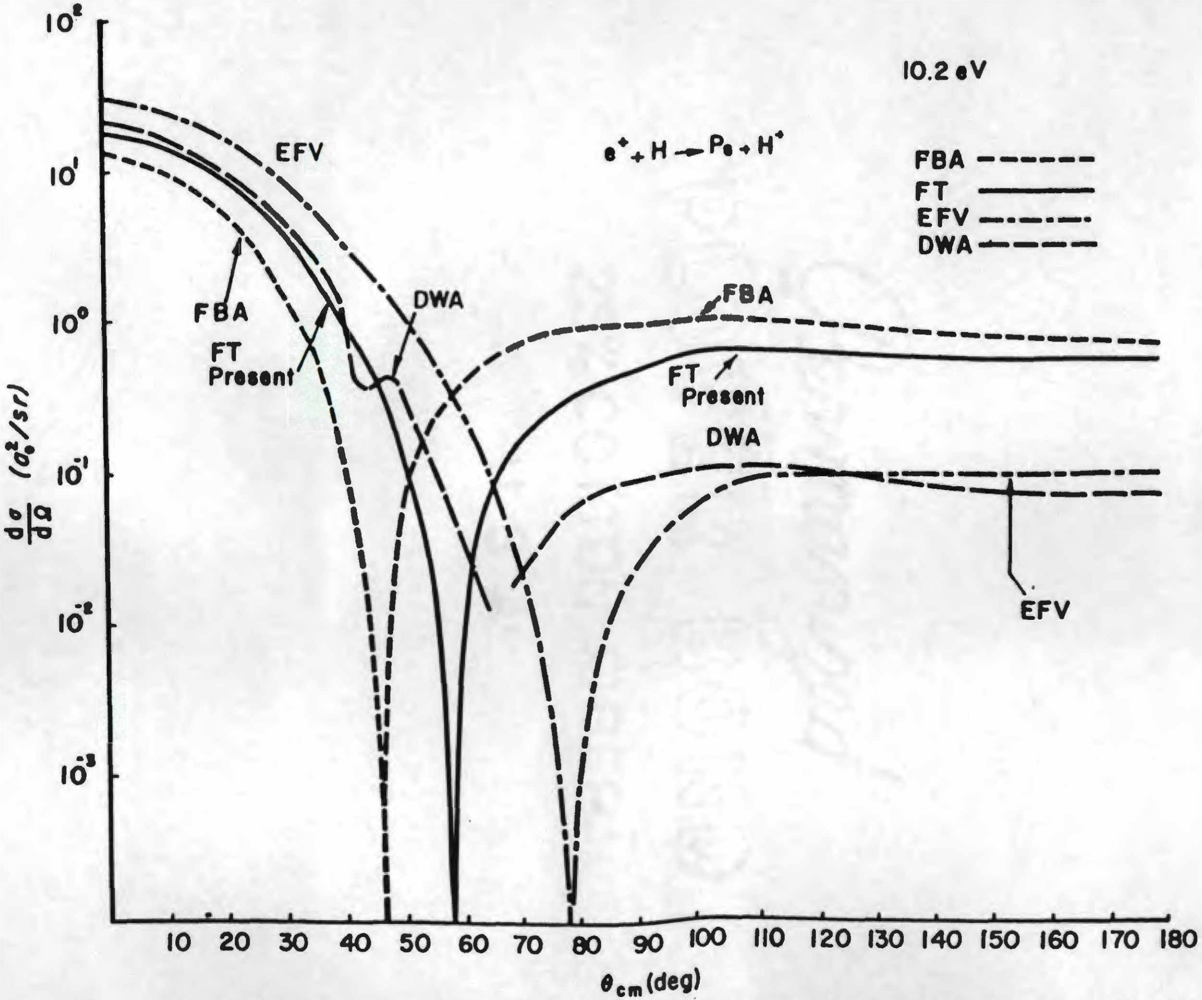

FIGURE 5. Differential cross section for positronium formation at 10.2 eV. The short-dashed curve is the FBA, the long-dashed curve is the DWA of Mandal et al.,[18] the dot-dashed curve is the Fock-Tani result of Ficocelli Varracchio and Girardeau[11] (EFV), and the solid curve is the present Fock-Tani result.

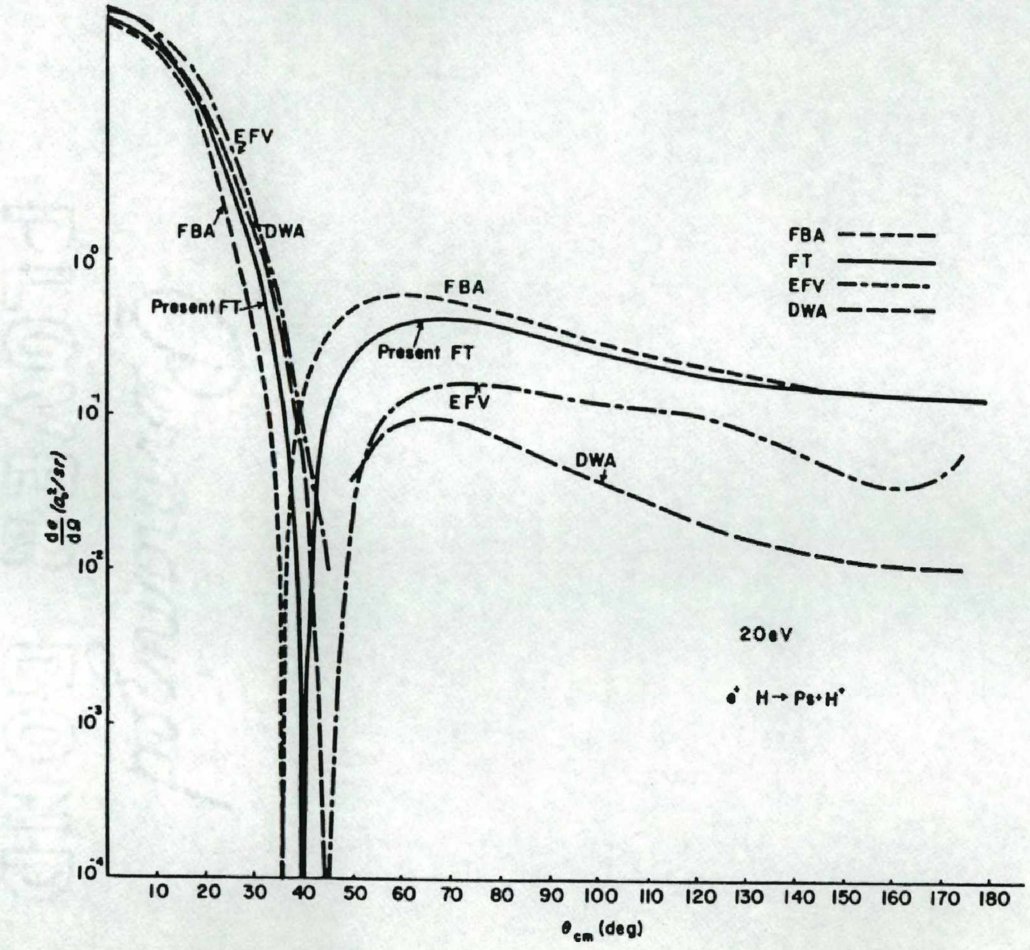

FIGURE 6. Differential cross section for positronium formation at 20 eV. The curves are labeled as in Fig. 5.

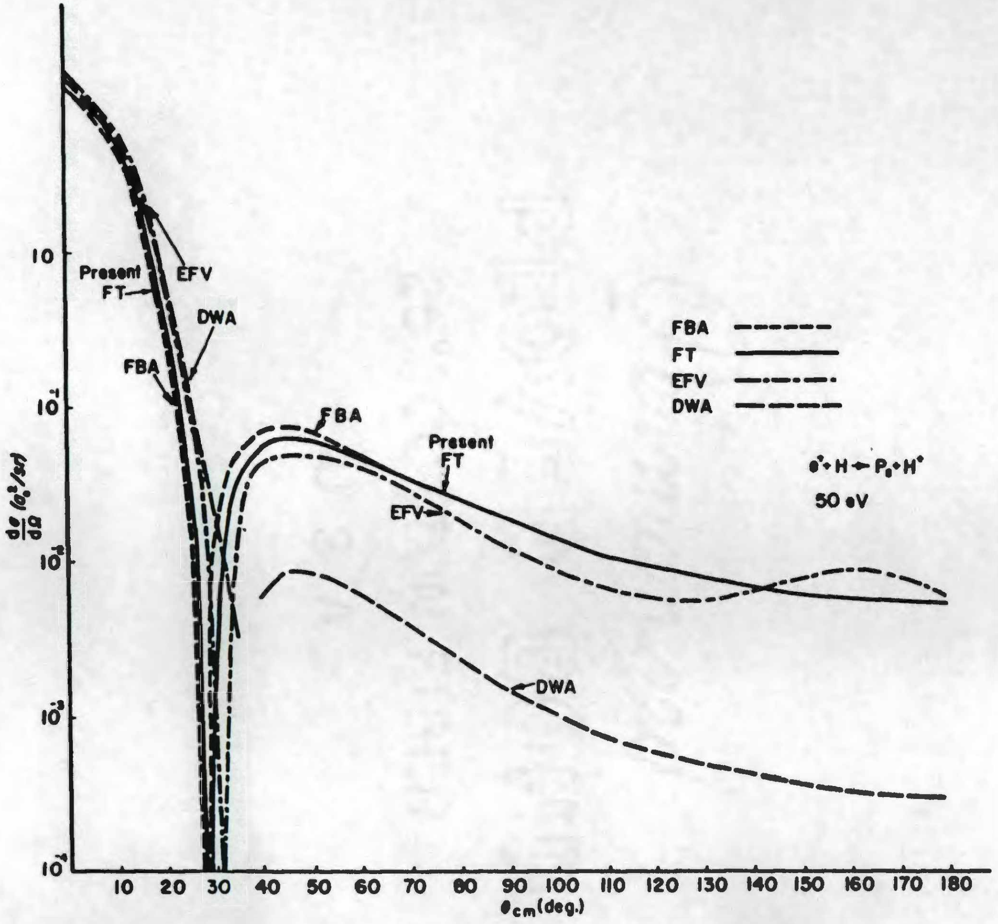

FIGURE 7. Differential cross section for positronium formation at 50 eV. The The curves are labeled as in Fig. 5.

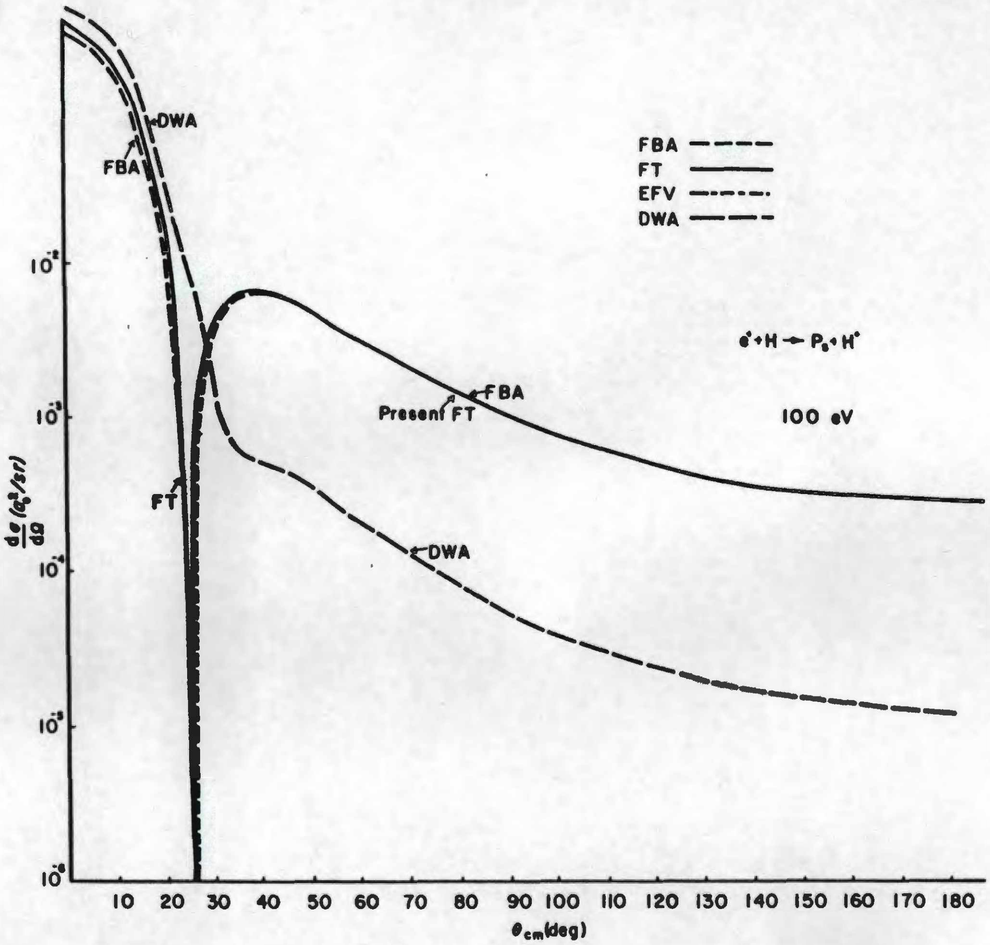

FIGURE 8. Differential cross section for positronium formation at 100 eV. The curves are labeled as in Fig. 5.

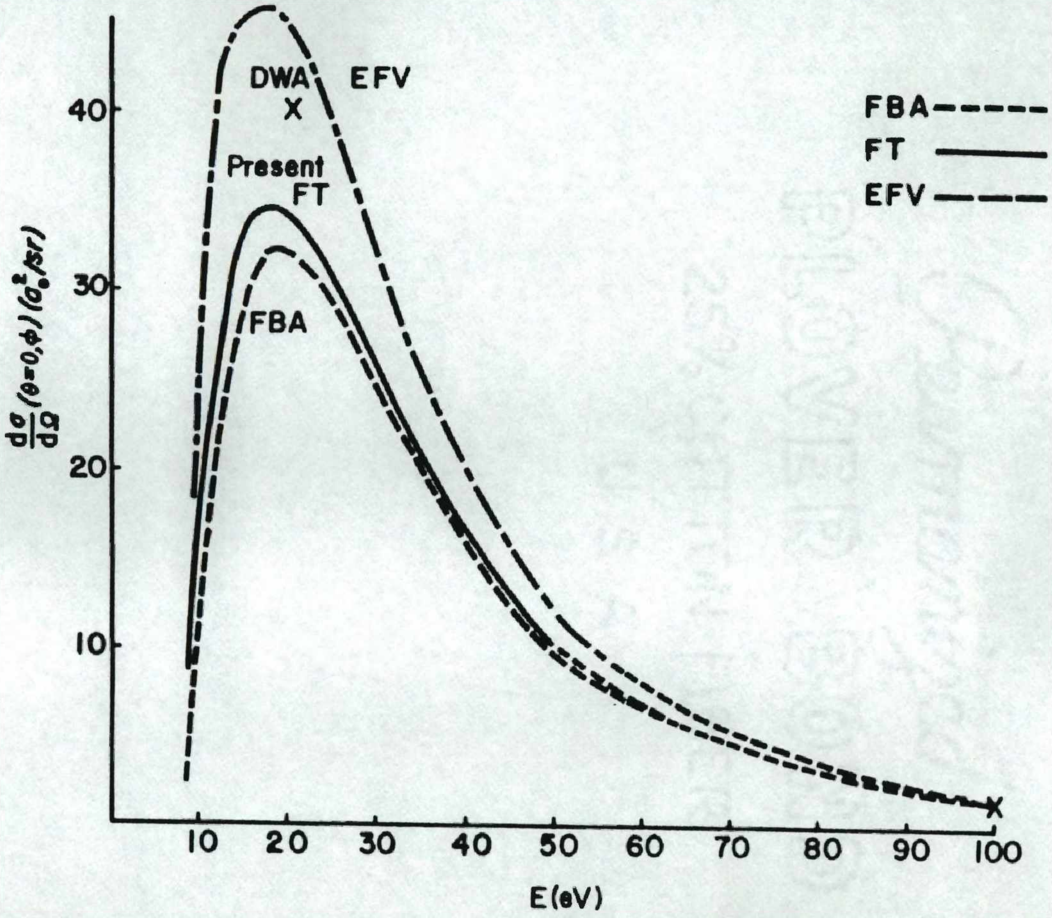

FIGURE 9. Forward scattering for positronium formation. The short-dashed curve is the FBA, the crosses are the DWA of Mandal et al.,[18] the dot-dashed curve is the Fock-Tani result of Ficocelli Varracchio and Girardeau[11] (EFV), and the solid curve is the present Fock-Tani result.

present program is capable of reproducing the $p^+ + H(1s) \rightarrow H(1s) + p^+$ reaction, it is also likely to give the correct result for $e^+ + H(1s) \rightarrow Ps(1s) + p^+$.

Equations (24) and (27)in Ficocelli Varrachio and Girardeau[11] contain errors. In the former the coefficient of B^2 should be 8 rather than 2, and in the latter the overall coefficient should be 2 rather than 8. But mimicking these by altering the present program does not reproduce their result. In any case, Professor Ficocelli Varracchio has assured me that the program he used has the correct values and that the discrepancy is probably due to a lack of convergence of their integrals and sums. (The program they used required much more computer time than the present one because it could be used for arbitrary initial and final atomic states.) Support for this interpretation comes from an examination of Figures 6 and 7. In the 100 to 180 degree region their results show oscillations characteristic of convergence problems.

Examining the total cross section, Fig. 10, it may be seen that the present Fock-Tani calculation gives a larger cross section than the first Born approximation, whereas the result of Ficocelli Varracchio and Girardeau is less than the FBA. In examining the differential cross sections it appears that the present result should fall between their result and the FBA. But a logarithmic graph can be deceiving

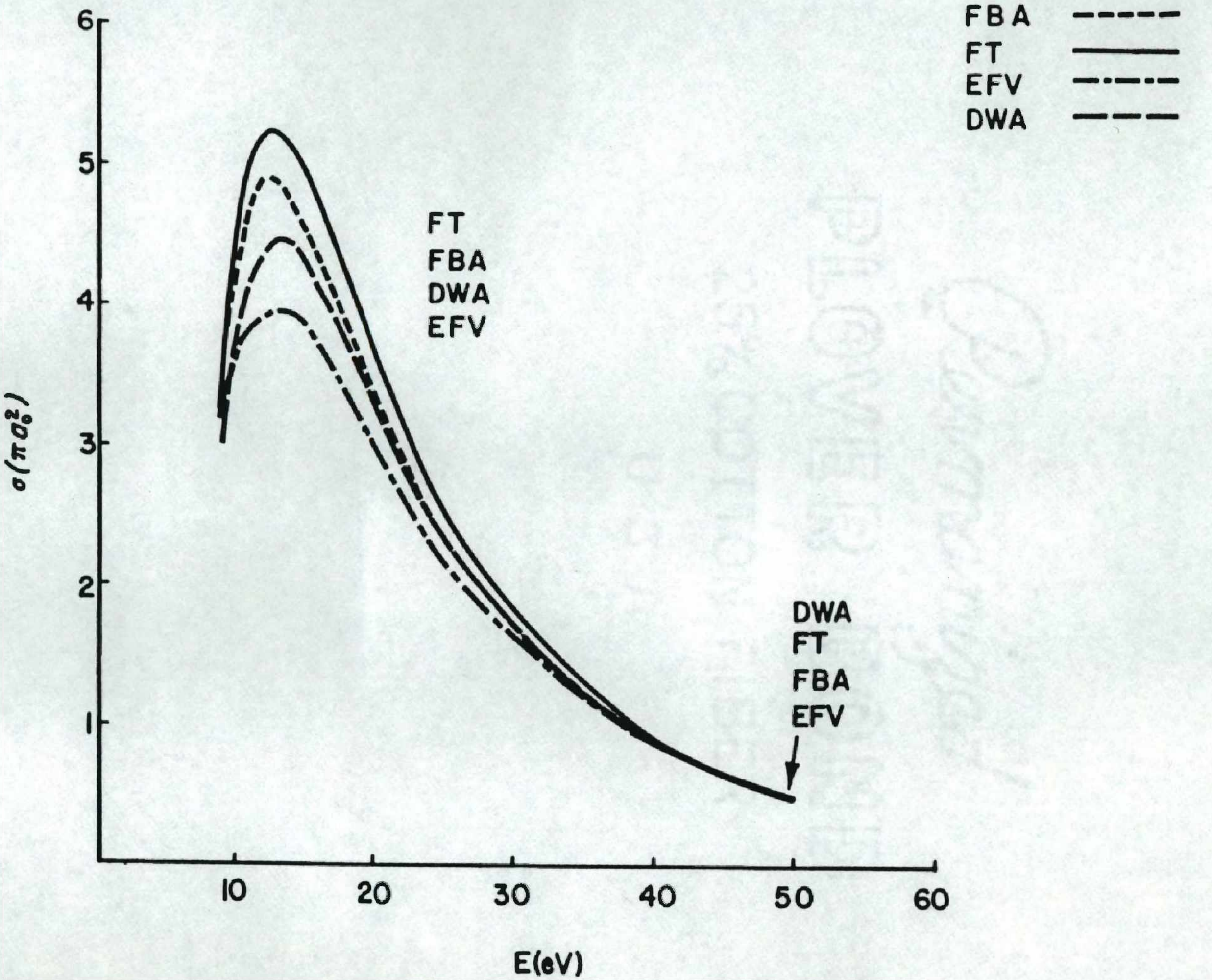

Figure 10. Total cross section for positronium formation. The curves are labeled in Fig. 5.

because the fluctuations are compressed. A calculation of the partial cross sections for the angles where FT > FBA, FT < FBA, and the transition region show the expected behavior. The sums of the results from these three regions add up in such a way that the total cross section for the FT result is greater than for the FBA except at 8.704 eV (where the ordering is FT < FBA < EFV).

Comparing the FT differential cross sections with the DWA and FBA results shows the former to be intermediate between the latter two. The first-order Fock-Tani T-matrix contains more physics than the non-orthogonal first Born approximation. In subtracting terms from the FBA T-matrix to make the incident plane waves orthogonal to the bound states, the Fock-Tani result accounts for some of the distortion that these incident (momentum) states should contain. Therefore it is not surprising that the Fock-Tani result is intermediate between the first Born and distorted wave approximations.

The total Fock-Tani cross section is not between the FBA and the DWA. There is a larger deficit for the DWA differential cross section relative to the FT result at large angles than for the FT relative to the FBA. And the surplus for the DWA relative to the FT result at small angles is roughly comparable to the surplus for the FT relative to the FBA result. Thus, the integration over scattering angles gives a total cross section for the DWA which is less than the FBA even though the FT result is greater than the FBA.

As a final note, the addition of the 3p orthogonalization term results in changes of order .1 percent. The 3s orthogonality corrections to each of the two potential terms are of the same order as the 2p corrections, but since the former cancel each other they don't contribute.

$(\mu^+\mu^-)$ from Muonic Hydrogen, Deuterium, and Tritium

A parallel to the formation of positronium, a bound state of an electron and its anti-particle, is the formation of the bound state $(\mu^+\mu^-)$. This has been given the name "mumuonium" because the more consistant name, "muonium" was used in the naming of the (μ^+e^-) bound state.[19] The muon is believed to be identical to the electron in all respects except that it is much more massive, ($m_\mu = 206.76859(29)m_e$ [20]), so that no hadronic interactions cloud the tests of electromagnetic interactions involving muons and electrons. Measurements of the Zeeman effect in the ground state of muonium have provided the most precise determination of the magnetic moment of the positive muon, a key test of quantum electrodynamics (QED).[21] But because the Bohr radii for mumuonium ($.00967265a_0$), muonic hydrogen [(μ^-p^+), .00538094], muonic deuterium [(μ^-d^+), $.00510877a_0$], and muonic tritium [(μ^-d^+), $.00501824a_0$][22] are so much smaller than that for muonium (.99518605), one would expect

QED effects to be much larger. Indeed, the magnification of the differences between energy levels in these muonic isotopes might allow greater sensitivity in measuring atomic hyperfine structure. Because the muonic hydrogen Bohr radius is only 100 times the proton radius, Hughes and Wu[23] have noted that a state of the art[24] calculation of the ground state splitting, together with a precise measurement, would be sensitive to models of proton structure. But a consideration of the correspondence between the Bohr radii of mumuonium and muonic hydrogen leads to an even more intriguing parallel. Would such a calculation and measurement process for mumuonium show that the muon is not a structureless Dirac particle? The calculation would be more difficult because one would have to consider the question of structure for both muons.

Muonic hydrogen isotopes are also of importance in catalyzed fusion, again because of the small Bohr radius. One of the most interesting processes from the Fock-Tani standpoint is the initial formation of $(d\mu)$, subsequent formation of $(d\mu d)^+$, followed rapidly by nuclear fusion. The muon is then free $(f \approx 87\%)$ to catalyze another fusion.[25] Charge transfer cross sections involving the $(ped)^+$ intermediate state have been studied in Fock-Tani representation by Hsu.[26] His techniques may be useful in the catalysis reaction.

The generalized program developed for the present calculation could be used for a full set of reactions involving positrons, electrons, muons, proton, deuterons, and tritons at a later date. For the present consider only the reactions

$$\mu^+ + (\mu^- p^+) \rightarrow (\mu^+ \mu^-) + p^+ \ , \tag{4.39}$$

$$\mu^+ + (\mu^- d^+) \rightarrow (\mu^+ \mu^-) + d^+ \ , \tag{4.40}$$

and

$$\mu^+ + (\mu^- t^+) \rightarrow (\mu^+ \mu^-) + t^+ \ . \tag{4.41}$$

Figures 11 and 12 show the differential cross sections for these processes at C.M. energies of 2.2024 keV and 25 keV, respectively, in first-order Born (FBA) and Fock-Tani (FT) approximations. The former is near the energy of the maximum in the total cross section for the proton case (2 keV_{LAB}). A comparison to the FBA and FT graphs in Fig. 5, the differential cross section at an energy near the positronium formation cross section maximum, 10.2eV, shows many similarities. Likewise, a comparison of the muonium differential cross section at about ten times the formation maximum, 25 keV, and the corresponding positronium differential cross section at about ten times the formation maximum, 100 eV (Fig. 8), shows similarities in overall shape. Note that the Fock-Tani and FBA differential cross

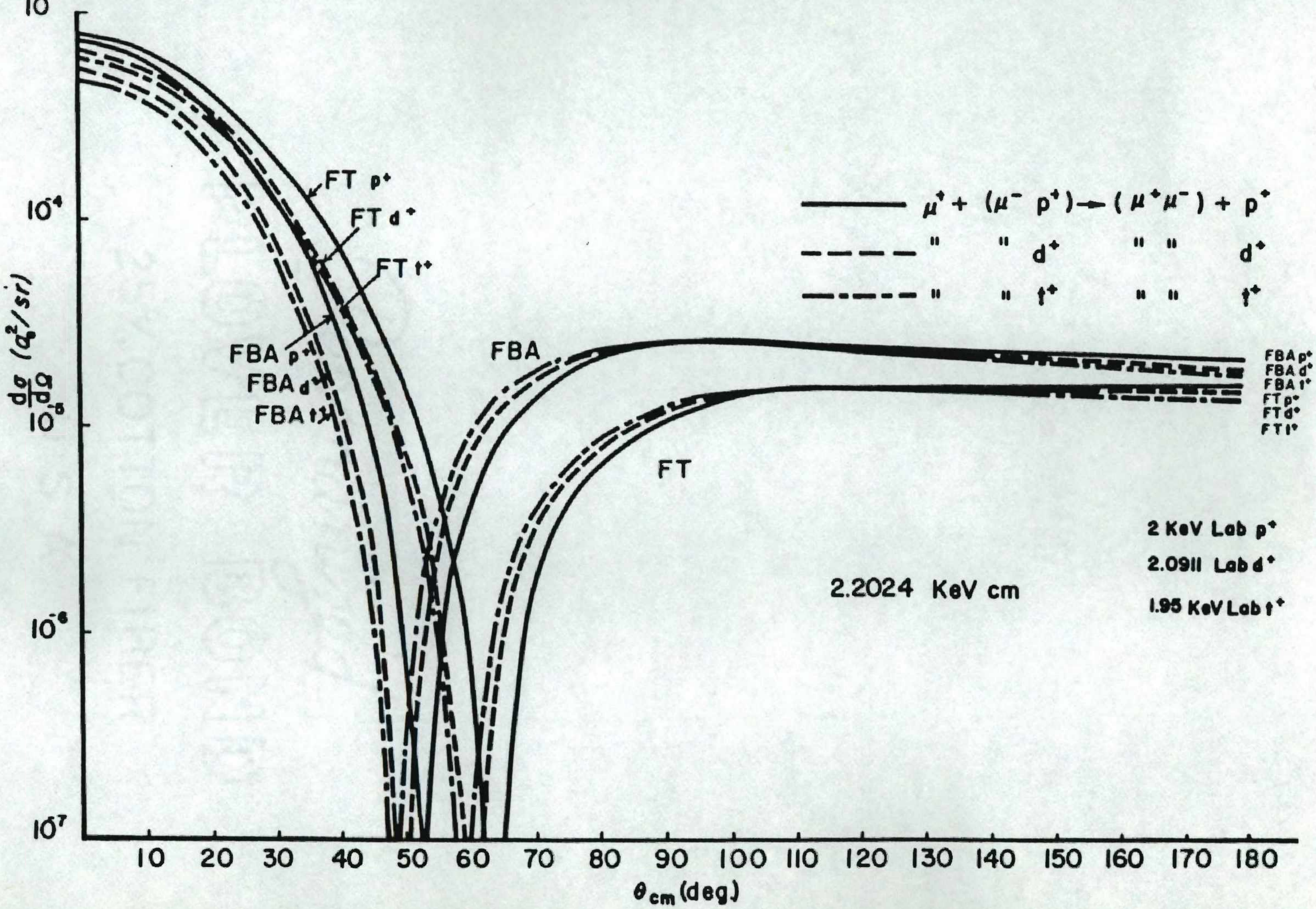

FIGURE 11. Differential cross section for mumuonium formation at 2.2024 keV. The solid, dashed and dot-dashed curves are for muonic hydrogen, muonic deuterium, and muonic tritium, respectively.

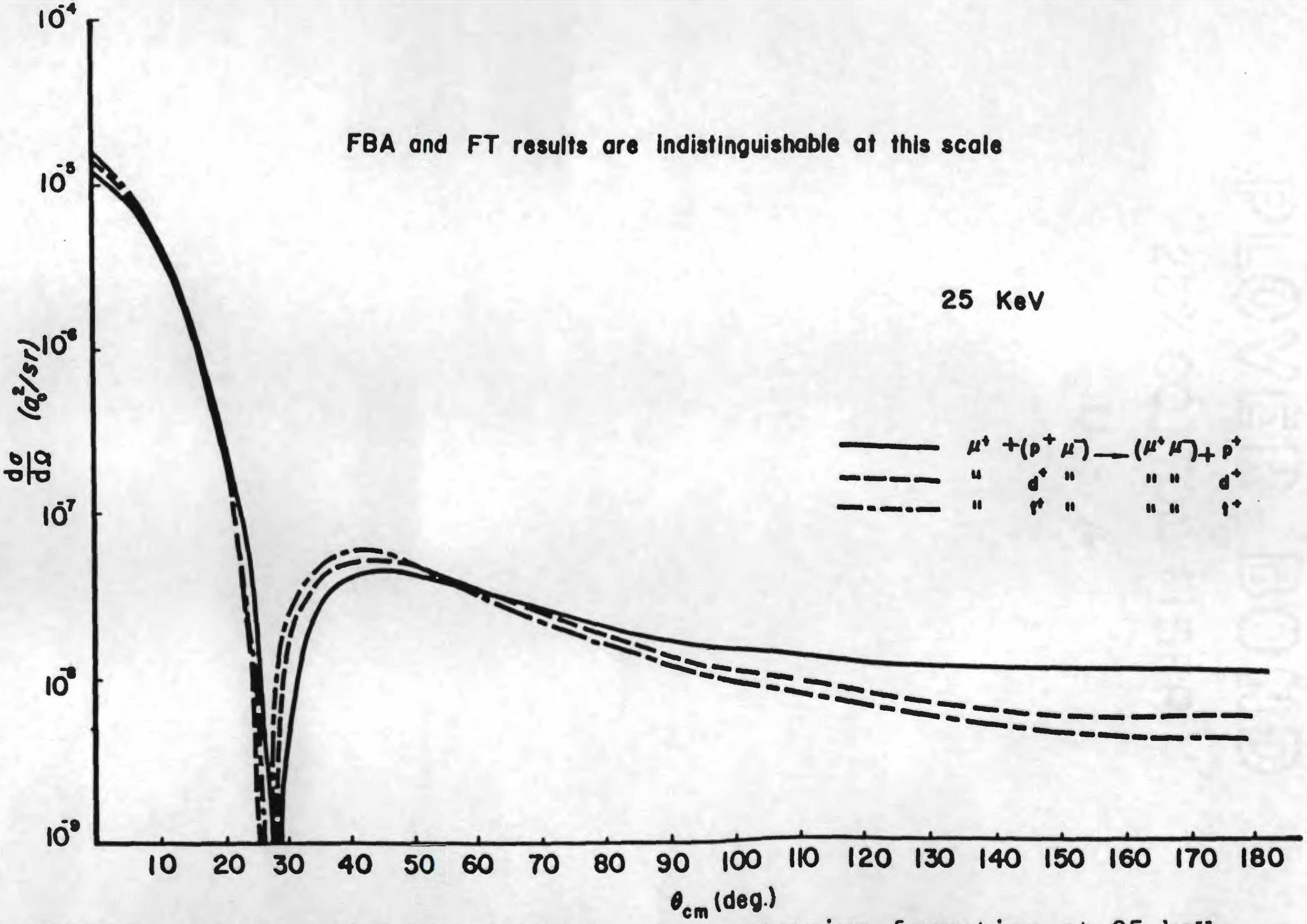

FIGURE 12. Differential cross section for mumuonium formation at 25 keV. The solid, dashed and dot-dashed curves are for muonic hydrogen, muonic deuterium, and muonic tritium, respectively.

sections for mumuonium are indistinguishable at these scales at 25 keV. This correspondence is not surprising considering the mass-scaling property demonstrated for the FBA total cross sections by Ma et al.[27] and by Ohsaki et al.[28] using a classical-trajectory Monte Carlo (CTMC) method.

As a final note on the differential cross section for these reactions, running the program at threshold (to error of order 0.00001 keV) produces an essentially constant value for all angles in both the FT and FBA theories. This is physically reasonable since at threshold the final momentum is zero and one has difficulty in even defining an angle between incident and final momenta. What is surprising result is that the FT result, $3.1\text{x}10^{-8}$, exceeds the FBA result, about $2.\text{x}10^{-11}$, by three orders of magnitude. A check on the positronium formation reaction produced FT and FBA threshold (.00680 eV) values of $2.\text{x}10^{-2}$ and $5.\text{x}10^{-4}$, respectively. The cross section for muon capture from muonic hydrogen by a positron at threshold (2.5172 keV) gave FT and FBA values of approximately $3.6\text{x}10^{-8}$ and $3.7\text{x}10^{-8}$, respectively. So the relative values appear to be mass-dependent. A broad survey of charge transfer reactions of this type could give a resolution of this dependence. Until this is done one should be cautious in accepting these threshold values.

Table 1 shows a comparison of the present first-order

Fock-Tani and FBA total cross section to the first-order distorted-wave approximation (DWBA) of Ma et al.,[27] and to the CTMC of Ohsaki et al.[28] The present FBA agrees with the result of Ma et al. except at 1.13 keV. This is probably because the energy they list is rounded to three places from the energy they calculated with, the cross section being very sensitive near threshold.

The FT and DWBA give remarkably good agreement for energies 1.7 through 7. keV , the range spanning the maximum in the cross section . This is much better agreement than for the positronium case, perhaps due to a somewhat different choice of distorting potentials.

Table 2 compares the muonic hydrogen, deuterium, and tritium cases. The total cross section is sensitive to variation among the heavy isotope initial states only near the threshold energies, which are

1.12189 keV_{LAB} (1.23544 keV_{CM}) for muonic hydrogen,

1.25729 keV_{LAB} (1.32434 keV_{CM}) for muonic deuterium, and

1.30465 keV_{LAB} (1.35195 keV_{CM}) for muonic tritium.

(Ma et al. use 1.13 for the hydrogen case.)

Therefore, since the differences in the momenta of the bound muon will be small, the ratio of projectile momenta to the probability of capture will be nearly the same except near threshold. A graph of the results of these tables is given in Fig. 13.

TABLE 1. Total Cross Sections for Reaction (4.39).

Lab Energy of Projectile	FBA	FT	DWBA[27]	CTMC*
		πa_0^2		
1.12190	1.090-10	1.608-7		
1.13000	9.928-7	1.285-5	1.47-10	
1.20000	2.445-5	5.234-5	4.80-5	
1.70000	1.617-4	1.772-3	1.79-4	
2.00000	1.768-4	1.869-4	1.89-4	
2.40000	1.670-4	1.738-4	1.75-4	4.-5
3.60000	1.046-4	1.085-4	1.09-4	3.8-5
5.00000	5.667-5	5.890-5		
6.00000	3.745-5	3.893-5		
7.00000	2.538-5	2.638-5	2.79-5	1.8-5
10.00000	9.057-6	9.402-6		
20.00000	7.506-7	7.878-7	9.76-7	4.8-7
100.00000	3.467-10†	3.471-10	6.02-10	

*Estimated from graph[28].

†The value given by Ma et al.[27] is 3.48-10 .

The notation 1.234-5 means $1.234x10^{-5}$

TABLE 4.2 Total Cross Sections for Reactions (4.39), (4.40), and (4.41).

Lab Energy of Projectile	hydrogen	deuterium		tritium	
	FT	FBA	FT	FBA	FT
		πa_0^2			
1.70000	1.772-3	1.075-4	1.173-4	2.456-5	7.133-5
2.00000	1.869-4	1.367-4	1.468-4	1.232-4	1.317-4
2.40000	1.738-4	1.420-4	1.513-4	1.323-4	1.421-4
3.00000		1.240-4	1.317-4	1.192-4	1.276-4
3.60000	1.085-4	1.005-4	1.066-4	9.834-5	1.051-4
5.00000	5.890-5	5.819-5	6.159-5	5.840-5	6.222-5
6.00000	3.893-5	3.970-5	4.193-5	4.033-5	4.285-5
7.00000	2.638-5	2.760-5	2.909-5	2.831-5	3.000-5
20.00000	7.878-7	9.459-7	9.975-7	1.026-6	1.084-6
100.00000	3.467-10†	3.471-10	6.02-10		

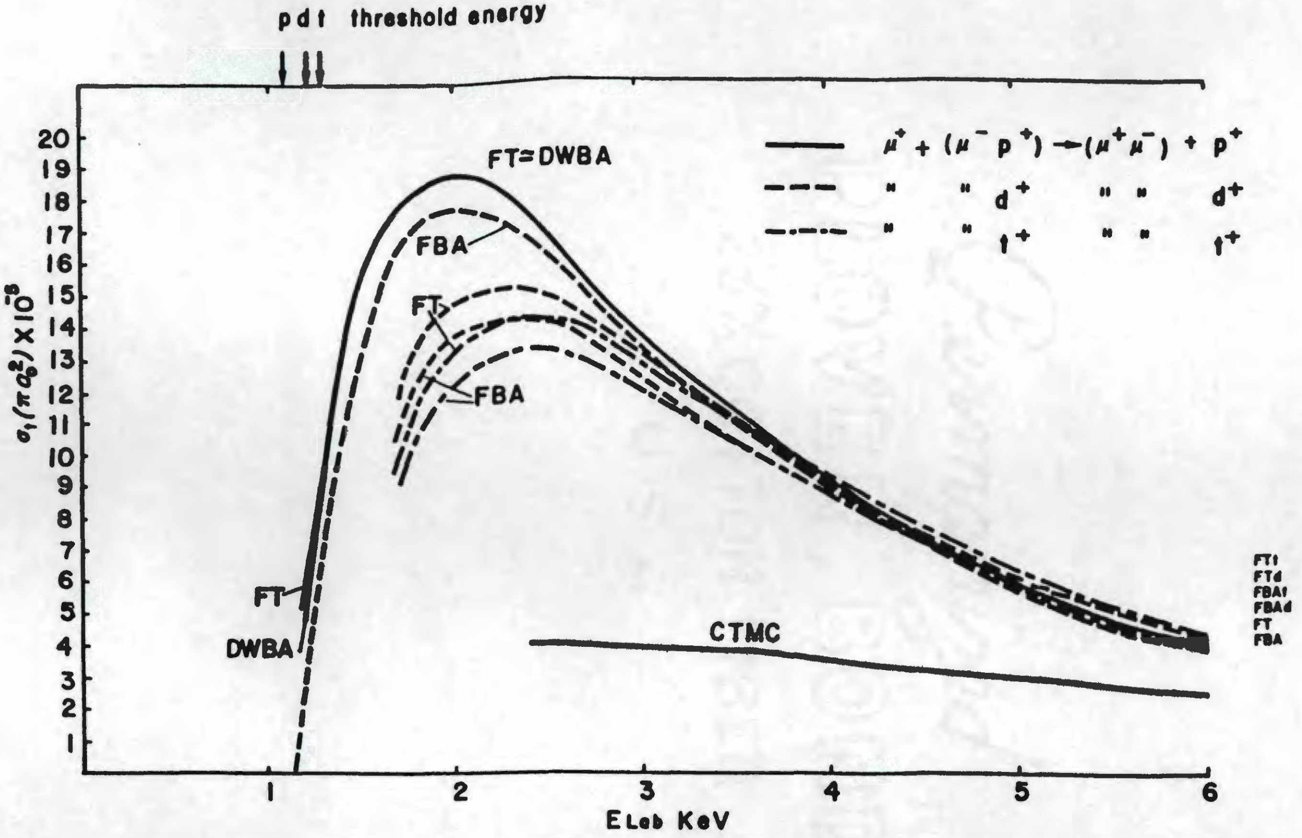

FIGURE 13. Total cross section for mumuonium formation. The solid, dashed and dot-dashed curves are for muonic hydrogen, muonic deuterium, and muonic tritium, respectively. The FBA and Fock-Tani results are given in each case. Note that the DWBA of Ma et al.[27] for muonic hydrogen is indistinguishable from the Fock-Tani result at this scale except near threshold. The CTMC result, of Ohsaki et al.,[28] for muonic hydrogen is also shown.

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CHAPTER V

POLARIZED WAVE FUNCTIONS FOR A HYDROGEN ATOM COUPLED TO A KINETIC EXTERNAL CHARGE

Introduction

The wave functions used in the first-order calculations ignore the distortion effects present in a system consisting of an atom and a charge. A comparison of the results of Ojha et al.[1] (see Appendix A) to the experimental data shows a lack of fit in the low energy region, where polarization feedback effects have more time to develop, and at larger angles, corresponding to smaller impact parameters, where all interactions should be greatest.

There has been much research done on the polarization problem. The polarized-orbital method was introduced by Bethe,[2] and revived by Temkin[3] and Callaway.[4] It is continually being modified and extended by various authors.[5] The essential approach is to calculate the polarized wave function of an atom in the presence of a fixed charge,[6,7] and from this the polarization potential in which the projectile moves. The wave function of the projectile is then found by numerical[5] or analytic[8] techniques. Seaton and Steenman-Clark,[9] using a close-coupling scheme, and Drachman,[10] by means of Feshbach projectors, have been able to include non-adiabatic effects in the polarization potential.

A self-consistant field theoretic approach[11] shows great promise and has been applied within the Fock-Tani representation by Ficocelli Varracchio.[12] His preliminary calculations of the s-wave phase shifts for elastic positronium scattering from hydrogen[13] show qualitative agreement with the benchmark variational calculations of Bhatia et al.[14] Further agreement might result from, among other refinements, inclusion of distortion in the propagator for the projectile.

In this chapter, a wave function will be found which contains distortion effects in both the atom and a moving projectile. It should be useful for refinement of both the polarized-orbital and field theoretic methods, as well as for refinement of the first-order Fock-Tani results of Chapters III and IV.

The Kinetic Equation

The problem involves a solution to the continuum Schrodinger equation for a system comprised of a moving charge and an atom in its ground state when the charge is at infinity. One cannot use bound state perturbation theory for this system since there is no energy shift in the system as a whole. But one can turn to scattering theory to solve for the Lippmann-Schwinger in-state,[15]

$$|\chi_i^+> = |\phi_i> + G_0^+V|\chi_i> \ , \tag{5.1}$$

where

$$G_0^+ = (E - H_0 + i\varepsilon) \ , \tag{5.2}$$

$$E = E_i = E_f \ , \tag{5.3}$$

and where the asymptotic state is defined by

$$(E_i - H_0)|\phi_i> = 0 \tag{5.4}$$

in the limit $\varepsilon \to 0^+$. The out-state is similarly defined, but with the opposite sign for ε.

Upon iterating (5.1), one produces the Born series

$$|\chi_i^+> = |\phi_i> + G_0^+V|\chi_i> + G_0^+VG_0^+V|\phi_i> + \ . \ . \ . \tag{5.5}$$

$$\equiv |\phi_i> + |\chi_i^{(1)}> + |\chi_i^{(2)}> + \ . \ . \ . \ . \tag{5.6}$$

Equating these two forms, term by term, produces the set of differential equations to be solved, (5.4) with

$$(E_i - H_0 + i\varepsilon)|\chi_i^{(1)}> = V|\phi_i> \qquad (5.7)$$

$$(E_i - H_0 + i\varepsilon)|\chi_i^{(w)}> = V|\chi_i^{(w-1)}> \text{ , for } w>1 \text{ .} \qquad (5.8)$$

Note that if one adds a term proportional to $|\phi_i>$ to the left-hand sides of each equation in (5.9) one still has a solution [because of (5.4)]. These proportionality constants are chosen so that

$$<\phi_i|\chi_i^{(w)}> = 0 \text{ .} \qquad (5.9)$$

To solve (5.7) a position dependent Dalgarno and Lewis[6] operator, F, is introduced, defined such that

$$\{[F,H_0] + i\varepsilon F\}|\phi_i> = V|\phi_i> \text{ .} \qquad (5.10)$$

Then

$$\{FE_i - H_0F + i\varepsilon F\} = V|\phi_i> \text{ ,} \qquad (5.11)$$

(5.7) and (5.9), give

$$|\chi_i^{(1)}> = F|\phi_i> - <\phi_i|F|\phi_i>|\phi_i> \text{ .} \qquad (5.12)$$

The Dalgarno and Lewis approach avoids the infinite sums and integrals one gets with an eigenfunction expansion of (5.7). In addition, solving the differential equation (5.10) is generally easier than solving (5.7) because F commutes with all potentials in H_0 on the left-hand side of (5.10). Furthermore, one can operate with H_0 and factor out the common $|\phi_i\rangle$ from both sides giving

$$\{\lambda(\nabla_R^2 + 2\vec{G}_{Rj}\cdot\vec{\nabla}_R) + (\nabla_r^2 + 2\vec{G}_{rj}\cdot\vec{\nabla}_r)\}F(\vec{R},\vec{r}) \equiv \{\lambda M[\vec{R}]+L[\vec{r}]\}F = $$
$$= -2P_0V/Z_A \quad , \tag{5.13}$$

where $\lambda = m/M$, $P_0 \equiv Z_A m$ $(m=1/a_0)$, and where the G-operators are defined by

$$\vec{G}_{\rho j} \equiv (1/\Phi_j)\vec{\nabla}_\rho \Phi_j \ . \tag{5.14}$$

In particular, for the present case (2.20), (2.21), and (2.23) give

$$\langle \vec{R}\vec{r}|\phi_i\rangle = (2\pi)^{-3/2}e^{i\vec{k}\cdot\vec{R}}(\pi)^{-1/2}e^{-P_0 r} \tag{5.15}$$

so that

$$\vec{G}_{R,k} = (i\vec{k}\cdot\hat{R})\hat{R} \qquad \text{and} \qquad \vec{G}_{r,100} = (-P_0)\hat{r} \ . \tag{5.16}$$

Chapter II contains a generic initial- or final-state Hamiltonian, (2.25) together with (2.26), for which we define V as the second two terms. It is convenient to scale the R coordinate vectors in this equation as

$$\vec{R}_1 = \frac{\vec{R}}{c(1-\nu)} \qquad \text{and} \qquad \vec{R}_2 = \frac{\vec{R}}{c\nu} \ , \tag{5.17}$$

where for initial states

$$c = +1 \text{ , and} \qquad \nu = \frac{m_1}{m_1 + m_2} \qquad (5.18)$$

and for final states

$$c = -1 \text{ , and} \qquad \nu = \frac{m_3}{m_3 + m_2} \; . \qquad (5.19)$$

Now one can expand the generic V in spherical harmonics,

$$V(\vec{R},\vec{r}) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{4\pi}{2\ell+1} \left(\frac{Z_A Z_P (-1)^{\ell} s_<^{\ell}}{(1-\upsilon) s_>^{\ell+1}} - \frac{Z_P \; t_<^{\ell}}{\upsilon t_>^{\ell+1}} \right) Y_{\ell m}^{*}(\hat{R}) Y_{\ell m}(\hat{r}) \; , \qquad (5.20)$$

where $s_<$ ($s_>$) is the lesser (greater) of R_1 and r and $t_<$ ($t_>$) is the lesser (greater) of R_2 and r. Notice that for $R \geq \upsilon r \geq (1-\upsilon) r$, the monopole terms of V exactly cancel if $Z_A = 1$, since

$$\frac{Z_A Z_P (-1)^0 r^0}{(1-\nu)|R/[c(1-\nu)]|^1} - \frac{Z_P r^0}{\nu |R/(c\nu)|^1} = \frac{Z_P (Z_A - 1)}{R} \; , \qquad (5.21)$$

so that the largest contribution from the inhomogeneous source in (5.13) arises from the dipole ($\ell = 1$) term in V. In fact one would expect, physically, that an external charge would induce a dipole moment in a spherically symmetric charge cloud.

The Large R Solution for the Multipole Terms

Equation (5.13) is solved by superposing the solutions for each source term of. Consider first the solution due to the multipole terms of V for the region $R_j > r$. The equation to be solved is

$$\{\lambda(\nabla_R^2 + 2\vec{G}_{Rj}\cdot\vec{\nabla}_R) + (\nabla_r^2 + 2\vec{G}_{rj}\cdot\vec{\nabla}_r)\}F^{>}(\vec{R},\vec{r}) \equiv \{\lambda M[\vec{R}]+L[\vec{r}]\}F =$$

$$= -2P_0\eta\frac{Z_P}{Z_A}\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{4\pi}{2\ell+1}\frac{\mu^\ell r^\ell}{R^{\ell+1}}Y_{\ell m}^{*}(\hat{R})\,Y_{\ell m}(\hat{r}) \;, \qquad (5.22)$$

where

$\eta = \{Z_A, -1\}$, $\mu = \{-1, +1\}$, and $R = \{R_1, R_2\}$ (5.23)

for the first and second terms of V, respectively.

If the angular parts of $F^{>}(\vec{R},\vec{r})$ are expanded in spherical harmonics with indices ℓm and LM, one finds that only the ℓ=L and m=M terms contribute, and that the radial part is independent of m, so that

$$F_\tau^{>}(\vec{R},\vec{r}) = -2P_0\eta\frac{Z_P}{Z_A}\sum_{\ell=1}^{\infty}\sum_{m=-\ell}^{\ell}\frac{4\pi}{2\ell+1}\mu^\ell\zeta_\nu(R>r)Y_{\ell m}^{*}(\hat{R})Y_{\ell m}(\hat{r}) \;, \qquad (5.24)$$

where τ is shorthand for the dependence on $\{\eta\mu k P_0\}$ and $\nu=\tau\ell$. Substituting (5.24) and (5.15) into (5.23), operating on the spherical harmonics with ∇^2, equating left- and right-hand sides, what remains is

$$\{\lambda M_{\nu}[R] + L_{\nu}[r]\}\zeta_{\nu}(R>r) = -\frac{r^{\ell}}{R^{\ell+1}} \quad , \tag{5.25}$$

where

$$M_{\nu}[R] = \frac{\partial^2}{\partial R^2} + 2\left(\frac{1}{R} + i\vec{k}\cdot\hat{R}\right)\frac{\partial}{\partial R} - \frac{\ell(\ell+1)}{R^2} \tag{5.26}$$

and

$$L_{\nu}[r] = \frac{\partial^2}{\partial r^2} + 2\left(\frac{1}{r} - P_0\right)\frac{\partial}{\partial r} - \frac{\ell(\ell+1)}{r^2} \; . \tag{5.27}$$

The method of solution is to expand ζ in the arbitrary parameter λ [given by the mass ratio m/M of (2.26)], equate equal powers of λ, and solve the resulting additional perturbation series order by order. Let

$$\zeta = \zeta^{(0)} + \lambda\zeta^{(1)} + \lambda^2\zeta^{(2)} + \; . \; . \; . \; . \tag{5.28}$$

Then one has the set of equations

$$L_{\nu}[r]\zeta_{\nu}^{(0)}(R>r) = -\frac{r^{\ell}}{R^{\ell+1}} \tag{5.29}$$

and

$$L_{\nu}[r]\zeta_{\nu}^{(w)}(R>r) = - M[R]\zeta_{\nu}^{(w-1)}(R>r) \; , \quad \text{for} \quad w>0 \; . \tag{5.30}$$

Bound-state double perturbation theory,[16] contains energy shift integrals to be calculated at each order for each perturbation expansion. Such coupled expansions must be solved simultaneously, to the same order. In contrast, the nested perturbation approach of the present method, expansions (5.2) and (5.28), contains no such energy terms so that an infinite-order solution of this expansion is possible. Indeed, an infinite order solution is realized for the present case of kinetically polarized s-state wave functions.

Equations (5.29) and (5.30) can be solved by defining

$$\zeta_\nu^{(w)}(R>r) = g_\nu^{(w)}(r) f_\nu^{(w)}(R) \ . \tag{5.31}$$

Then (5.30) separates into the set

$$L_\nu[r] g_\nu^{(0)}(r) = - r^\ell \ , \tag{5.32}$$

$$L_\nu[r] g_\nu^{(w)}(r) = \begin{cases} 0 \quad \text{if} \quad f_\nu^{(w-1)}(R) = 0 \\ \\ -g^{(w-1)}(r) \quad \text{otherwise} \end{cases} \quad \text{for} \quad w>0 \ , \tag{5.33}$$

$$f_\nu^{(0)}(R) = \frac{1}{R^{\ell+1}} \ , \text{ and} \tag{5.34}$$

$$f_\nu^{(w)}(R) = M[R] f_\nu^{(w-1)}(R) \ , \qquad \text{for} \quad w>0 \ . \tag{5.35}$$

The r-Dependent Solution

Because the solution to (5.32) generates a source for the w=1 equation (5.33) that is a polynomial, and the solution to the latter, in turn, generates a polynomial source for the w=2 equation (5.33), one should solve an equation for a generic monomial source,

$$L_\nu[r]h_\nu^{(w)}(r) = - r^{\ell+w} , \qquad (5.36)$$

and then superpose to obtain the solutions to (5.32) and (5.33).

The indicial equation associated with (5.36) has roots $r = \ell$ and $-\ell-1$. Each differs from $w + \ell + 2$ by an integer, admitting a particular solution containing an $\ln^2$ term, a logarithm multiplied by a series and a pure series[17]. One must eliminate the logarithmic terms on the physical grounds that the wave function should be non-singular at r=0. It will be shown in (5.41) that the coefficients of the remaining series are greater than the corresponding coefficients of the expansion of $\exp(+2P_0R)$, so the exponential fall-off of the hydrogenic wave function, which multiplies the polarization correction, is not sufficient to guarantee that the resulting function is finite for large r . We must therefore truncate the series at some point. Because (5.36) gives a two term recursion relation, this truncation causes all coefficients of terms with an exponent $j>w+1$ to be zero.

Let

$$h_\nu^{(w)}(r) = \sum_{q=0}^{j} a_q^w \, r^{\ell+q} \; . \tag{5.37}$$

Then

$$L_\nu[r]h_\nu^{(w)}(r) = \sum_{q=0}^{j} a_q^w \, r^{\ell+q}\{q(q+2\ell+1)r^{-2} - 2P_0(\ell+q)r^{-1}\} =$$

$$= -r^{\ell+w} \qquad , \tag{5.38}$$

where we have used the identity,

$q(q+2\ell+1) = (\ell+q) + 2(\ell+q) - \ell(\ell+1)$.

Equating powers of r on the left- and right-hand sides, one has

$$a_q^w = 0 \; , \qquad \text{for} \quad q > w+1 \; , \tag{5.39}$$

$$a_{w+1}^w = \frac{1}{2P_0(\ell+w+1)} \quad , \text{ and} \tag{5.40}$$

$$a_q^w = a_{q+1}^w \frac{(q+1)(q+2\ell+2)}{2P_0(\ell+w)} \quad , \qquad \text{for} \quad q < w+1 \; . \tag{5.41}$$

To solve for the zeroth- and first-order g's, one needs

$$a_1^0 = \frac{1}{2P_0(\ell+1)} \; , \tag{5.42}$$

$$a_0^0 = a_1^0 \, \frac{2\ell+1}{2P_0\ell} = \frac{1}{2P_0^2\ell} \quad , \tag{5.43}$$

$$a_2^1 = \frac{1}{2P_0(\ell+2)} , \tag{5.44}$$

$$a_1^1 = a_2^1 \frac{2(2\ell+3)}{2P_0(\ell+1)} = \frac{2\ell+3}{2P_0{}^2(\ell+1)(\ell+2)} , \tag{5.45}$$

and

$$a_0^1 = a_1^1 \quad \frac{2\ell+2}{2P_0\ell} = \frac{2\ell+3}{2P_0{}^3(\ell+2)} . \tag{5.46}$$

Then the solution to (5.32) is immediate:

$$g_\nu^{(0)}(r) = h_\nu^{(0)}(r) = a_0^0 r^\ell + a_1^0 r^{\ell+1} \equiv D_0^0 r^\ell + D_1^0 r^{\ell+1}$$

$$= \frac{1}{2P_0}(\frac{r^\ell}{P_0\ell} + \frac{r^{\ell+1}}{\ell+1}) \quad . \tag{5.47}$$

Substituting (5.47) and (5.34) into (5.31), substituting the resulting expression into (5.24), and setting $\eta = -1$ and $\mu = +1$ (τ for the second term of (5.20)) gives

$$F_2^>(\vec{R}_2,\vec{r}) \simeq \frac{Z_P}{Z_A} \sum_{\ell=1}^{\infty} (\frac{r^\ell}{P_0\ell} + \frac{r^{\ell+1}}{\ell+1}) \frac{1}{R_2{}^{\ell+1}} P_\ell(\cos\theta) , \tag{5.48}$$

which is the adiabatic result of Dalgarno and Stewart.[18] Note that in the limit $m_1 \to \infty$ (so that $R_1 \to \infty$) , $F_1^>(\vec{R}_1,\vec{r}) \to 0$. It is shown in (5.72) that $f_\nu^{(w)}(R) = 0$ for $w>0$ if the momentum vector, $\vec{k}$, is zero. Then (from (5.33)) $g_\nu^{(w)}(r) = 0$ for $w > 0$. So the (present) non-adiabatic exterior solution has the proper adiabatic (and infinite nucleus mass) limit.

Now the first-order equation (5.33),

$$L_\nu[r]g_\nu^{(1)}(r) = -\, g_\nu^{(0)}(r) = D_0^0 r^\ell + D_1^0 r^{\ell+1} \quad , \tag{5.49}$$

has a solution, given as a superposition of solutions to (5.36),

$$g_\nu^{(1)}(r) = D_0^0 h_\nu^{(0)}(r) + D_1^0 h_\nu^{(1)}(r) = \tag{5.50}$$

$$= D_0^0 a_0^0 r^\ell + D_0^0 a_1^0 r^{\ell+1}$$

$$+ D_1^0 a_0^1 r^\ell + D_1^0 a_1^1 r^{\ell+1} + D_1^0 a_2^1 r^{\ell+2} \tag{5.51}$$

$$\equiv C_{00}^1 r^\ell + C_{01}^1 r^{\ell+1}$$

$$+ C_{10}^1 r^\ell + C_{11}^1 r^{\ell+1} + C_{12}^1 r^{\ell+2} \tag{5.52}$$

$$\equiv D_0^1 r^\ell + D_1^1 r^{\ell+1} + D_2^1 r^{\ell+2} \quad . \tag{5.53}$$

This pattern also continues for $w > 1$, so that the general solution to (5.33), for non-zero f's, is

$$g_{\nu}^{(w)}(r) = \sum_{t=0}^{w+1} D_t^w \, r^{\ell+t} , \tag{5.54}$$

where

$$D_0^0 \equiv a_0^0 , \qquad D_1^0 \equiv a_1^0 , \tag{5.55}$$

$$D_t^w \equiv \sum_{u=t-1}^{w} C_{ut}^{\ w} , \qquad \text{for } w > 0 , \tag{5.56}$$

$$C_{-1\ t}^{\ w} \equiv 0 , \tag{5.57}$$

and

$$C_{ut}^{\ w} \equiv D_u^{w-1} a_t^u , \qquad \text{for } u > -1 . \tag{5.58}$$

The a's are given by (5.40) and (5.41). The P_0 and ℓ labeling for the a's, C's, and D's has been suppressed for simplicity.

The solution for the ns wave function, n>1, follows this pattern but with (5.39), (5.40), (5.41), and (5.55) altered due to the changes in the sources and in (5.14).

Using these definitions,

$$C_{00}^{\ 1} = a_0^0 a_0^0 = \frac{1}{4P_0{}^4 \ell^2} , \tag{5.59}$$

$$C_{10}^{1} = a_1^0 a_0^1 = \frac{2P+3}{4P_0{}^4 \ell(\ell+1)(\ell+2)} , \tag{5.60}$$

$$C_{01}^{1} = a_0^0 a_1^0 = \frac{1}{4P_0{}^3 \ell(\ell+1)} , \tag{5.61}$$

$$C_{11}^{1} = a_1^0 a_1^1 = \frac{2P+3}{4P_0{}^3 (\ell+1)^2(\ell+2)} . \tag{5.62}$$

and

$$C_{12}^{1} = a_1^0 a_2^1 = \frac{1}{4P_0{}^2 (\ell+1)(\ell+2)} . \tag{5.63}$$

These give

$$D_0^1 = \frac{1}{4P_0{}^4 \ell} \left(\frac{1}{\ell} + \frac{2\ell+3}{(\ell+1)(\ell+2)}\right) = \frac{3\ell^2+6\ell+2}{4P_0{}^4 \ell^2(\ell+1)(\ell+2)} , \tag{5.64}$$

$$D_1^1 = \frac{1}{4P_0{}^3 (\ell+1)} \left(\frac{1}{\ell} + \frac{2\ell+3}{(\ell+1)(\ell+2)}\right) = \frac{3\ell^2+6\ell+2}{4P_0{}^3 \ell(\ell+1)^2(\ell+2)} , \tag{5.65}$$

and

$$D_2^1 = C_{12}^1 , \tag{5.66}$$

which is given by (5.63).

Substituting these coefficients into (5.54) gives the r-dependent part of lowest-order kinetic contribution to the polarized orbitals (5.2),

$$g_{\nu}^{(1)}(r) = \frac{1}{4P_0{}^2(\ell+1)(\ell+2)} \{ \frac{3\ell^2+6\ell+2}{P_0\ell} [\frac{r^{\ell}}{P_0\ell} + \frac{r^{\ell+1}}{\ell+1}] + r^{\ell+2} \} . \tag{5.67}$$

Note that the term in square brackets is proportional to $g_{\nu}^{(0)}(r)$, but this pattern does not hold for $w>1$. This result multiplied by the ground-state wave function is proportional to the function given in Seaton and Steenman-Clark[9] (their Equation 4.7) from a similar iterative solution for only the r-dependent part.

The R-dependent Solution

Solutions to (5.35) generate operands for the next-order solution which are sums of inverse powers. Again one starts by defining a generic solution:

$$I_{\nu}^{(w)}(R) \equiv M[R]\frac{1}{R^{\ell+w}} = \tag{5.68}$$

$$= - \frac{(\ell+w)(2i\vec{k}\cdot\hat{R})}{R^{\ell+w+1}} + \frac{w(w+2\ell+1) - 2(\ell+w)}{R^{\ell+w+2}} \tag{5.70}$$

$$\equiv \frac{b^{w}_{w+1}}{R^{\ell+w+1}} + \frac{b^{w}_{w+2}}{R^{\ell+w+2}} \quad . \tag{5.71}$$

Note that the second term is zero for $w=1$, so that the

R-dependent part of the lowest-order kinetic contribution to the polarized orbitals is

$$f_{\ell}^{(1)}(R) = -\frac{(\ell+1)(2i\vec{k}\cdot\hat{R})}{R^{\ell+2}} . \tag{5.72}$$

For $\vec{k} = 0$, (5.35) gives $f_{\nu}^{(w)}(R) = 0$ for $w>0$. Then from (5.33), $g_{\nu}^{(w)}(r) = 0$ for $w>0$, which is the conventional adiabatic result[19] in the limit $m_1 \to \infty$.

In applying (5.35) for successive w's, one can see that the general-order solution is

$$f_{\nu}^{(w)}(R) = \sum_{v=w+1}^{2w} B_{v}^{w} \frac{1}{R^{\ell+v}} , \tag{5.73}$$

where

$$B_{w+1}^{w} = B_{w}^{w-1} b_{w+1}^{w} , \tag{5.74}$$

$$B_{q}^{w} = B_{q-2}^{w-1} b_{q}^{q-2} + B_{q-1}^{w-1} b_{q}^{q-1} , \qquad \text{for} \quad w+1<q<2w , \tag{5.75}$$

$$B_{2w}^{w} = B_{2w-1}^{w-1} b_{2w}^{2w-2} , \qquad \text{for } w>1 , \tag{5.76}$$

and

$$B_{1}^{0} \equiv 1 . \tag{5.77}$$

The b's are given in (5.70). The k and ℓ labeling of the B's and b's has been suppressesd for simplicily.

Substitution of (5.73) and (5.54) into (5.31), (5.28) and (5.24) gives the complete series solution to the large-R part of the kinetic polarized orbital problem. A computer can easily handle the calculation of coefficients.

One must still consider whether the series converges. In the region $r \leq a_0 \leq R$ ($a_0 = 1/P_0$) succeding terms go as $[\lambda k(a_0)^2/R]^w$ (or as $k[\lambda(a_0)2/R^2]^w$ for small k), in leading order. For a hydrogen bound state and a positron external charge, $\lambda = m/M \simeq 1-\varepsilon^2$ ($\varepsilon = 1/m_{prot}$) and $a_0 = 1-\varepsilon$. For a positronium bound state and a proton external charge $\lambda \simeq 1/4$ and $a_0 = 2$. For charge transfer the final momentum is of the same order of magnitude as the initial momentum so the solution for both cases must be restricted to the region $R \geq a_0{}^2 k$. The range of incident kinetic energies in the lab frame (≃ the CM energy) for charge transfer are 6.8 eV to about 50 eV, corresponding to k = .7 and 2., respectively, in atomic units. So the series converges within the same region in which the particle at R can (semi-classically) be said to be outside of the atomic cloud, self-consistant with the region in which the solution was developed from (5.22).

For a proton incident on a hydrogen atom, $\lambda \simeq 2\varepsilon$. So the series converges for $R \geq a_0{}^2 k/918$. For resonant charge transfer, the first-order cross section is appreciable for lab kinetic energies ≤ 100 Kev, or for $k \leq 2$. In such a case the series converges rapidly, requiring at most the w=1 term. In fact, the series converges at energies to

774 MeV, far beyond the range of validity of a non-relativistic theory. Indeed, one would expect that the corrections to the momentum eigenstate, of one proton relative to the other, would hardly be affected by atomic polarization over a wide range of high energies.

What is surprising in the present result is that the polarization corrections to the R and r parts of the wave function increase rather than decrease with k . However, Seaton and Steenman-Clark[9] and Drachman[10] calculated the non-adiabatic correction to the asymptotic effective dipole polarization potential (in the close-coupling and Feshbach projector methods, respectively), and obtained a result which is also proportional to k^2 .

The Kinetic Polarization Potential

The quantal virial theorem[18] will be used to calculate the lowest-order non-adiabatic correction to the polarization potential for the present formulation. In deriving the set of perturbation equations (5.4), (5.7), and (5.8), an energy shift was not defined because in a scattering process the energy of the system as a whole does not shift. However it is correct to say that there is a change in the energy of the atom as long as one sees that this energy shift is compensated for elsewhere. The change in energy of the atom will be calculated as a function of the distance to the external charge.

The standard first-order energy shift for the atom is found by taking the expectation value of the potential between zeroth-order wave functions and integrating only over the atomic coordinates (the momentum wave functions cancel),

$$E^{(1)}(R) = \langle \phi_i | V | \phi_i \rangle_r$$

$$= \langle u_{n\ell m} | V | u_{n\ell m} \rangle \ . \qquad (5.78)$$

This is just the static potential for elastic scattering. For n=1, this is given by

$$E^{(1)}(\vec{R}) = V_s(\vec{R}) = \frac{Z_A Z_P}{1-\upsilon} P_0 W^{1s}_{1s}(\vec{R}_1) - \frac{Z_P}{\upsilon} P_0 W^{1s}_{1s}(\vec{R}_2) \ , \qquad (5.79)$$

where R_1, R_2, and ν are given by (5.17) through (5.19), and

$$P_0 W^{1s}_{1s}(\vec{\rho}) = \frac{1}{\rho} - \exp(-2P_0\rho)(P_0 + \frac{1}{\rho}) \ . \qquad (5.80)$$

If one takes the limit $m_1 \rightarrow \infty$, then $\upsilon \rightarrow 1$ and

$$E^{(1)}(\vec{R}) \rightarrow \frac{Z_A Z_P}{R} - \frac{Z_P}{\upsilon} P_0 W^{1s}_{1s}(\vec{R}_2) \ , \qquad (5.81)$$

which is Robinson's result[20] for the static potential. In addition to this limit, Dalgarno and Lewis[6] also neglected the exponential terms in their result. For $Z_A = 1$,the 1/R terms cancel, leaving only the exponential terms, as in Joachian's version[21] for $Z_P = -1$.

One can check the importance of the the inertial potentials, W, of Chapter II by calculating this energy shift starting with the symmetrical reduced Hamiltonian, (2.22), but neglecting W. One recovers (5.20) because μ_3 of (2.22) equals m of (2.25), and since the kinetic energy of the external charge does not enter in. This approximation differs from the exact result in that the exponential in R_1 is neglected. So for such a problem one can conclude that the momentum dependent potentials can be neglected for external charge radii of order $R \geq 1/2m_1$.

It is interesting that for the case of positronium, (e^+e^-), and mumuonium, $(\mu^+\mu^-)$, atoms, $Z_A=1$ so that the monopole terms of (5.20) cancel. Furthermore $\upsilon=1/2$ gives $R_1= R_2$, so that the exponential terms also cancel, giving a zero first-order energy shift for positronium and mumuonium. Dalgarno and Stewart[18] noted that the n^{th}-order wave function gives the $(2n+1)^{st}$-order energy shift. The expectation values of the positions of electron and atomic nucleus are two diffuse spheres superposed with a common center. For the positronium case the spheres are identical, whereas for hydrogen they are of different sizes. A semi-classical snap-shot would show, on the average, positions for the two particles which are not charge symmetric relative to the average center-of-mass for the hydrogen system, the origin of the two spheres. But positronium has the added symmetry of a balanced charge distribution, on the average, relative to the center-of-mass. Consider a classical analogue consisting of two oppositely charged particles fixed to the ends of a rigid rotor of constant angular velocity, pivoting about the center-of-mass. The inverse-square force between these charges and an external charge would yield a net attraction for the case of unequal (rotor) masses, in a time average, and no net attraction for the equal mass case.

Equation (5.78) is a positional average of the attraction of the "external" charge to the system decribed by the zeroth-order wave function, so that in cases where the centers of mass and charge are identical, one would expect no first-order energy shift. Furthermore, since the first-order wave functions contain polarization, which is eight times larger for positronium than for hydrogen, one would expect second- and third-order energy shifts to be larger for positronium. This is confirmed in (5.85).

The second-order energy shift is given by the expectation value of the potential between zeroth- and first-order wave functions. Again we want this as a function of R so integration will be only over the r coordinates (the momentum wave functions cancel). Then the polarization energy is

$$E^{(2)}(R) = \langle \phi_i | V | \chi_i^{(1)} \rangle$$

$$= \langle u_{n\ell m} | V(F - a) | u_{n\ell m} \rangle \; , \qquad (5.82)$$

where

$$a \equiv \langle \phi_i | F | \phi_i \rangle \; . \qquad (5.83)$$

In the limit $m_1 \to \infty$, and neglecting any terms in exp(-R) arising from the part of the r-integrals where r>R,

$$F(\vec{R}\, ,\vec{r}) \simeq \frac{Z_P}{Z_A} \sum_{\ell=1}^{\infty} ([\frac{r^{\ell}}{P_0{}^{\ell}} + \frac{r^{\ell+1}}{\ell+1}] \frac{1}{R^{\ell+1}}$$

$$- \frac{\lambda}{P_0(\ell+2)} \{ \frac{3\ell^2+6\ell+2}{P_0{}^{\ell}} [\frac{r^{\ell}}{P_0{}^{\ell}} + \frac{r^{\ell+1}}{\ell+1}] + r^{\ell+2} \} \frac{i\vec{k}\cdot\hat{R}}{R^{\ell+2}}) P_{\ell}(\cos\theta)$$

$$(5.84)$$

and

$$V(R,r) \simeq - Z_P \sum_{L=1}^{\infty} \frac{r^L}{R^{L+1}} P_L(\cos\theta) \; . \qquad (5.85)$$

Then the lowest-order kinetic contribution to a of (5.83) will be of order $1/R^4$ (ℓ=2) and is, therefore, neglected in comparison to the lowest-order kinetic contribution from *F* (ℓ=1) . Then the second-order (polarization) energy (in the large R approximation) is

$$E^{(2)}(R) \simeq - \frac{Z_P{}^2\, a_0{}^3}{Z_A{}^4}\left(\frac{9}{4R^4} - \frac{129\lambda}{12P_0{}^2}\,\frac{i\vec{k}\cdot\hat{R}}{R^5}\right) . \qquad (5.86)$$

As noted earlier, the second-order energy shift is eight times larger for positronium (where $a_0=2$) than for hydrogen. The first term (when multiplied by 2 to change to rydbergs) is given in Dalgarno and Stewart.[19] These authors previously[18] showed that the quantal virial theorem is satisfied by the zeroth- and first-order wave functions so that the potential energy is given by

$$W(R) = 2E + R\,\frac{\partial E}{\partial R}. \qquad (5.87)$$

Then the polarization potential in which the projectile moves is given by the second-order term in this expression divided by the charge of the projectile:

$$V^{(2)}(R) \simeq \frac{Z_P a_0{}^3}{Z_A{}^4}\left(\frac{9}{2R^4} - \frac{129\lambda}{4P_0{}^2}\,\frac{i\vec{k}\cdot\hat{R}}{R^5}\right) . \qquad (5.88)$$

The first term is the well-known adiabatic polarization potential, where $Z_P= -1$ in Seaton and Steenman-Clark[9] and in Drachman.[10] Like these authors' results, the present non-adiabatic correction is an increasing function of k and leads to a repulsive force, which is an indication that the k-dependence of (5.73), though counter-intuitive , is qualitatively correct. However, the present non-adiabatic correction enters in at a slightly lower order in 1/R and is dependent on k rather than k^2 .

The Small R Solution for the Multipole Terms

One can formally develop the R<r multipole solution using the same expansion, (5.28), as for the R>r solution by interchanging R and r in the source terms of (5.22) through (5.35). However, (5.35), in which there are no boundary-condition choices to be made (no constant of integration), inevitably gives terms which are singular at the origin of R. The function

$$f_{\nu}^{(1)<}(R) = 2i\vec{k}\cdot\hat{R} + \frac{2 - \ell(\ell+1)}{R} \tag{5.89}$$

is singular at R=0 unless $\ell=1$. Furthermore, for $\ell=1$,

$$f_{\ell=1}^{(2)<}(R) = -4i\vec{k}\cdot\hat{R}/R^2 \tag{5.90}$$

is singular. Because succeeding w's are even more singular this approach doesn't bear fruit unless the dipole approximation is valid and λ is small enough to neglect terms with w>1 .

An alternate possibility would be to interchange the roles of L and M [(5.26) and (5.27)] so that one can choose boundary conditions for the f's. This is done by expanding

$$\zeta^{<} = \zeta^{(0)<} + 1/\lambda\ \zeta^{(1)<} + 1/\lambda^{2}\ \zeta^{(2)<} + \ldots \qquad (5.91)$$

and defining

$$\zeta_{\nu}^{(w)}(R<r) \equiv g_{\nu}^{(w)<}(r) f_{\nu}^{(w)<}(R)\ . \qquad (5.92)$$

The solution is then given by the replacements

$$g_{P_0}^{(w)<}(r) = f_{-i\vec{k}\cdot\hat{R}}^{(w)}(R) \quad \text{and} \quad f_{-i\vec{k}\cdot\hat{R}}^{(w)<}(R) = g_{P_0}^{(w)}(r) \qquad (5.93)$$

where the ℓ dependence is not shown.

However, this solution also has its problems. The expansion coefficient $1/\lambda$ is greater than one. And one would expect the adiabatic limit ($k\rightarrow 0$) to be the ground state of the H_2^+ molecule. In fact the adiabatic limit diverges term by term as $1/k^{2w}$!

It should be noted that the expansion in λ, (5.28), is not the only way to solve the large R equation, (5.25). One can expand ζ in a series of increasing powers of $1/R$, with coefficients that are functions of r. The first two terms in this series are identical to the first two of (5.28) because the second term of (5.71) is zero. However, higher-order terms involve mixing of the $g^{(w)}$'s so that discerning a general series would be much more difficult than the decoupled (product) solution, (5.31).

Likewise, for the small-R case, the alternate expansion of ζ in powers of R with coefficients that are functions of r gives the same result and, hence, the same problems.

The small-R part of the multipole problem appears to be unsolvable by obvious means. So one must be satisfied, at present, to approximate the polarization part of the wave function with the R>r solution restricted to the region essentially outside of the densest part of the atomic electron cloud; $R>5a_0$. A number of authors[22] use an adiabatic wavefunction which is cut off in this way. So the final, approximate solution is

$$F_\tau(\vec{R},\vec{r}) \approx F_\tau^{>}(\vec{R},\vec{r})\Theta(\vec{R}-\vec{r}) \ , \tag{5.94}$$

where Θ is the Heaviside step function.

Higher-order Terms

The solution to (5.7) in the large R (external charge coordinate) limit, effectively useful for $R \geq 5a_0$, is now complete. The solution was explicitly labeled initial, but is the same for final states as well, with the alternate definition of ν in (5.19). Because there are no energy shift terms to calculate the present machinery can easily be applied to the solution of the second-order equation, (5.8) with w=2 . Define a position-dependent Dalgarno and Lewis[6] operator, $F^{(2)}$, such that

$$\{[F^{(2)},H_0] + i\varepsilon F\}|\phi_i> = V|\chi_i^{(1)}> . \qquad (5.95)$$

One can again factor out the exponential parts of the wave function on both sides and solve for the rest. The seed equations, (5.32) and (5.34), will have more complicated sources. But using the superposition principle, together with the generic equations, (5.37), (5.38), and (5.68), the problem is reduced to a matter of efficient bookkeeping. And given this solution to (5.8) for w=2, one can solve for w=3 and so on. Thus continuum perturbation theory is necessary for a solution to this problem. But since it generates no energy shift terms (found in bound state perturbation theory), this form of perturbation theory actually facilitates a solution to arbitrary order.

Notes

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CHAPTER VI

HIGHER-ORDER EFFECTS IN FOCK-TANI REPRESENTATION

Introduction

The first-order Fock-Tani results[1] for the reaction $p^+ + H \rightarrow H + p^+$ match the experimental data[2,3] well for differential angles less than 3 mrad and for energies greater than 10 keV. The improvement over the first Born approximation is due to the inclusion of higher-order effects within the first order Fock-Tani T-matrix. Because the orthogonalization corrections of the Fock-Tani theory remove the double counting of the plane-wave states superimposed over the bound state, which occurs in conventional representations, the Fock-Tani T-matrix may be considered as a type of distorted wave T-matrix. It would be desirable to account for additional sources of distortion.

In this chapter the framework for a distorted-wave T-matrix is developed, and the solution to the equation for the distorted states, which includes some additional effects to infinite order while neglecting others, is outlined. Finally, a method for including these neglected terms to second- and third-order is considered.

The Distorted-Wave T-matrix

Girardeau's development[*] of a distorted-wave T-matrix, which accounts for some initial- and final-state effects to infinite order and the remaining terms to arbitrary order, is presented. However, the result is extended to the case where there may be different distortion potentials for initial- and final-states. One starts with the general definition of the T-matrix from Chapter IV:

$$T_{fi} = (\phi_f|\hat{V}|\psi_i^+) \ , \tag{6.1}$$

where the final asymptotic state, $(\phi_f|$, is given by (3.73), the Lippmann-Schwinger in-state, $|\psi_i^+)$, is given by

$$|\psi_i^+) = |\phi_i) + \hat{G}_0^+\hat{V}|\psi_i^+) \ , \tag{6.2}$$

and $\hat{V}$ is given by (3.57). In this equation the initial asymptotic state, $|\phi_i)$, is given by (3.71) and

$$\hat{G}_0^+ = (E - \hat{H}_0 + i\varepsilon) \ , \tag{6.3}$$

where the limit $\varepsilon \to 0^+$ is implied and $\hat{H}_0$ given by (3.56). If the full potential is split into initial-state distortion terms and a remainder,

$$\hat{V} = \hat{V}_d + \hat{U}_d \ , \tag{6.4}$$

then one can define a distorted initial state by

$$|\chi_i^{+d}) = |\phi_i) + \hat{G}_0^+\hat{V}_d|\chi_i^{+d}) \ . \tag{6.5}$$

One may also split the potential into final-state distortion terms and a remainder,

$$\hat{V} = \hat{V}_b + \hat{U}_b \ , \tag{6.6}$$

where *b* may or may not equal *d*. Then one defines the final distorted state as

$$(\chi_f^{-b}| = (\phi_f| + (\chi_f^{-b}|\hat{V}_b\hat{G}_0^+ \ . \tag{6.7}$$

Substituting (6.7) and (6.2) into (6.1) and rearranging terms gives the conventional two-potential T-matrix,[5]

$$T_{fi} = (\chi_f^{-d}|\hat{U}_b|\psi_i^+) + (\chi_f^{-d}|\hat{V}_b|\phi_i) \ . \tag{6.8}$$

Since ionization and recombination terms are allowed in the distorting potential, the second term is not zero. Equating $|\phi_i)$ in (6.2) and (6.5), using the operator relation $(AB)^{-1} = (B^{-1})(A^{-1})$ one can show that

$$\begin{aligned} |\psi_i^+) &= (E - \hat{H}_0 - \hat{V} + i\varepsilon)^{-1}(E - \hat{H}_0 - \hat{V}_d + i\varepsilon)|\chi_i^{+d}) \\ &= (1 - \hat{G}^{+d}\hat{U}_d)^{-1}|\chi_i^{+d}) \\ &= (1 + \hat{G}^{+d}\hat{U}_d + \hat{G}^{+d}\hat{U}_d\hat{G}^{+d}\hat{U}_d + \ . \ . \ .)|\chi_i^{+d}) \ , \end{aligned} \tag{6.9}$$

where the distorted-wave Green's operator is given by

$$\hat{G}^{+d} = (E - \hat{H}_0 - \hat{V}_d + i\varepsilon)^{-1} \quad . \qquad (6.10)$$

Then the distorted wave T-matrix, which now includes distortion interactions to infinite order in the initial, intermediate, and final states and in the distorted-wave propogator $\hat{G}^{+d}$, is given by

$$T_{fi} = (\chi_f^{-b}|\hat{U}_b|\chi_i^{+d}) + (\chi_f^{-b}|\hat{V}_b|\phi_i) + (\chi_f^{-b}|\hat{U}_b\hat{G}^{+d}\hat{U}_d|\chi_i^{+d})$$

$$+ (\chi_f^{-b}|\hat{U}_b\hat{G}^{+d}\hat{U}_d\hat{G}^{+d}\hat{U}_d|\chi_i^{+d}) + \ldots . \qquad (6.11)$$

The choice of what to include in V_b and V_d is physically motivated. It is found that some terms that are initially included in V_b and V_d must later be neglected. These should be shifted to U_b and U_d, respectively.

Determining the Distorted States

First the Fock-Tani potential is rewritten in a shorthand form, where the left and right hand subscripts indicate the creation and annihilation operators found in that term of V [e represents a continuum electron, ε an electron bound to the origin, a a free a-particle, and α an (a^+e^-) bound state]:

$$\hat{V} = {}_{e}\hat{V}_{e} + {}_{\alpha}\hat{V}_{\alpha} + ({}_{\alpha}\hat{V}_{ea} + {}_{ae}\hat{V}_{\alpha}) + ({}_{\alpha}\hat{V}_{\varepsilon a} + {}_{a\varepsilon}\hat{V}_{\alpha}) + {}_{ae}\hat{V}_{ea}$$

$$+ ({}_{ae}\hat{V}_{\varepsilon a} + {}_{a\varepsilon}\hat{V}_{ea}) + {}_{a\varepsilon}\hat{V}_{\varepsilon a} \, . \qquad (6.12)$$

If one iterates (6.4), the only non-zero terms are

$$|\chi_{i}^{+d}) = |\phi_{i}) + \hat{G}_{0}^{+}\hat{V}_{d}|\phi_{i}) + \hat{G}_{0}^{+}\hat{V}_{d}\hat{G}_{0}^{+}\hat{V}_{d}|\phi_{i}) + \ldots$$

$$= |\phi_{i}) + \hat{G}_{0}^{+}({}_{ae}\hat{V}_{\varepsilon a} + {}_{a\varepsilon}\hat{V}_{\varepsilon a})|\phi_{i})$$

$$+ \hat{G}^{+}({}_{ae}\hat{V}_{\varepsilon a} + {}_{a\varepsilon}\hat{V}_{\varepsilon a} + {}_{ae}\hat{V}_{ea} + {}_{a\varepsilon}\hat{V}_{ea} + {}_{e}\hat{V}_{e})\hat{G}_{0}^{+}({}_{ae}\hat{V}_{\varepsilon a} + {}_{a\varepsilon}\hat{V}_{\varepsilon a})|\phi_{i})$$

$$+ \ldots \qquad (6.13)$$

if the charge transfer terms, $({}_{\alpha}\hat{V}_{a\varepsilon} + {}_{\alpha}\hat{V}_{ae} + {}_{ae}\hat{V}_{\alpha} + {}_{a\varepsilon}\hat{V}_{\alpha})$, are excluded. Note that if one had started with the Fock-Tani Hamiltonian, (3.18), derived from the non-specialized Fock Hamiltonian, (3.1), $\hat{V}_{d}$ would have had a ${}_{a}\hat{V}_{a}$ term. The contribution from this process is included in each of the present V's as the monopole part in the expansion of the first term of (3.68).

To find the distorted initial state one must solve the equation

$$(E - \hat{H}_0 - \hat{V}_d)|\chi_i^{+d}) = 0 \ , \qquad (6.14)$$

subject to outgoing boundary conditions ($\varepsilon \to 0^+$). The solution follows the non-pertubative approach of Tripathy and Rao[6], but will differ in substance. The primary differences are that continuum states are included in the present expansions and the internuclear potential is not neglected. The former slightly complicates the formulas. The latter fundamentally alters the result because this potential cancels the monopole term that is their largest source of distortion.

First a complete set of {bound, continuum} states, is defined by

$$\{|\xi_G)\} = \{\hat{\varepsilon}_\gamma^\dagger|0>, \ (2\pi)^{-3/2}\int d\vec{r} e^{i\vec{g}\cdot\vec{r}}\hat{e}^\dagger(\vec{r})|0>\} \ , \qquad (6.15)$$

using a generic label G for either γ or $\vec{g}$, and likewise H for either η or $\vec{h}$. The energy of the state, E_G, stands for either E_γ , given by (3.54), or $g^2/2m$, given by (3.42) and (3.43). The total energy of the system is

$$E = E_{1s} + k^2/2M \ , \qquad (6.16)$$

for an 1s initial bound state, where $\vec{k}$ is the initial momentum vector and M is the 3-body reduced mass, (3.43).

The normalization condition is

$$(\xi_G|\xi_H) = \delta_{GH} \equiv \delta_{\gamma\eta} \text{ or } \delta(\vec{g}-\vec{h}) \ . \tag{6.17}$$

If one expands χ in this complete set,

$$|\chi_i^{+d}) = \sum\!\!\!\!\!\!\int_H d\vec{R}_1\, \chi_H^{+d}(\vec{R}_1\vec{k})\hat{a}^\dagger(\vec{R}_1)|\xi_H) \ , \tag{6.18}$$

substitutes into (6.14), and multiplies from the left by $(\xi_G|\hat{a}(\vec{R})$, one gets the equation

$$[E - E_G - T_a(\vec{R})]\chi_G^{+d}(\vec{R}\vec{k}) = \sum\!\!\!\!\!\!\int_H d\vec{R}_1\,(\xi_G|\hat{a}(\vec{R})\hat{V}_d\hat{a}^\dagger(\vec{R}_1)|\xi_H)\chi_H^{+d}(\vec{R}_1\vec{k}) \ . \tag{6.19}$$

Using the definition of the distortion potential, (6.13) and (3.57), this splits into two sets of coupled equations:

$$[k^2 - 2M(E_{1s} - E_\gamma) + \nabla^2]\chi_\gamma^{+d}(\vec{R}\vec{k}) =$$

$$= 2M\sum_\eta\int d\vec{R}_1\,(\vec{R}\gamma|H_{ae}|\vec{R}_1\eta)'\chi_\eta^{+d}(\vec{R}_1\vec{k})$$

$$+ 2M(2\pi)^{-2/3}\int d\vec{h}\,d\vec{R}_1\,d\vec{r}\,(\vec{R}\gamma|H_{ae}|\vec{R}_1\vec{r})''e^{i\vec{h}\cdot\vec{r}}\chi^{+d}(\vec{h}\vec{R}\vec{k}) \tag{6.20}$$

and

$$[k^2 - 2M(E_{1s} - h^2/2m) + \nabla^2]\chi^{+d}(\vec{h}\vec{R}\vec{k}) =$$

$$= 2M(2\pi)^{-3/2}\sum_{\eta}\int d\vec{R}_1 d\vec{r} e^{-i\vec{h}\cdot\vec{r}}(\vec{R}\vec{r}|H_{ae}|\vec{R}_1\eta)''\chi_{\eta}^{+d}(R_1k)$$

$$+ 2M(2\pi)^{-3}\int d\vec{g} d\vec{R}_1 d\vec{r} d\vec{r}_1 e^{-i\vec{h}\cdot\vec{r}}(\vec{R}\vec{r}|H_{ae}|\vec{R}_1\vec{r}_1)'' e^{i\vec{g}\cdot\vec{r}_1}\chi^{+d}(\vec{g}\vec{R}\vec{k}) \ . \tag{6.21}$$

The source terms on the right hand side simplify if one neglects the non-local orthogonality corrections, giving

$$[k^2 - 2M(E_{1s} - E_{\gamma}) + \nabla^2]\chi_{\gamma}^{+d}(\vec{R}\vec{k}) =$$

$$= \sum_{\eta}U_{\gamma\eta}(\vec{R})\chi_{\eta}^{+d}(\vec{R}\vec{k}) + \int d\vec{h} U_{\gamma}^{*}(\vec{h}\vec{R})\chi^{+d}(\vec{h}\vec{R}\vec{k}) \tag{6.22}$$

and

$$[k^2 - 2M(E_{1s} - h^2/2m) + \nabla^2]\chi^{+d}(\vec{h}\vec{R}\vec{k}) =$$

$$= \sum_{\gamma}U_{\gamma}(\vec{h}\vec{R})\chi_{\gamma}^{+d}(\vec{R}\vec{k}) + \int d\vec{g} U(\vec{h}\vec{g}\vec{R})\chi^{+d}(\vec{g}\vec{R}\vec{k}) \ , \tag{6.23}$$

where

$$U_{\gamma\eta}(\vec{R}) = 2M\int d\vec{r} u_{\gamma}^{E^*}(\vec{r})(V_{ab}(\vec{R}\vec{r}) + V_{ae}(\vec{R}\vec{r}))u_{\eta}^{E}(\vec{r}) \ , \tag{6.24}$$

$$U_{\gamma}(\vec{h}\vec{R}) = 2M(2\pi)^{-3/2}\int d\vec{r} e^{-i\vec{h}\cdot\vec{r}}(V_{ab}(\vec{R}\vec{r}) + V_{ae}(\vec{R}\vec{r}))u_{\gamma}^{E}(\vec{r}) \ , \tag{6.25}$$

$$U(\vec{g}\vec{h}\vec{R}) = 2M(2\pi)^{-3}\int d\vec{r}\,(V_{ab}(\vec{R}\vec{r}) + V_{ae}(\vec{R}\vec{r}))e^{-i(\vec{h}-\vec{g})\cdot\vec{r}} \;, \qquad (6.26)$$

$$V_{ab}(\vec{R}\vec{r}) + V_{ae}(\vec{R}\vec{r}) = \frac{Z_a Z_b}{|\vec{R}+\lambda\vec{r}|} - \frac{Z_a}{|\vec{R}-\nu\vec{r}|} \;, \qquad (6.27)$$

$$\nu = \frac{m_b}{m_b + m_e} \;, \text{ and } \qquad \lambda = \frac{m_e}{m_b + m_e} \;. \qquad (6.28)$$

If one expands (6.27) in spherical harmonics one notes that the monopole terms cancel for R>r and Z_b=1 . The dipole potential terms is then dominant in this region, as one would expect. But Tripathy and Rao[6] neglected the internuclear potential, V_{ab}, in their Hamiltonian [their equation (21)] so that this cancellation did not occur. They were left with a monopole term as dominant.

Given the cancellation of the bare internuclear potential by the corresponding term in the orthogonalization potential noted by Ojha et al.,[1] for the reaction $p^+ + H \rightarrow H + p^+$, an approximation confirmed to give only 10 percent error in Chapter IV, one might wonder if such cancellation might occur between the bare terms included in (6.22) and (6.23) and the presently neglected orthogonality corrections. In fact, in this approximation, such a cancellation occurs only between V_{ab} in $U_\gamma(\vec{h}\vec{R})$, (6.25), and the corresponding orthogonality correction for the

E-bound states. However, the monopole term of V_{ae} in (6.25), for R>r, is also canceled by the monopole term in the orthogonality correction, so one is still left with the dipole potential dominant.

Satapathy, Tripathy, and Rao, in a later paper[7], improved their calculations for $p^+ + H \rightarrow H + p^+$ by introducing a screening parameter to account for the neutrality of the atom. The present potential, in which the dipole term is dominant, rests on firmer physical ground and contains no arbitrary parameter. It is shown that the dipole case also yields a solution.

The coupled equations (6.22) and (6.23), could be solved numerically. However, "infinity" of the radial integrals must typically be taken to be several hundred Bohr radii. This increases computer time and accumulates roundoff errors.[8] To avoid this, an analytic solution is found in the region $R>R_{max}$, where the latter is an intermediate value chosen by trial. Tripathy and Rao[6] were able to find an analytic solution in this region for the monopole potential; a Coulomb wave. However in subsequent calculations they also appear to have used this function for small values of R . The use of an asymptotic solution for a monopole potential might be justified in the R<r region, since the dominant term in the latter region is of monopole form, although involving the electron radius, r, rather than the projectile radius, R . But using the

asymptotic solution for a dipole potential as the solution for small R for the present system would not be a good approximation since monopole terms dominate for R<r.

Since the dipole potential generated by an atom arises from virtual transitions between the ground state and bound and contiuum states with angular momentum one, it is consistent to restrict the U's in (6.22) and (6.23) to such transitions. Any e^{-R} terms arising in $\ell=1$ part of (6.24), (6.25), and (6.26) are also neglected. Then the coupled equations become

$$[k^2 + \nabla^2]\chi^{+d}_{1s}(\vec{R}\vec{k}) \simeq$$

$$\simeq \sum_{np} U_{1s,np}(\vec{R})\chi^{+d}_{np}(\vec{R}\vec{k}) + \int d\vec{h}U^{*}_{1s}(\vec{h}\vec{R})\Big|_{\ell=1}\chi^{+d}(\vec{h}\vec{R}\vec{k}) \ , \qquad (6.29)$$

$$[k^2 - 2M(E_{1s} - E_{np}) + \nabla^2]\chi^{+d}_{np}(\vec{R}\vec{k}) \simeq$$

$$\simeq U_{np,1s}(\vec{R})\chi^{+d}_{1s}(\vec{R}\vec{k}) \ , \qquad (6.30)$$

and

$$[k^2 - 2M(E_{1s} - h^2/2m) + \nabla^2]\chi^{+d}(\vec{h}\vec{R}\vec{k}) \simeq$$

$$\simeq U_{1_{\sigma}}(\vec{h}\vec{R})\Big|_{\ell=1}\chi^{+d}_{1s}(\vec{R}\vec{k}) \ . \qquad (6.31)$$

The outgoing boundary condition implied in (6.14) gives an asymtotic form for the solution of (6.29),

$$\chi_{1s}^{+d}(\vec{R}\vec{k}) \xrightarrow[R\to\infty]{} A\left(e^{i\vec{k}\cdot\vec{R}} + f_{1s}(\theta\phi)\frac{e^{ikR}}{R}\right) \tag{6.32}$$

for which

$$\nabla^2\chi_{1s}^{+d}(\vec{R}\vec{k}) \xrightarrow[R\to\infty]{} -k^2\chi_{1s}^{+d}(\vec{R}\vec{k}) + O(1/R^3) \ . \tag{6.33}$$

Following the discussion in Tripathy and Rao, for potentials $U \sim 1/R^{p+1}$, one considers the relations

$$\nabla^2[U(\vec{R})\chi_{1s}^{+d}(\vec{R}\vec{k})] = \chi\nabla^2 U + 2\vec{\nabla}U\cdot\vec{\nabla}\chi + U\nabla^2\chi =$$

$$\simeq U\nabla^2\chi + O(1/R^{p+2})$$

$$\simeq -k^2U(\vec{R})\chi_{1s}^{+d}(\vec{R}\vec{k}) \ , \tag{6.34}$$

where the last relation comes from (6.33). If

$$[k^2 - 2M(E_{1s} - E_{np})]U_{1s,np}\chi_{1s}^{+d}(\vec{R}\vec{k}) \tag{6.35}$$

is added to both sides of (6.34) and if $U\chi$ on the right-hand side of the resulting equation is replaced with the left-hand side of (6.30), one obtains

$$[k^2 - 2M(E_{1s} - E_{np}) + \nabla^2]U_{1s,np}(\vec{R})\chi^{+d}_{1s}(\vec{R}\vec{k}) \simeq$$

$$\simeq [k^2 - 2M(E_{1s} - E_{np}) - k^2]U_{1s,np}(\vec{R})\chi^{+d}_{1s}(\vec{R}\vec{k})$$

$$\simeq [2M(E_{np} - E_{1s})][k^2 - 2M(E_{1s} - E_{np}) + \nabla^2]\chi^{+d}_{np}(\vec{R}\vec{k}) \tag{6.36}$$

or

$$\chi^{+d}_{np}(\vec{R}\vec{k}) \simeq \frac{U_{1s,np}(\vec{R})}{2M(E_{np} - E_{1s})}\,\chi^{+d}_{1s}(\vec{R}\vec{k}) \;. \tag{6.37}$$

By a similar process, one can show that

$$\chi^{+d}(\vec{h}\vec{R}\vec{k}) \simeq \frac{U_{1s}(\vec{h}\vec{R})\Big|_{\ell=1}}{2M(h^2/2m - E_{1s})}\,\chi^{+d}_{1s}(\vec{R}\vec{k}) \;. \tag{6.38}$$

Inserting (6.37) and (6.38) into (6.29) one obtains

$$(k^2 + \nabla^2 + \frac{M\alpha}{R^4})\chi^{+d}_{1s}(\vec{R}\vec{k}) \simeq 0 \;, \tag{6.39}$$

where

$$\alpha = \frac{R^4}{2M^2}\sum_{np}\frac{\left|U_{1s,np}(\vec{R})\right|^2}{\left|E_{np} - E_{1s}\right|} + R^4\int d\vec{h}\,\frac{\left|U_{1s}(\vec{h}\vec{R})\Big|_{\ell=1}\right|^2}{\left(h^2/2m + \left|E_{1s}\right|\right)} \tag{6.40}$$

is the conventional dipole polarizability[6] (if the e^{-R}

terms in the U's are neglected) plus a term with the same interpretation arising from virtual transitions to the continuum. A minus sign was factored out from these terms (where $E<0$) to indicate the attractive nature of the potential in (6.39). If the e^{-R} terms in the U's are neglected then α is independent of R and the integral may be calculated prior to other numerical integrals. In this case the computation time is not significantly increased.

The solution to (6.39) for all R has been given by Holzwarth[9], but the asymptotic expansion found by Hunter and Kuriyan[8] is more useful for the present purpose because it consists of simple triginometric functions multiplied by a 1/R series, so the need to determine characteristic exponants is avoided, and it is non-iterative. If one expands χ

$$\chi^{+d}_{1s}(Rk) = \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{X(Rk)}{R} Y_{\ell m}(\hat{R}) Y^{*}_{\ell m}(\hat{k}) \quad , \tag{6.41}$$

the solution to (6.39) and (6.41) is, for $z \equiv kR$,

$$X(z) = \gamma(P(z)\cos z - Q(z)\sin z) + \beta(P(z)\sin z + Q(z)\cos z) \tag{6.42}$$

where γ and β are arbitrary constants to be determined by equating the numerical solution of (6.22) and (6.23), for small R, to (6.42) at some intermediate value of R, R_{max}, chosen so that variations in R_{max} give variations in the result that are less than the tolerable error. The functions P and Q are series in 1/z ,

$$P(z) = \sum_{j=0}^{\infty} (-1)^j T_{2j}(z) , \quad Q(z) = \sum_{j=0}^{\infty} (-1)^j T_{2j+1} , \qquad (6.43)$$

where T_0 is an arbitrary normalization constant which may be set equal to one, and where

$$2zT_1 = \ell(\ell+1)T_0 ,$$

$$4zT_2 = [\ell(\ell+1) - 2]T_1 \text{ , and}$$

$$2jzT_j = [\ell(\ell+1) - j(j-1)]T_{j-1} + M\alpha k^2 T_{j-3}/z^2 . \qquad (6.44)$$

$M\alpha$ is the numerator in (6.39). The ℓ indices on *P, Q,* and the *T*'s have been suppressed.

Hunter and Kuriyan[8] found that for terms with j>30, the contribution of subsequent terms was less than the tolerable error. Their criterion was sufficient to guarantee an accurate solution for moderate to large R even if (6.43) are asymptotic series.

The asymptotic limit is

$$X(Rk) \xrightarrow[R\to\infty]{} \gamma\cos Rk + \beta\sin Rk . \qquad (6.45)$$

If one substitutes the asymptotic solution to (6.41), which contains a factor of 1/R, and the $1/R^2$ potentials into the right-hand sides of (6.30) and (6.31) then, by a dimensional argument, $x_{np}^{+d}(\vec{R}\vec{k})$ and $x^{+d}(\vec{h}\vec{R}\vec{k})$ also go as 1/R asymptotically. However, even if one uses the full formula for X(z), (6.30) and (6.31) are just wave equations for a series of $(\alpha\cos Rk + \beta\sin Rk)1/R^{3+j}$ sources, so their solution is straightforward. An approximate solution for the initial distorted state is now complete. The solution for the final distorted state follows the same format. From these the first-order distorted-wave T-matrix in (6.11) can then be evaluated.

The Second- and Third-order Distorted T-matrices

Madison[10] has developed a method for calculating an exact second-order T-matrix element, and the extension to third-order is obvious. One could calculate a second-order undistorted T-matrix element, but this is essentially equivalent to the first order term of (6.8), with ψ replaced by ϕ. To include higher-order effects one should begin with the second- and third-order terms of (6.11),

$$T_{fi}^{2} = (\chi_f^{-b}|\hat{U}_b\hat{G}^{+d}\hat{U}_d|\chi_i^{+d}) \qquad (6.46)$$

and

$$T^3_{fi} = (\chi_f^{-b}|\hat{U}_b\hat{G}^{+d}\hat{U}_d\hat{G}^{+d}\hat{U}_d|\chi_i^{+d}) \ . \qquad (6.47)$$

The intermediate states in these expressions involve multidimensional integrals. The standard approximation,[12] replacing the energy variable in the denominator of such integrals by an "average" energy, is not acceptable for a process allowing transitions to the continuum. How does one define the average of energies ranging to infinity? Instead the problem is transformed to the solution of differential equations, a general method pioneered by Dalgarno and Lewis.[11] If one defines

$$|\zeta_i^{+d}) = \hat{G}^{+d}\hat{U}_d|\chi_i^{+d}) \qquad (6.48)$$

and

$$(\zeta_f^{-bd}| = (\chi_f^{-b}|\hat{U}_b\hat{G}^{+d} \ , \qquad (6.49)$$

the second- and third-order T-matrix elements are reduced to integrals over a single set of variables:

$$T^2_{fi} = (\chi_f^{-b}|\hat{U}_b|\zeta_i^{+d}) = (\zeta_f^{-bd}|\hat{U}_d|\chi_i^{+d}) \qquad (6.50)$$

and

$$T^3_{fi} = (\zeta_f^{-bd}|\hat{U}_d|\zeta_i^{+d}) \ . \qquad (6.51)$$

There are no intermediate loops to integrate over. Equation (6.50) has 4 or 6 fewer dimensions to be integrated over or summed (depending whether the intermediate state is bound or continuum, respectively) than (6.46). The reduction in going from (6.47) to (6.51) is 6 or 12 fewer integral dimensions (or sums). The tradeoff is the need to solve the differential equations

$$(E - \hat{H}_0 - \hat{V}_d)|\zeta_i^{+d}) = \hat{U}_d|\chi_i^{+d}) \tag{6.52}$$

and

$$(E - \hat{H}_0 - \hat{V}_d)|\zeta_i^{-bd}) = \hat{U}_b|\chi_f^{+b}) \ , \tag{6.53}$$

which generally requires less computer time than does multidimensional integration. Madison has demonstrated that the an exact calculation of (6.50) is a tractable problem, whereas an exact calculation of (6.46) would be extremely difficult. It is possible that the techniques of the previous section could yield an approximate solution for the third-order T-matrix.

Notes

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CHAPTER VII

CONCLUSION

The primary goal of this work was to more closely examine 3-body scattering so that an extension of the Fock-Tani transformation to larger systems would be firmly grounded. It has been shown that the difficulty of carrying out this transformation can be considerably reduced by working in reduced-mass coordinate systems. The choice of whether to use the symmetrical center-of-mass system, with one particle fixed at the origin, or to use either the initial- or final-state inertial center-of-mass system is shown to depend on the application.

A transformation using the symmetrical system is greatly simplified for "knock out" reactions in which there are two types of particles that can bind to the origin. It has the drawback of giving a first-order T-matrix with an error of $1/m_{proton}$ in the initial state momentum wave function. However, an examination of the physics of the reaction easily leads to an ad hoc correction. The Fock-Tani transformation using the inertial reduced-mass system is much more difficult than that using the symmetrical reduced-mass system for this reaction.

It was also found that setting up any problem in the symmetric $n \rightarrow (n-1)$-body system initially , for $n<6$, may facilitate eventual calculations done in the inertial systems because this may be the easiest coordinate transformation path to the latter. In the process, relations between initial- and final-state inertial systems are generated. Finding such relations by other methods may be much more difficult.

The first-order results were examined in detail and computer programs giving differential and total cross sections for reactions of the type

$$a^+ + (b^+c^-) \rightarrow (a^+c^-) + b^+ \,, \tag{7.1}$$

for arbitrary masses, were generated . It was found that the inertial $3\rightarrow 2$-body systems gave the same result, in first-order, as the full 3-body Fock-Tani transformation. This transformation can be done with half the work of the 3-body transforation.

Results for (abc) = (ppe) were compared to Fock-Tani results of Ojha et al.[1] Their neglect of the internuclear potential was found to give an error of order 10 percent, but their neglect of 3s, 3p, and 3d orthogonality corrections was found to give an error of only one percent. The more general, present result removes small oscillations found in their differential cross sections at small angles.

Present results for (abc) = (epe) and the previous Fock-Tani result of Ficocelli Varracchio and Girardeau[2] were found to disagree, probably due to lack of convergence in the previous result. Fock-Tani cross sections for (abc) = (μpμ) were also calculated and compared to first Born, distorted-wave[3], and classical-trajectory Monte-Carlo[4] calculations. It was found that the Fock-Tani and distorted-wave results are in excellent agreement for a wide range of energies. Finally, Fock-Tani results for (abc) = {(μpμ), (μdμ), and (μtμ)} were compared with each other and found to be somewhat different near threshold and nearly the same for larger energies.

Because the Fock-Tani results for resonant charge transfer in proton-hydrogen collisions agreed with the experiment for energies greater than 10 keV and for differential angles less than 1 mrad at 25, 60, and 125 keV, but did poorly outside these regions, it was thought that including higher-order effects in the calculations might give a better overall result.

For this reason a solution was found to the equation for the first-order wave function for a system containing a hydrogenic atom coupled to a kinetic external charge. The solution is easily extended to higher orders. The lowest-order kinetic correction to the much-used adiabatic wave function was found to depend on k/R^3, where k is the momentum and R the coordinate of the external ($R \geq 5a_0$) charge. In a subsequent calculation of the polarization potential, using this wave function and the virial theorem, the lowest-order kinetic contribution was found to be of a similar form to the result of Seaton and Steenman-Clark[5] and Drachman,[6] but was shown to enter in at a lower order in (large) R, depending on k/R^5 rather than k^2/R^6.

Techniques for evaluating the distorted-wave Fock-Tani T-matrix were also developed. The equation for the distorted states was shown to give an approximate analytical solution for large R, to be coupled to a numerical solution in the small-R region. The solution of the second- and third-order distorted-wave T-matrices was outlined.

It is my intention to apply the polarized wave function and distorted-wave techniques to the reactions calculated at first-order in this dissertation. In addition, the general-mass computer programs of Appendix B could provide differential and total cross section theoretical results for reactions (7.1) not presently available in the literature.

Also the techniques and understanding gained throughout the work on this dissertaion will be used in calculating the differential and total cross sections for charge transfer in the 4-body scattering problem

$$es + H^- \rightarrow Ps(n\ell) + H(1s) \tag{7.2}$$

during the coming year under the auspices of a National Research Council-NASA Research Associateship, for which I am very grateful.

The significance of this dissertation from my perspective lies not so much in the specific answers generated for the present problems, even though they should be very useful to researchers in this field, but, rather, in the refinement of a style of perceiving, thinking, and imagining which will be of benefit to my future research. I have learned that science, like any other art, requires two things: a willingness to clearly see and acknowledge the world as it presents itself; and the technical skills necessary to share such understanding with others.

Notes

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APPENDIX A

THE 3-BODY RESULTS OF OJHA ET AL.

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Fock-Tani transformation and a first-order theory of charge transfer

P. C. Ojha, M. D. Girardeau, J. D. Gilbert, and J. C. Straton
Department of Physics, Institute of Chemical Physics and Institute of Theoretical Science,
University of Oregon, Eugene, Oregon 97403

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A unitary (Fock-Tani) transformation of the second-quantized Hamiltonian breaks the interaction into its component parts, e.g., elastic scattering, inelastic scattering, rearrangement interaction, etc. The interaction for a particular process is "weaker" than the overall interaction; this is reflected in certain orthogonality corrections which appear in a perturbation expansion of the T-matrix element. As a result, the internuclear potential makes a negligible contribution of order m_e/m_p to the first-order amplitude for charge transfer. We find very good agreement with experimental and the best available theoretical results for the total cross section for the reaction $p+\text{H}(1s)\to\text{H}(1s)+p$ for energies greater than 10 keV and for the differential cross section at 25, 60, and 125 keV in an angular range of ~ 1 mrad about the forward direction.

I. INTRODUCTION

Atomic physics provides the ideal setting for testing new approaches to the quantum-mechanical scattering problem mainly because the interaction potential is known but also because of the variety and richness of phenomena open to investigation. This paper is part of a broader program to investigate the suitability of one such approach based on unitary (Fock-Tani) transformation of the second-quantized Hamiltonian. The motivation for this transformation is discussed and its basic features illustrated for the simple case of potential scattering in Sec. II; the mathematical details relevant to present application are given in Sec. III and the complete result is enumerated in Appendix A. Here we merely note the final result that the interaction is broken into its component parts, e.g., elastic scattering, inelastic scattering, rearrangement interaction, etc. This gives one considerably more latitude in introducing physically motivated approximations, for example, in a Born series expansion of the scattering amplitude. The effective interaction for a particular process is, in a sense, "weaker" than the overall interaction which is the sum of all interactions. It is found that to each order in the perturbation, certain orthogonality corrections to the usual (Fock) scattering amplitude appear. In this paper we restrict ourselves to a first-order (Born-type) approximation, in which case the orthogonality correction becomes negligible at high energies. We therefore expect the Fock-Tani formalism to extend the range of validity of the first-order approximation to lower energies.

This formalism has been applied previously to the calculation of the scattering amplitude for positronium formation[1] and for positron-hydrogen elastic scattering[2] in collisions of positrons with hydrogen atoms. The numerical results of the second of these papers clearly demonstrate the superiority of the Fock-Tani representation over close-coupling representations in some cases where channel coupling plays an important role. In this paper we consider the closely related problem of resonant charge transfer,

$$p+\text{H}(1s)\to\text{H}(1s)+p\ , \tag{1.1}$$

with the understanding that at collision energies under consideration (relative velocities of order 1 a.u.) proton-proton exchange plays no role. This problem, in spite of a long history of quantum-mechanical analysis going back to the early days of quantum mechanics,[3,4] is still under vigorous investigation as indicated by a recent review article[5] and numerous other publications. An early difficulty was caused by the Coulomb repulsion of the nuclei. This was neglected by Oppenheimer[3] and Brinkman and Kramers[4] on physical grounds but the resulting cross sections were too large by a factor of 3 or 4. Its inclusion in a mathematically consistent first-order theory[6,7] brought the total cross section in line with experiment but clashed with the physical argument that the internuclear potential cannot significantly affect the cross section for charge transfer. In Sec. IV we show that in the Fock-Tani formalism, as a consequence of the orthogonality correction, the Coulomb interaction of the nuclei contributes a negligible term of order m_e/m_p to the first-order reaction amplitude, a result pleasingly consistent with an observation about the *exact* scattering amplitude originally made by Wick (see footnote in Ref. 6).

The first-order orthogonality correction is reduced to a numerically tractable form in Sec. V, and computed differential and total cross sections are compared with experiment and the best available theoretical results (two-state atomic expansion introduced by Bates[8]) in Sec. VI. In Sec. VII we summarize our results and outline possible future extension of this work.

II. FOCK-TANI TRANSFORMATION FOR POTENTIAL SCATTERING

The basic idea behind Fock-Tani transformation and its consequence for scattering are best explained for scattering of a single particle from a fixed potential $V(\mathbf{r})$ which is sufficiently strong to support a number of bound states $\{|\mu\rangle, \mu=1,2,3,\ldots\}$ with energies $\{\epsilon_\mu, \mu=1,2,3,\ldots\}$.

This formulation was first considered by Tani[9] but the following summary is closer in its mathematical detail to the generalization due to Girardeau.[10]

We begin with the second-quantized form of the Hamiltonian (Fock Hamiltonian)

$$\hat{H}_F = \int d\mathbf{r}\,\hat{a}^\dagger(\mathbf{r})[T(\mathbf{r})+V(\mathbf{r})]\hat{a}(\mathbf{r}) , \tag{2.1}$$

where $T(\mathbf{r})$ is the kinetic-energy operator and $\hat{a}^\dagger(\mathbf{r})$ and $\hat{a}(\mathbf{r})$ are "elementary" creation and annihilation operators defined in the Fock space $\mathscr{F}$. These satisfy canonical commutation relations

$$[\hat{a}(\mathbf{r}),\hat{a}(\mathbf{r}')]=[\hat{a}^\dagger(\mathbf{r}),\hat{a}^\dagger(\mathbf{r}')]=0 \tag{2.2a}$$

and

$$[\hat{a}(\mathbf{r}),\hat{a}^\dagger(\mathbf{r}')]=\delta(\mathbf{r}-\mathbf{r}') . \tag{2.2b}$$

If the wave functions $\{\psi_\mu(\mathbf{r}),\ \mu=1,2,\ldots\}$ of the bound states are known, one may introduce "bound-state" creation and annihilation operators

$$\hat{\psi}^\dagger_\mu = \int d\mathbf{r}\,\psi_\mu(\mathbf{r})\hat{a}^\dagger(\mathbf{r}) \tag{2.3a}$$

and

$$\hat{\psi}_\mu = \int d\mathbf{r}\,\psi^*_\mu(\mathbf{r})\hat{a}(\mathbf{r}) . \tag{2.3b}$$

Note that the commutation relations of these operators with $\hat{a}(\mathbf{r})$ and $\hat{a}^\dagger(\mathbf{r})$ are not always simple. In particular,

$$[\hat{a}(\mathbf{r}),\hat{\psi}^\dagger_\mu]=\psi_\mu(\mathbf{r}) \tag{2.4a}$$

and

$$[\hat{a}^\dagger(\mathbf{r}),\hat{\psi}_\mu]=-\psi^*_\mu(\mathbf{r}) \tag{2.4b}$$

are noncanonical. This complicates the mathematical analysis whenever one has to make explicit the existence of bound states of the system.

It is therefore desirable to introduce operators which can be associated with the bound states and which satisfy canonical commutation relations instead of (2.4). With this in mind, we introduce an "ideal-state" space $\mathscr{B}$ in which creation and annihilation operators $\{\hat{b}^\dagger_\mu,\ \hat{b}_\mu,\ \mu=1,2,\ldots\}$ are defined. These are further assumed to satisfy the following commutation relations:

$$[\hat{b}_\mu,\hat{b}_\nu]=[\hat{b}^\dagger_\mu,\hat{b}^\dagger_\nu]=0 \tag{2.5a}$$

and

$$[\hat{b}_\mu,\hat{b}^\dagger_\nu]=\delta_{\mu\nu} . \tag{2.5b}$$

We next construct the direct-product space $\mathscr{H}\equiv\mathscr{F}\otimes\mathscr{B}$. In this space all annihilation and creation operators previously introduced are defined. However, the "ideal-state" operators $\hat{b}_\mu$, $\hat{b}^\dagger_\mu$, etc., unlike the "real-state" operators $\hat{\psi}_\mu$, $\hat{\psi}^\dagger_\mu$, etc., *commute* with the elementary operators $\hat{a}(\mathbf{r})$ and $\hat{a}^\dagger(\mathbf{r})$:

$$\begin{aligned}[\hat{a}(\mathbf{r}),\hat{b}_\mu]&=[\hat{a}(\mathbf{r}),\hat{b}^\dagger_\mu]\\ &=[\hat{a}^\dagger(\mathbf{r}),\hat{b}_\mu]=[\hat{a}^\dagger(\mathbf{r}),\hat{b}^\dagger_\mu]=0 .\end{aligned} \tag{2.6}$$

The subspace $\mathscr{H}_F\subset\mathscr{H}$ defined by the condition

$$\sum_\mu \hat{b}^\dagger_\mu\hat{b}_\mu|\chi\rangle=0 \text{ iff } |\chi\rangle\in\mathscr{H}_F , \tag{2.7}$$

is quite obviously isomorphic to the Fock space $\mathscr{F}$. Any calculations in $\mathscr{F}$ may as well be done in $\mathscr{H}_F$. We will, however, make a unitary transformation which will give the physical meaning of the real states $\hat{\psi}^\dagger_\mu|0\rangle$ to the ideal states $\hat{b}^\dagger_\mu|0\rangle$. This transformation will carry the subspace $\mathscr{H}_F\subset\mathscr{H}$ to the Fock-Tani subspace $\mathscr{H}_{FT}\subset\mathscr{H}$ in which all calculation with the transformed Hamiltonian should be done. This transformation, schematically indicated in Fig. 1, is defined via the unitary operator

$$\hat{U}=\exp\left[\frac{\pi}{2}\sum_\mu(\hat{\psi}^\dagger_\mu\hat{b}_\mu-\hat{b}^\dagger_\mu\hat{\psi}_\mu)\right] . \tag{2.8}$$

The transform $\hat{U}^{-1}\hat{O}\,\hat{U}$ of any operator is evaluated using the Campbell-Hausdorff formula. It is easily verified that the transformed Hamiltonian (Fock-Tani Hamiltonian) is given by

$$\begin{aligned}\mathscr{H}_{FT}&\equiv\hat{U}^{-1}\mathscr{H}_F\hat{U}\\ &=\sum_\mu\epsilon_\mu\hat{b}^\dagger_\mu\hat{b}_\mu+\int d\mathbf{r}\,\hat{a}^\dagger(\mathbf{r})[T((\mathbf{r})+V(\mathbf{r})]\hat{a}(\mathbf{r})\\ &\quad-\sum_\mu\epsilon_\mu\int d\mathbf{r}\,d\mathbf{r}'\,\hat{a}^\dagger(\mathbf{r})\psi_\mu(\mathbf{r})\psi^*_\mu(\mathbf{r}')\hat{a}(\mathbf{r}') ,\end{aligned} \tag{2.9}$$

and that

$$\hat{U}^{-1}\hat{b}_\mu\hat{U}=-\hat{\psi}_\mu \tag{2.10a}$$

and

$$\hat{U}^{-1}\hat{\psi}_\mu\hat{U}=\hat{b}_\mu . \tag{2.10b}$$

From (2.10) it is clear that the role of $\hat{b}_\mu$ and $\hat{\psi}_\mu$ is interchanged. In fact, a weaker condition [which holds in the general case of scattering from targets with internal structure even when (2.10) does not]

$$\hat{\psi}^\dagger_\mu|0\rangle\to\hat{b}^\dagger_\mu|0\rangle ,$$

i.e., a real state $\hat{\psi}^\dagger_\mu|0\rangle$ is transformed into an ideal state

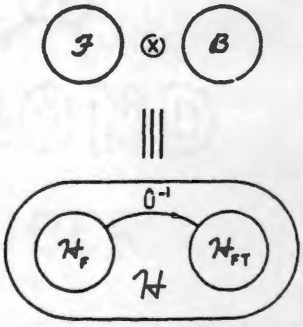

FIG. 1. Schematic connection between various Hilbert spaces defined in the text. Fock-Tani transformation is effected by the operator $\hat{U}^{-1}$ which carries $\mathscr{H}_F$ into $\mathscr{H}_{FT}$.

$\hat{b}_\mu^\dagger|0\rangle$, is sufficient proof that the transformation gives physical meaning to the ideal states.

The subsidiary condition (2.7) transforms to

$$\sum_\mu \hat{\psi}_\mu^\dagger \hat{\psi}_\mu |\chi\rangle = 0 \text{ iff } |\chi\rangle \in \mathscr{H}_{\mathrm{FT}} . \tag{2.11}$$

Equation (2.9) may be viewed as a formal expression of the following operator identity:

$$\hat{H} \equiv \sum_\mu \epsilon_\mu P_\mu + (1-P)\hat{H}(1-P) , \tag{2.12}$$

where the projection operator $P_\mu = |\mu\rangle\langle\mu|$ and $P = \sum_\mu P_\mu$.

In Eq. (2.12) [as well as (2.9)] the Hamiltonian is divided into a bound-state part (first term) and a scattering part (remaining terms) with the understanding that in considering $(1-P)\hat{H}(1-P)$ one ignores the states $|\mu\rangle$ which formally are its eigenfunctions of zero energy. The subsidiary condition (2.11) appears because the Fock space $\mathscr{F}$ was initially expanded to accommodate ideal-state operators $\hat{b}_\mu$, $\hat{b}_\mu^\dagger$, etc., and merely serves to restrict us to the appropriate subspace of the enlarged space $\mathscr{H}$. There is no analogous condition when considering (2.12).

In the case of realistic scattering or reaction problems where the bound states are composites (atoms, molecules, etc.), the one-particle Fock-Tani representation outlined above can be straightforwardly generalized[11] and leads naturally to a separation of the Hamiltonian into portions representing physically distinct processes (elastic scattering, inelastic scattering, various rearrangement processes). Such a second-quantization representation also has other advantages over separation based on projection operators, in that powerful field-theoretic techniques previously found useful in electron scattering from atoms[12] now become applicable to reactive scattering. A review of the field-theoretic formulation of three-particle reactive scattering in terms of the Fock-Tani representation has been given recently by Ficocelli Varracchio.[13]

Normally, imposition of the subsidiary condition (2.11) would make the solution of any practical problem difficult and we would have merely traded the difficulty inherent in the noncanonical commutation relations of the real-state operators $\hat{\psi}_\mu$, $\hat{\psi}_\mu^\dagger$, etc. [see Eq. (2.4)], for something equally difficult. However, an enormous simplification which makes the rigmarole of the Fock-Tani transformation worthwhile occurs if we consider scattering from a time-dependent point of view. At $t \to -\infty$ we construct a wave packet infinitely far away from the scattering center. It is orthogonal to all bound states by virtue of their finite spatial range, and the subsidiary condition (2.11) is satisfied in the limit $t \to -\infty$. Now, since $\sum_\mu \hat{\psi}_\mu^\dagger \hat{\psi}_\mu$ commutes with the Hamiltonian $\mathscr{H}_{\mathrm{FT}}$ (this is easily seen for the corresponding operators $\sum_\mu \hat{b}_\mu^\dagger \hat{b}_\mu$ and $\hat{H}_F$ *before* the transformation), Eq. (2.11) is satisfied at all times and may be ignored altogether. This essential simplification is then justified for the time-independent view of scattering in the usual manner.

The Hamiltonian in (2.9) can be divided as usual into an unperturbed part $\hat{H}_0$ [one possibility is $\hat{H}_0 = \sum_\mu \epsilon_\mu \hat{b}_\mu^\dagger \hat{b}_\mu + \int d\mathbf{r}\, \hat{a}^\dagger(\mathbf{r}) T(\mathbf{r}) \hat{a}(\mathbf{r})$] and a perturbation $\hat{V}$ and the full scattering function $|\chi^{(\pm)}\rangle$ may be expanded in powers of $\hat{V}$. Since a truncated expansion $|\chi_{\mathrm{app}}^{(\pm)}\rangle$ is defined in terms of the creation operator $\hat{a}^\dagger(\mathbf{r})$ only, it is orthogonal to all bound states $\{\hat{b}_\mu^\dagger|0\rangle, \mu = 1,2,\ldots\}$. This is quite unlike the perturbation expansion in the Fock space where an *approximate* scattering function is *not* orthogonal to the bound states and this lack of orthogonality introduces an error in the scattering amplitude which is tolerably small at sufficiently high energies only. Forcing appropriate orthogonality on the *approximate* scattering states $|\chi_{\mathrm{app}}^{(\pm)}\rangle$ leads to orthogonality corrections to the Fock-space scattering amplitude—mathematically these arise from the last term in (2.9)—which serve to extend the range of validity of the perturbation approximation to lower energies. In fact, our approach can be regarded as a generalization of Weinberg's "quasiparticle method"[14] to which it is closely related both in concept and in the form of orthogonalization corrections. Weinberg showed, within the context of one-particle scattering from a potential supporting bound states, that such orthogonalization greatly improves the convergence of the Born expansion. We expect a similar benefit in the case of the composite-particle generalization employed here.

An important proviso must be added to the remarks of previous paragraphs. We are justified in ignoring the subsidiary condition (2.11) only as long as we calculate the *exact* scattering state $|\chi^{(\pm)}\rangle$. The approximate state $|\chi_{\mathrm{app}}^{(\pm)}\rangle$ does not lie entirely in the Fock-Tani subspace $\mathscr{H}_{\mathrm{FT}}$ but contains an admixture of states outside $\mathscr{H}_{\mathrm{FT}}$. Thus, truncation of the perturbation expansion for $|\chi^{(\pm)}\rangle$ in the Fock-Tani space introduces an error in the scattering amplitude analogous to the error in the truncated Fock-space amplitude. It is not possible to make any definite general statement about the relative magnitudes of these errors. However, such numerical evidence as is already available[2] indicates that this representation can yield rather accurate results for rearrangement processes even in first order. We take this as adequate justification for use of this approach herein. Additional *a posteriori* evidence is supplied by the accuracy of our calculated cross sections.

III. FOCK-TANI TRANSFORMATION FOR REARRANGEMENT COLLISIONS:
1 + (23)→(12) + 3

A similar transformation was previously considered by Girardeau[15] for scattering of positrons from hydrogen atoms. In that case the transformation was somewhat simplified because the nuclear coordinate was frozen by virtue of the (supposedly) infinite mass of the nucleus. In the more general case of charge transfer, one may still eliminate a coordinate from consideration; the center-of-mass coordinate is the most convenient choice. We therefore introduce elementary annihilation and creation operators $\{\hat{a}_i(\mathbf{r}_i), \hat{a}_i^\dagger(\mathbf{r}_i), i = 1,2,3\}$ for the particles 1, 2, and 3. These are assumed to be distinguishable so that we may require $\hat{a}_i(\mathbf{r}_i)$, $\hat{a}_j^\dagger(\mathbf{r}_j)$, etc. to satisfy boson commutation relations.

Assuming pairwise interaction, the Fock Hamiltonian is

$$\hat{H}_F=\sum_{i=1}^{3}\int d\mathbf{r}_i\hat{a}_i^{\dagger}(\mathbf{r}_i)T_i(\mathbf{r}_i)\hat{a}_i(\mathbf{r}_i)$$
$$+\sum_{i=1}^{3}\int d\mathbf{r}_i d\mathbf{r}_{i+1}\hat{a}_i^{\dagger}(\mathbf{r}_i)\hat{a}_{i+1}^{\dagger}(\mathbf{r}_{i+1})$$
$$\times V_{i,i+1}(\mathbf{r}_i,\mathbf{r}_{i+1})\hat{a}_{i+1}(\mathbf{r}_{i+1})\hat{a}_i(\mathbf{r}_i)\,, \qquad (3.1)$$

where the subscript 4 is to be regarded as 1.

The interactions V_{12} and V_{23} are assumed sufficiently strong to support a number of bound states. In analogy with Eq. (2.3) we introduce the following bound-state creation operators:

$$(\hat{\psi}_{\mu_\alpha}^{\alpha})^{\dagger}=(2\pi)^{-3/2}\int d\mathbf{r}_i d\mathbf{r}_j \psi_{\bar{\mu}_\alpha}^{\alpha}(\mathbf{r}_\alpha)$$
$$\times\exp(i\mathbf{k}_\alpha\cdot\mathbf{R}_\alpha)\hat{a}_i^{\dagger}(\mathbf{r}_i)\hat{a}_j^{\dagger}(\mathbf{r}_j)\,,$$
$$\alpha\equiv(ij)=(12)\text{ or }(23)\,. \qquad (3.2)$$

In our notation, the superscript $\alpha=(ij)$ labels the pair of particles, $\mathbf{r}_\alpha$ and $\mathbf{R}_\alpha$ are the relative and center-of-mass coordinates of the pair, and μ_α is a collective label for the internal state $\bar{\mu}_\alpha$ and the center-of-mass momentum $\mathbf{k}_\alpha$. Annihilation operators are defined by Hermitian conjugation of (3.2). The commutation relations of these operators are obtained from the commutation relations for the elementary operators $\hat{a}_i^{\dagger}(\mathbf{r}_i)$, $\hat{a}_j(\mathbf{r}_j)$, etc.

We next introduce "ideal-state" operators $\hat{b}_{\mu}^{\alpha}$ and $(\hat{b}_{\mu}^{\alpha})^{\dagger}$ for $\alpha=(12)$ and (23) and define the following unitary operators in analogy with Eq. (2.8):

$$\hat{U}^{\alpha}=\exp\left[\frac{\pi}{2}\sum_{\mu_\alpha}[(\hat{\psi}_{\mu_\alpha}^{\alpha})^{\dagger}\hat{b}_{\mu_\alpha}^{\alpha}-(\hat{b}_{\mu_\alpha}^{\alpha})^{\dagger}\hat{\psi}_{\mu_\alpha}^{\alpha}]\right]. \qquad (3.3)$$

The Fock-Tani transformation is now made by successive application of the transformations generated by $\hat{U}^{(12)}$ and $\hat{U}^{(23)}$, but unlike (2.9) there are now two possibilities. Alternative transformations,

$$\hat{H}_{\mathrm{FT1}}=(\hat{U}^{(23)})^{-1}(\hat{U}^{(12)})^{-1}\hat{H}_F\hat{U}^{(12)}\hat{U}^{(23)} \qquad (3.4a)$$

and

$$\hat{H}_{\mathrm{FT2}}=(\hat{U}^{(12)})^{-1}(\hat{U}^{(23)})^{-1}\hat{H}_F\hat{U}^{(23)}\hat{U}^{(12)}\,, \qquad (3.4b)$$

are not identical because $[\hat{U}^{(12)},\hat{U}^{(23)}]\neq0$. In this paper we work with (3.4a) because for the reaction under consideration, $1+(23)\rightarrow(12)+3$, the corresponding first-order amplitude is easily interpreted; it is a sum of the first-order Fock amplitude and an orthogonality correction, much as in the case of potential scattering. The zeroth-order wave functions for *all* possible initial and final states are now orthogonal, thus satisfying the same orthogonality relation as the *exact* scattering states. The first- and higher-order wave functions are, however, not exactly orthogonal due to the possibility of rearrangement, but exact orthogonality is restored at infinite order. We leave the investigation of the implication of this for future work when we shall extend our analysis to higher perturbative corrections. We note here only that the orthogonality obtaining in first order in our approach is a distinct improvement over approaches in which such orthogonality is violated.

The transformed Hamiltonian is rather lengthy to write and we have relegated the complete expression to Appendix A. Parts of the Hamiltonian relevant to this paper are the zeroth-order Hamiltonian

$$\hat{H}_0=\sum_{\alpha,\mu_\alpha}\epsilon_{\mu_\alpha}^{\alpha}(\hat{b}_{\mu_\alpha}^{\alpha})^{\dagger}\hat{b}_{\mu_\alpha}^{\alpha}+\sum_{i=1}^{3}\int d\mathbf{r}_i\hat{a}_i^{\dagger}(\mathbf{r}_i)T_i(\mathbf{r}_i)\hat{a}_i(\mathbf{r}_i) \qquad (3.5a)$$

and the rearrangement interaction

$$V_{\mathrm{rearr}}=\sum_{\mu_{\alpha_1},\mu_{\alpha_2}}\int d\mathbf{r}_3 d\mathbf{r}_1(\hat{b}_{\mu_{12}}^{(12)})^{\dagger}\hat{a}_3^{\dagger}(\mathbf{r}_3)\langle\mu_{12}\mathbf{r}_3|V|\mu_{23}\mathbf{r}_1\rangle$$
$$\times\hat{a}_1(\mathbf{r}_1)\hat{b}_{\mu_{12}}^{(12)}+\mathrm{H.c.}\,, \qquad (3.5b)$$

where the interaction $\langle\mu_{12}\mathbf{r}_3|V|\mu_{23}\mathbf{r}_1\rangle$ is given in (A5) and H.c. denotes Hermitian conjugation. The first-order approximation to the T matrix is then given by the matrix element of V_{rearr} between appropriate eigenstates of $\hat{H}_0$.

IV. FIRST-ORDER T-MATRIX ELEMENT FOR REARRANGEMENT

We will use three alternative sets of coordinates, shown in Fig. 2: (i) $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$, which are coordinates of the particles 1, 2, and 3, respectively, in a fixed coordinate system; (ii) $\mathbf{R}$ (center-of-mass coordinate), $\mathbf{r}_{3\alpha_1}$ [vector from particle 3 to the center of mass of (1,2)], and $\mathbf{r}_{12}$ [relative coordinate of (1,2)]; and (iii) $\mathbf{R}$, $\mathbf{r}_{\alpha_2 1}$ [vector from the center of mass of (2,3) to particle 1] and $\mathbf{r}_{23}$ [relative coordinate of (2,3)].

The initial and final-state wave functions

$$|\psi_i\rangle=(2\pi)^{-3/2}\int d\mathbf{r}_1'\exp(i\mathbf{k}_1\cdot\mathbf{r}_1')$$
$$\times\hat{a}_1^{\dagger}(\mathbf{r}_1')(\hat{b}_{\mu_{23}}^{(23)})^{\dagger}|0\rangle \qquad (4.1a)$$

and

$$|\psi_f\rangle=(2\pi)^{-3/2}\int d\mathbf{r}_3'\exp(i\mathbf{k}_3\cdot\mathbf{r}_3')$$
$$\times\hat{a}_3^{\dagger}(\mathbf{r}_3')(\hat{b}_{\nu_{12}}^{(12)})^{\dagger}|0\rangle \qquad (4.1b)$$

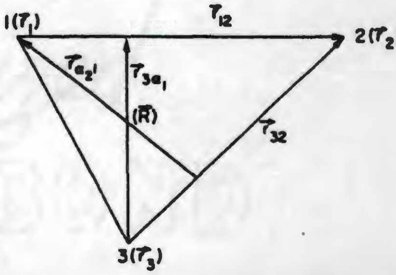

FIG. 2. Alternative coordinates for the three-particle system. The vector from the origin (not shown in the figure) to a specified point is indicated in parentheses beside the point in question. Thus, $\mathbf{r}_1$ is the vector from the origin to particle 1, etc.

are eigenfunctions of $\hat{H}_0$ and represent plane waves of $\bar{\alpha}$ impinging on bound states of α. We recall that the label μ_{α_1} includes the internal state $\bar{\mu}$ of the pair α_1 and its center-of-mass momentum $\mathbf{k}_\mu$.

The first-order T-matrix element is given quite simply by

$$T^{(1)}_{\nu_{12}\leftarrow\mu_{23}}=\langle\psi_f\,|\,V_{\text{rearr}}\,|\,\psi_i\rangle$$

$$=(2\pi)^{-3}\int d\mathbf{r}_3 d\mathbf{r}_1 e^{-i\mathbf{k}_3\cdot\mathbf{r}_3}$$

$$\times\langle\nu_{12}\mathbf{r}_3\,|\,V\,|\,\mu_{23}\mathbf{r}_1\rangle e^{i\mathbf{k}_1\cdot\mathbf{r}_1} \qquad (4.2)$$

and splits into a sum of two terms arising from the $[\delta(\mathbf{r}_1-\mathbf{r}_1')\delta(\mathbf{r}_2-\mathbf{r}_2')-\Delta^{12}(\mathbf{r}_1',\mathbf{r}_2';\mathbf{r}_1,\mathbf{r}_2)]$ factor in the definition of $\langle\mu_{12}\mathbf{r}_3\,|\,V\,|\,\mu_{23}\mathbf{r}_1\rangle$ [see Eq. (A5)]. It will emerge later that the first term gives the Jackson-Schiff-Bates Dalgarno (JSBD) approximation to the T matrix and the second term represents orthogonality corrections characteristic of the present formalism. Thus

$$T^{(1)}_{\nu_{12}\leftarrow\mu_{23}}=T^{\text{JSBD}}_{\nu_{12}\leftarrow\mu_{23}}+T^{\text{ortho}}_{\nu_{12}\leftarrow\mu_{23}}\,. \qquad (4.3)$$

In substituting (A5) into (4.2) we note that

$$\psi^{(12)}_{\nu_{12}}(\mathbf{r}_1,\mathbf{r}_2)=(2\pi)^{-3/2}\exp(i\mathbf{k}_\nu\cdot\mathbf{R}_{12})\psi^{(12)}_{\bar{\nu}}(\mathbf{r}_{12}) \qquad (4.4a)$$

and

$$\psi^{(23)}_{\mu_{23}}(\mathbf{r}_2,\mathbf{r}_3)=(2\pi)^{-3/2}\exp(i\mathbf{k}_\mu\cdot\mathbf{R}_{23})\psi^{(23)}_{\bar{\mu}}(\mathbf{r}_{23})\,. \qquad (4.4b)$$

In this equation $\mathbf{k}_\mu$ and $\mathbf{k}_\nu$ are the center-of-mass momenta of the pairs $\alpha_2=(23)$ and $\alpha_1=(12)$, respectively. As a first step in factoring the overall center-of-mass momentum, we replace the momenta $\mathbf{k}_1$ and $\mathbf{k}_\mu$ by $\mathbf{k}_i$ [relative momentum of particle 1 and pair (23)] and the overall center-of-mass momentum $\mathbf{K}_i$,

$$\mathbf{K}_i=\mathbf{k}_1+\mathbf{k}_\mu \qquad (4.5a)$$

and

$$\mathbf{k}_i=[(m_2+m_3)\mathbf{k}_1-m_1\mathbf{k}_\mu]/(m_1+m_2+m_3)\,, \qquad (4.5b)$$

where m_i denotes the mass of the ith particle. Similarly, the pair $(\mathbf{k}_3,\mathbf{k}_\nu)$ is replaced by $(\mathbf{k}_f,\mathbf{K}_f)$ with obvious physical significance.

The first term $T^{\text{JSBD}}_{\nu_{12}\leftarrow\mu_{23}}$, which is written as an integral over $\mathbf{r}_1$, $\mathbf{r}_2$, and $\mathbf{r}_3$, can be simplified by switching to $(\mathbf{R},\mathbf{r}_{3\alpha_1},\mathbf{r}_{12})$ coordinates. Integration over the center-of-mass coordinate $\mathbf{R}$ gives a factor $\delta(\mathbf{K}_i-\mathbf{K}_f)$ which expresses conservation of center-of-mass momentum.

The final result

$$\begin{aligned}T^{\text{JSBD}}_{\nu_{12}\leftarrow\mu_{23}}=&(2\pi)^{-3}\delta(\mathbf{K}_i-\mathbf{K}_f)\int d\mathbf{r}_{3\alpha_1}d\mathbf{r}_{12}\exp(-i\mathbf{k}_f\cdot\mathbf{r}_{3\alpha_1})\\&\times[\psi^{(12)}_{\bar{\nu}}(\mathbf{r}_{12})]^*\left[V_{13}\left[\mathbf{r}_{3\alpha_1}-\frac{m_2}{m_1+m_2}\mathbf{r}_{12}\right]+V_{23}\left[\mathbf{r}_{3\alpha_1}+\frac{m_1}{m_1+m_2}\mathbf{r}_{12}\right]\right]\\&\times\psi^{(23)}_{\bar{\mu}}\left[\mathbf{r}_{3\alpha_1}+\frac{m_1}{m_1+m_2}\mathbf{r}_{12}\right]\exp\left[i\mathbf{k}_i\cdot\left[\frac{m_3}{m_2+m_3}\mathbf{r}_{3\alpha_1}-\frac{m_2(m_1+m_2+m_3)}{(m_1+m_2)(m_2+m_3)}\mathbf{r}_{12}\right]\right]\end{aligned} \qquad (4.6)$$

is just the matrix element considered by Jackson and Schiff[6] and Bates and Dalgarno.[7] In Eq. (4.6) we have written coordinates $\mathbf{r}_{13}$, $\mathbf{r}_{23}$, and $\mathbf{r}_{\alpha_2 1}$ explicitly in terms of integration variables $\mathbf{r}_{3\alpha_1}$ and $\mathbf{r}_{12}$ by referring to Fig. 2.

From Eq. (4.2), the second term $T^{\text{ortho}}_{\nu_{12}\leftarrow\mu_{23}}$ is given as an integral over the coordinates $\mathbf{r}_1$, $\mathbf{r}_2$, $\mathbf{r}_3$, $\mathbf{r}_1'$, and $\mathbf{r}_2'$. The first step in its simplification is to replace $(\mathbf{r}_1,\mathbf{r}_2)$ by the relative and center-of-mass coordinates $(\mathbf{r}_{12},\mathbf{R}_{12})$ for the pair (12) and $(\mathbf{r}_1',\mathbf{r}_2')$ by $(\mathbf{r}_{12}',\mathbf{R}_{12}')$. The bound-state kernel,

$$\Delta^{(12)}(\mathbf{r}_1',\mathbf{r}_2';\mathbf{r}_1,\mathbf{r}_2)=\delta(\mathbf{R}_{12}'-\mathbf{R}_{12})\sum_\lambda\psi^{(12)}_\lambda(\mathbf{r}_{12}')[\psi^{(12)}_\lambda(\mathbf{r}_{12})]^*\,,$$

is then seen to contain a δ function and integration over $\mathbf{R}_{12}$ is immediate. We then revert to $(\mathbf{r}_1',\mathbf{r}_2')$ before introducing new coordinates $(\mathbf{R}',\mathbf{r}_{3\alpha_1}',\mathbf{r}_{12}')$ instead of $(\mathbf{r}_1',\mathbf{r}_2',\mathbf{r}_3)$ in analogy with $(\mathbf{R},\mathbf{r}_{3\alpha_1},\mathbf{r}_{12})$ in Fig. 2. Integration over $\mathbf{R}'$ then yields a δ function in initial and final center-of-mass momenta $\mathbf{K}_i$ and $\mathbf{K}_f$. The final form of the orthogonality correction is

$$\begin{aligned}T^{\text{ortho}}_{\nu_{12}\leftarrow\mu_{23}}=&-(2\pi)^{-3}\delta(\mathbf{K}_i-\mathbf{K}_f)\sum_\lambda\int d\mathbf{r}_{12}d\mathbf{r}_{3\alpha_1}'d\mathbf{r}_{12}'\exp(-i\mathbf{q}_1\cdot\mathbf{r}_{3\alpha_1}')[\psi^{(12)}_{\bar{\nu}}(\mathbf{r}_{12}')]^*\\&\times\left[V_{13}\left[\mathbf{r}_{3\alpha_1}'-\frac{m_2}{m_1+m_2}\mathbf{r}_{12}'\right]+V_{23}\left[\mathbf{r}_{3\alpha_1}'+\frac{m_1}{m_1+m_2}\mathbf{r}_{12}'\right]\right]\\&\times\psi^{(12)}_\lambda(\mathbf{r}_{12}')[\psi^{(12)}_\lambda(\mathbf{r}_{12})]^*\exp(-i\,m\,\mathbf{k}_i\cdot\mathbf{r}_{12})\psi^{(23)}_{\bar{\mu}}\left[\mathbf{r}_{3\alpha_1}'+\frac{m_1}{m_1+m_2}\mathbf{r}_{12}\right]\end{aligned} \qquad (4.7)$$

with

$$\mathbf{q}_1=\mathbf{k}_f-\frac{m_3}{m_2+m_3}\mathbf{k}_i \tag{4.8a}$$

and

$$\mathfrak{m}=\frac{m_2(m_1+m_2+m_3)}{(m_1+m_2)(m_2+m_3)}\ . \tag{4.8b}$$

In this expression λ ranges over all bound states of the pair (12) and all coordinates have been written in terms of integration variables with reference to Fig. 2.

The orthogonality correction can be interpreted in two alternative ways. It arises from a potential, say V_{nonre}, which must be subtracted from the overall potential to give the rearrangement part of the interaction, V_{rearr}. V_{nonre} consists of a sum of terms, each associated with a bound state of (12). The $\lambda=\bar{\nu}$ term, i.e., when the intermediate state is the same as the final bound state of the composite (12), is just the static interaction in the final channel. Remaining terms, arising from other intermediate states, give nonlocal contributions to V_{nonre}. Alternatively, $T^{\text{ortho}}_{\nu_{12}\leftarrow\mu_{23}}$ can be regarded as correcting for the lack of orthogonality between the initial state and *all* possible final states, the $\lambda=\bar{\nu}$ term corresponding to the particular final state in question.

In the special case of charge transfer, particles 1 and 3 are nuclei and particle 2 is an electron. Then $m_2 \ll m_1$, m_3 and $m_1 \sim m_3$. We note that it is a good approximation to neglect all terms of order m_e/m_p unless they are multiplied by a nuclear momentum k which may be large.

$T^{\text{JSBD}}_{\nu_{12}\leftarrow\mu_{23}}$ also consists of two terms. The second term

$$V_{23}\left[\mathbf{r}_{3\mathfrak{m}_1}+\frac{m_1}{m_1+m_2}\mathbf{r}_{12}\right]\ [=V_{23}(\mathbf{r}_{23})]$$

alone constitutes the Oppenheimer-Brinkman-Kramers (OBK) approximation.[3,4] The first term

$$V_{13}\left[\mathbf{r}_{3\mathfrak{m}_1}-\frac{m_2}{m_1+m_2}\mathbf{r}_{12}\right]=V_{13}(\mathbf{r}_{13})$$

represents internuclear interaction and it is very nearly canceled by the first term in (4.7). To see this, note that to a very good approximation we can replace

$$V_{13}\left[\mathbf{r}'_{3\mathfrak{m}_1}-\frac{m_2}{m_1+m_2}\mathbf{r}'_{12}\right]\longrightarrow V_{13}(\mathbf{r}'_{3\mathfrak{m}_1}) \tag{4.9}$$

in Eq. (4.7) and also make a corresponding approximation in (4.6). Integration over $\mathbf{r}'_{12}$ in the first term of (4.7) then gives $\delta_{\lambda\bar{\nu}}$ and only the $\lambda=\bar{\nu}$ term makes a nonzero contribution in the sum over λ. Substituting (4.8a) and (4.8b) for $\mathbf{q}_1$ and $\mathfrak{m}$, respectively, in the resulting expression, a simple rearrangement of terms and comparison with the first term in (4.6) shows that the two cancel. In making the approximation (4.9), we incur a small error of order $m_2/(m_1+m_2)\sim m_e/m_p$ so that the cancellation is not exact but nearly so. In light of the observation made by Wick (quoted in a footnote in Ref. 6) that the internuclear potential makes a negligible contribution of order m_e/m_p to the *exact* reaction amplitude, our result for the corresponding *first-order* amplitude is very satisfying. In subsequent analysis, we therefore completely disregard nuclear repulsion.

The role of internuclear potential in charge transfer has received much attention and it has been long known that one must correct for the lack of orthogonality between the initial and final states.[8] In a particularly relevant paper, Bassel and Gerjuoy[16] achieved this limited objective by subtracting the static interaction in the final channel from the total interaction in the post form of the transition matrix element. In light of our comments following Eq. (4.8), this is a special case of our result which we have obtained starting from a much more general objective of considering scattering in the presence of bound states.

V. EVALUATION OF THE T MATRIX

It follows from the discussion of Sec. IV that to a very good approximation the T-matrix element is given by

$$T_{\nu_{12}\leftarrow\mu_{23}}=T^{\text{OBK}}_{\nu_{12}\leftarrow\mu_{23}}+T^{\text{ortho}}_{\nu_{12}\leftarrow\mu_{23}}\ , \tag{5.1}$$

where

$$T^{\text{OBK}}_{\nu_{12}\leftarrow\mu_{23}}=(2\pi)^{-3}\int d\mathbf{r}_{3\mathfrak{m}_1}d\mathbf{r}_{12}\exp(-i\mathbf{q}_1\cdot\mathbf{r}_{3\mathfrak{m}_1})[\psi^{12}_{\bar{\nu}}(\mathbf{r}_{12})]^*$$
$$\times V_{23}\left[\mathbf{r}_{3\mathfrak{m}_1}+\frac{m_1}{m_1+m_2}\mathbf{r}_{12}\right]\psi^{23}_{\mu}\left[\mathbf{r}_{3\mathfrak{m}_1}+\frac{m_1}{m_1+m_2}\mathbf{r}_{12}\right]\exp(-i\,\mathfrak{m}\,\mathbf{k}_i\cdot\mathbf{r}_{12}) \tag{5.2a}$$

and

$$T^{\text{ortho}}_{\nu_{12}\leftarrow\mu_{23}}=-(2\pi)^{-3}\sum_{\lambda}\int d\mathbf{r}_{12}d\mathbf{r}'_{3\mathfrak{m}_1}d\mathbf{r}'_{12}\exp(-i\mathbf{q}_1\cdot\mathbf{r}_{3\mathfrak{m}_1})[\psi^{(12)}_{\bar{\nu}}(\mathbf{r}'_{12})]^*V_{23}\left[\mathbf{r}'_{3\mathfrak{m}_1}+\frac{m_1}{m_1+m_2}\mathbf{r}'_{12}\right]$$
$$\times\psi^{(12)}_{\lambda}(\mathbf{r}'_{12})[\psi^{(12)}_{\lambda}(\mathbf{r}_{12})]^*\exp(-i\,\mathfrak{m}\,\mathbf{k}_i\cdot\mathbf{r}_{12})\psi^{(23)}_{\mu}\left[\mathbf{r}'_{3\mathfrak{m}_1}+\frac{m_1}{m_1+m_2}\mathbf{r}_{12}\right]\ . \tag{5.2b}$$

Equations (5.2a) and (5.2b) for $T^{\text{OBK}}_{\nu_{12}\leftarrow\mu_{23}}$ and $T^{\text{ortho}}_{\nu_{12}\leftarrow\mu_{23}}$ are obtained from Eqs. (4.6) and (4.7) for $T^{\text{JSBD}}_{\nu_{12}\leftarrow\mu_{23}}$ and $T^{\text{ortho}}_{\nu_{12}\leftarrow\mu_{23}}$, respectively, by dropping the internuclear potential. We have also suppressed the δ function denoting conservation of overall center-of-mass momentum.

$T^{\mathrm{OBK}}_{\nu_{12}\to\mu_{23}}$ is easily evaluated by reverting to independent variables $\mathbf{r}_{12}$ and $\mathbf{r}_{32}$. We quote the final result from Appendix I of Jackson and Schiff[6] after transcribing it into our notation. It is first necessary to define another momentum-transfer vector

$$\mathbf{q}_2=\mathbf{k}_i-\frac{m_1}{m_1+m_2}\mathbf{k}_f \tag{5.3}$$

analogous to $\mathbf{q}_1$ defined by Eq. (4.8a). Then

$$T^{\mathrm{OBK}}_{\nu_{12}\to\mu_{23}}=-\left[\frac{m_1+m_2}{2m_1m_2}q_2^2+\epsilon_{\bar\nu}\right]\Phi_{\beta}(-\mathbf{q}_1)\Phi^*_{\bar\nu}(\mathbf{q}_2)\,, \tag{5.4}$$

where $\epsilon_{\bar\nu}$ is the binding energy of the pair (12) in the internal state $\bar\nu$ and $\Phi_{\beta}(-\mathbf{q}_1)$ and $\Phi_{\bar\nu}(\mathbf{q}_2)$ are momentum-space wave functions.

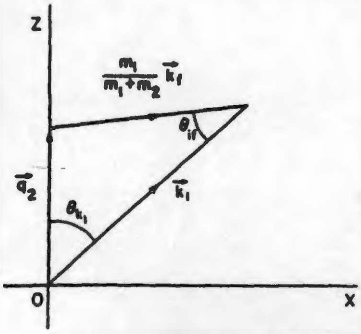

FIG. 3. Spatial arrangement of vectors $\mathbf{k}_i$, $\mathbf{k}_f$, and $\mathbf{q}_2$ for the evaluation of the integral in Eq. (5.6).

In order to evaluate the orthogonality correction, we first rewrite the coordinate-space wave functions $[\psi_\lambda^{e_1}(\mathbf{r}_{12})]^*$ and $\psi_\beta^{e_2}(\mathbf{r}'_{3m_1}+(m_1/m_1+m_2)\mathbf{r}_{12})$ as Fourier transforms of corresponding momentum-space wave functions $\Phi^*_\lambda(\mathbf{p})$ and $\Phi_\beta(\mathbf{p}_1)$ and also rewrite the Coulomb interaction as a Fourier transform,

$$\left|\mathbf{r}'_{3m_1}+\frac{m_1}{m_1+m_2}\mathbf{r}_{12}\right|^{-1}=\frac{1}{2\pi^2}\int d\mathbf{p}_2\frac{1}{p_2^2}\exp\left[-i\mathbf{p}_2\cdot\left[\mathbf{r}'_{3m_1}+\frac{m_1}{m_1+m_2}\mathbf{r}_{12}\right]\right]. \tag{5.5}$$

This introduces three new integration variables $\mathbf{p}$, $\mathbf{p}_1$, and $\mathbf{p}_2$, but integration over $\mathbf{r}_{3m_1}$ and $\mathbf{r}_{12}$ immediately gives a delta function each, $\delta(\mathbf{q}_1+\mathbf{p}_2-\mathbf{p}_1)$ and $\delta(\mathbf{p}-(m_1/m_1+m_2)\mathbf{p}_1+m\,\mathbf{k}_i)$. This allows us to integrate over $\mathbf{p}_1$ and $\mathbf{p}_2$. After some simple algebraic rearrangement to show that $m\,\mathbf{k}_i-(m_1/m_1+m_2)\mathbf{q}_1=\mathbf{q}_2$, the orthogonality correction is rewritten as

$$\begin{aligned}T^{\mathrm{ortho}}_{\nu_{12}\to\mu_{23}}=-\frac{Z_2Z_3}{2\pi^2}\frac{m_1+m_2}{m_1}\sum_\lambda\int d\mathbf{p}\,d\mathbf{r}'_{12}\frac{1}{|\mathbf{p}+\mathbf{q}_2|^2}\exp[-i(\mathbf{p}+\mathbf{q}_2)\cdot\mathbf{r}'_{12}]\\ \times[\psi_{\bar\nu}^{(12)}(\mathbf{r}'_{12})]^*\psi_\lambda^{(12)}(\mathbf{r}'_{12})\Phi^*_\lambda(\mathbf{p})\Phi_\beta\left[\frac{m_1+m_2}{m_1}(\mathbf{p}+m\,\mathbf{k}_i)\right].\end{aligned} \tag{5.6}$$

In the following discussion we assume without loss of generality that the vector $\mathbf{q}_2$ lies along the z axis and $\mathbf{k}_i$ and $\mathbf{k}_f$ lie in the x-z plane (Fig. 3). For specific final state $\bar\nu$ and intermediate state λ, the integral

$$I_{\bar\nu\lambda}(\mathbf{p}+\mathbf{q}_2)=\int d\mathbf{r}'_{12}\exp[-i(\mathbf{p}+\mathbf{q}_2)\cdot\mathbf{r}'_{12}][\psi_{\bar\nu}^{e_1}(\mathbf{r}'_{12})]^*\psi_\lambda^{e_1}(\mathbf{r}'_{12}) \tag{5.7}$$

which appears in (5.6) can be evaluated analytically. (Particular results for the $1s$ final state and $1s$, $2s$, and $2p$ intermediate states are given in Appendix B.) Moreover, for a spherically symmetric final state (i.e., $l_{\bar\nu}=0$), it factors into a spherical harmonic and a part depending on $|\mathbf{p}+\mathbf{q}_2|$ only:

$$I_{\bar\nu\lambda}(\mathbf{p}+\mathbf{q}_2)_{l_{\bar\nu}=0}=I_{\bar\nu\lambda}(|\mathbf{p}+\mathbf{q}_2|)_{l_{\bar\nu}=0}Y_{l_\lambda m_\lambda}(\Omega_{\mathbf{p}+\mathbf{q}_2})\,. \tag{5.8}$$

We can then sum over m_λ on the right-hand side of (5.6)—the sum over λ is really a triple sum over n_λ, l_λ, and m_λ—and use the addition theorem for spherical harmonics to obtain

$$\sum_{m_\lambda}Y^*_{l_\lambda m_\lambda}(\Omega_{\mathbf{p}})Y_{l_\lambda m_\lambda}(\Omega_{\mathbf{p}+\mathbf{q}_2})=\frac{2l_\lambda+1}{4\pi}P_{l_\lambda}\left[\frac{\mathbf{p}\cdot(\mathbf{p}+\mathbf{q}_2)}{p\,|\mathbf{p}+\mathbf{q}_2|}\right]. \tag{5.9}$$

Note that with the assumption that $\mathbf{q}_2$ lies along the z axis, the argument of the Legendre polynomial depends on p and θ_p but does not depend on the azimuthal angle ϕ_p.

The only ϕ_p dependence of the integrand in (5.6) comes from the initial-state wave function $\Phi_\beta((m_1+m_2/m_1)\times(\mathbf{p}+m\,\mathbf{k}_i))$. For a spherically symmetric state ($l_\beta=0$) it is contained in the $\mathbf{p}\cdot\mathbf{k}_i$ term in the argument; moreover, for the $1s$ initial state, integration over ϕ_p can be done analytically (see Appendix B).

These manipulations reduce the orthogonality correction to its final form which is used for numerical calculation:

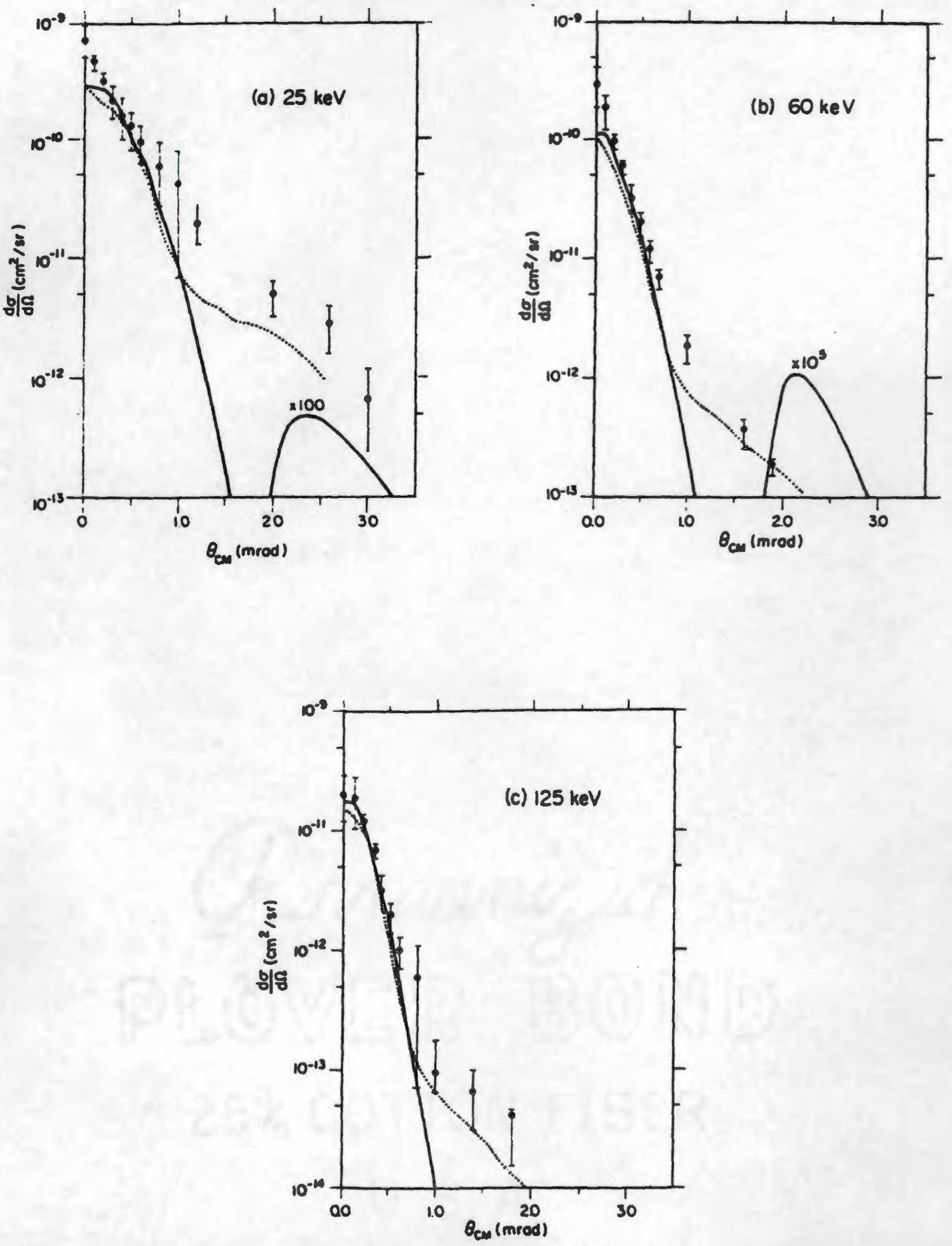

FIG. 4. Center-of-mass differential cross section for resonant charge transfer, $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p$, at (a) 25, (b) 60, and (c) 125 keV. The experimental points are from Martin *et al.* (Ref. 17), the dotted curve is from the two-state atomic expansion calculation quoted by Martin *et al.*, and the solid curve is the Fock-Tani result with orthogonality corrections due to $1s$, $2s$, and $2p$ intermediate states. Note that the experimental cross section is for capture into all bound states and it is expected to be 20% greater than the cross section for capture into the ground state. The secondary peak in (a) and (b) has been scaled up by the indicated factor.

$$T^{\text{ortho}}_{\nu_{1s}\to(1s)_{23}}=-\frac{Z_2Z_3}{\sqrt{2}\pi^3}\left[\frac{m_1}{m_1+m_2}\right]^3\sum_{n_\lambda,l_\lambda}(2l_\lambda+1)\int dp\,d\theta_p\,\sin\theta_p\frac{p^2}{|\mathbf{p}+\mathbf{q}_2|^2}R_{n_\lambda l_\lambda}(p)I_{\nu\lambda}(|\mathbf{p}+\mathbf{q}_2|)_{l_\nu=0}$$

$$\times P_{l_\lambda}\left[\frac{\mathbf{p}\cdot(\mathbf{p}+\mathbf{q}_2)}{p\,|\mathbf{p}+\mathbf{q}_2|}\right]\frac{A}{(A^2-B^2)^{3/2}}\quad\text{for } l_\nu=0\,. \tag{5.10}$$

VI. DIFFERENTIAL AND TOTAL CROSS SECTIONS

The integral appearing in Eq. (5.10) is evaluated easily and rapidly by two-dimensional numerical integration. When the electron mass is neglected in relation to the nuclear mass, this integral can be evaluated analytically for each value of n_λ and l_λ, the intermediate-state quantum numbers. We have done this for all states up to $n_\lambda=3$ as a check on the result of numerical integration.

In the numerical results that we quote, only the 1*s*, 2*s*, and 2*p* intermediate states have been retained in the sum in Eq. (5.10). This a very good approximation at all energies for which we present differential cross section (25, 60, ad 125 keV) in Fig. 4 but is somewhat suspect at the lower end of the energy scale ($E<10$ keV) of Fig. 5 where we present the total cross section. However, the error is estimated to be no more than 20%, and at these low energies, a first-order approximation is inadequate anyway.

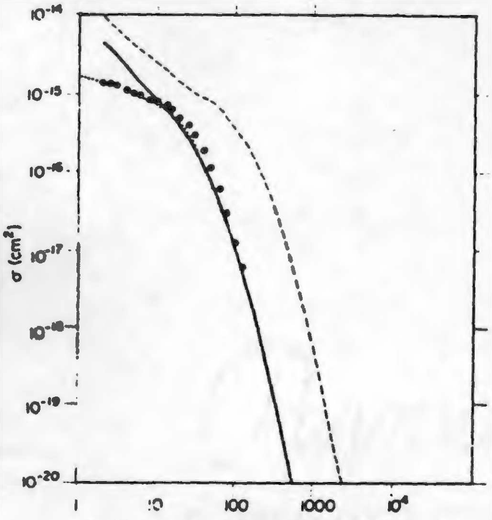

FIG. 5. Total cross section for resonant charge transfer, $p+\mathrm{H}(1s)\to\mathrm{H}(1s)+p$, as a function of laboratory collision energy. The experimental points are from McClure (Ref. 19), the dotted curve is from the two-state atomic expansion calculation of McCarroll (Ref. 20), and the solid curve is the Fock-Tani result with orthogonality corrections due to 1*s*, 2*s*, and 2*p* intermediate states. The experimental cross section in this case is also for capture into all bound states. The dashed curve gives the Fock-Tani cross section for $d+\mathrm{H}(1s)\to\mathrm{D}(1s)+p$.

We compare our calculated differential cross section with the experimental results (Martin *et al.*[17]) in Fig. 4 and also with the two-state atomic expansion (TSAE) results quoted by Martin *et al.* The TSAE approximation was picked out of a number of theoretical results because it seems to give the best fit to differential and total cross sections over a large range of angles and energies. It is satisfying to see that our calculation agrees very well with the TSAE and experimental results over angular range of 1 mrad about the forward direction and over a comparable range at 60 and 125 keV also. The discrepancy at larger angles is no doubt due to the neglect of higher-order corrections and we expect much of it to disappear upon the inclusion of second-order correction. In fact, even the minima in the first-order differential cross section at the energies we have considered are spurious.[18]

We also compare the Fock-Tani total cross section with the experimental results of McClure[19] and the TSAE calculation of McCarroll[20] in Fig. 5. Once again we find that our calculation agrees very well with both these results for $E>10$ keV; in fact, for $E>60$ keV, our results are identical with those of McCarroll. The discrepancy at low energies is to be expected of a first-order approximation. In the same figure, we also show the Fock-Tani total cross section for $d+\mathrm{H}(1s)\to\mathrm{D}(1s)+p$.

We close our discussion of the numerical results by remarking that the two-state atomic expansion was introduced by Bates[8] with the express purpose of correcting for the lack of orthogonality of the initial- and final-state wave functions. This, along with other orthogonality corrections, is contained in the Fock-Tani approximation, too. Close agreement between the results of these approximations is, then, just as it should be.

VII. SUMMARY AND CONCLUSION

In this paper we have developed a unitary transformation of the second-quantized Hamiltonian of a three-particle system which breaks the overall interaction into its component parts corresponding to permissible physical processes and have applied it to the problem of resonant charge transfer, $p+\mathrm{H}(1s)\to\mathrm{H}(1s)+p$. In this scheme, zeroth-order wave functions for initial and final states are mutually orthogonal, thus satisfying the same orthogonality relation as the *exact* scattering states. As a consequence of this, an orthogonality correction to the usual first-order reaction amplitude appears and the internuclear potential makes a negligible contribution of order

m_e/m_p to the T-matrix element. This result is consistent with the physical result that the internuclear potential cannot significantly affect the passage of a light, charged particle from one nucleus to another. We have computed differential and total cross sections over a range of angles and energies and compared our results with experiment and with the best available theoretical results based on a two-state atomic expansion. Except at angles larger than 1 mrad and energies less than 10 keV, we find very good agreement. The discrepancy is attributed to the omission of second- and higher-order perturbative effects. The agreement with TSAE results is a reflection of the fact that this method also corrects for the lack of orthogonality of the zeroth-order initial and final states in Fock representation. The agreement with experiment underlines the importance of proper orthogonality of approximate scattering states, a fact recognized long back by Bates.[8]

An obvious extension of the present work is to include second-order corrections and thus attempt to remove the remaining discrepancy between our results and the experiment. Such an extension is currently being investigated. We are also contemplating application of Fock-Tani formalism to other problems of atomic scattering, particularly ionization of the hydrogen atom by electron impact.

ACKNOWLEDGMENT

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APPENDIX A: FOCK-TANI TRANSFORMATION FOR THE THREE-PARTICLE SYSTEM

We have evaluated the Fock-Tani Hamiltonian (3.4a) by a diagrammatic technique.[21] The interaction is now broken up into various parts corresponding to the possible physical processes for this system:

$$
\begin{aligned}
\hat{H}_{\mathrm{FT1}} = {} & \sum_{\alpha,\mu_\alpha} \epsilon^{\alpha}_{\mu_\alpha} (\hat{b}^{\alpha}_{\mu_\alpha})^{\dagger} \hat{b}^{\alpha}_{\mu_\alpha} + \sum_{i} \int d\mathbf{r}_i\, \hat{a}^{\dagger}_{i}(\mathbf{r}_i) T_i(\mathbf{r}_i) \hat{a}_i(\mathbf{r}_i) \\
& + \sum_{\substack{i,j \\ (j>i)}} \int d\mathbf{r}_i\, d\mathbf{r}_j\, d\mathbf{r}'_i\, d\mathbf{r}'_j\, \hat{a}^{\dagger}_{i}(\mathbf{r}_i) \hat{a}^{\dagger}_{j}(\mathbf{r}_j) \langle \mathbf{r}_i \mathbf{r}_j | V | \mathbf{r}'_i \mathbf{r}'_j \rangle \hat{a}_j(\mathbf{r}'_j) \hat{a}_i(\mathbf{r}'_i) \\
& + \sum_{\alpha,\mu_\alpha,\nu_\alpha} \int d\mathbf{r}_{\bar\alpha}\, d\mathbf{r}'_{\bar\alpha} (\hat{b}^{\alpha}_{\mu_\alpha})^{\dagger} \hat{a}^{\dagger}_{\bar\alpha}(\mathbf{r}_{\bar\alpha}) \langle \mu_\alpha \mathbf{r}_{\bar\alpha} | V | \nu_\alpha \mathbf{r}'_{\bar\alpha} \rangle \hat{a}_{\bar\alpha}(\mathbf{r}'_{\bar\alpha}) \hat{b}^{\alpha}_{\nu_\alpha} \\
& + \left[\sum_{\alpha,\mu_\alpha} \int d\mathbf{r}_{\bar\alpha}\, d\mathbf{r}'_i\, d\mathbf{r}'_j\, d\mathbf{r}'_{\bar\alpha} (\hat{b}^{\alpha}_{\mu_\alpha})^{\dagger} \hat{a}^{\dagger}_{\bar\alpha}(\mathbf{r}_{\bar\alpha}) \langle \mu_\alpha \mathbf{r}_{\bar\alpha} | V | \mathbf{r}'_i \mathbf{r}'_j \mathbf{r}'_{\bar\alpha} \rangle \hat{a}_{\bar\alpha}(\mathbf{r}'_{\bar\alpha}) \hat{a}_j(\mathbf{r}'_j) \hat{a}_i(\mathbf{r}'_i) + \text{H.c.} \right] \\
& + \left[\sum_{\mu_{12},\mu_{23}} \int d\mathbf{r}_3\, d\mathbf{r}_1 (\hat{b}^{(12)}_{\mu_{12}})^{\dagger} \hat{a}^{\dagger}_{3}(\mathbf{r}_3) \langle \mu_{12} \mathbf{r}_3 | V | \mu_{23} \mathbf{r}_1 \rangle \hat{a}_1(\mathbf{r}_1) \hat{b}^{(23)}_{\mu_{23}} + \text{H.c.} \right] \\
& + \int \left[\prod_i d\mathbf{r}_i\, d\mathbf{r}'_i \right] \hat{a}^{\dagger}_{1}(\mathbf{r}_1) \hat{a}^{\dagger}_{2}(\mathbf{r}_2) \hat{a}^{\dagger}_{3}(\mathbf{r}_3) \langle \mathbf{r}_1 \mathbf{r}_2 \mathbf{r}_3 | V | \mathbf{r}'_1 \mathbf{r}'_2 \mathbf{r}'_3 \rangle \hat{a}_3(\mathbf{r}'_3) \hat{a}_2(\mathbf{r}'_2) \hat{a}_1(\mathbf{r}'_1) \,. \qquad \text{(A1)}
\end{aligned}
$$

In our notation $\alpha \equiv (ij)$ labels the pair (i,j) and $\bar{\alpha}$ labels the remaining particle. The sum over α ranges from $\alpha_1 = (12)$ to $\alpha_2 = (23)$ and correspondingly $\bar{\alpha}_1 = 3$ and $\bar{\alpha}_2 = 1$. Indices i and j, when summed, range from 1 to 3 but are otherwise defined by associated α. All interactions are written formally as brackets, $\langle \,|\,|\, \rangle$, and the symbol H.c. denotes Hermitian conjugation.

The first two terms in (A1) constitute the unperturbed Hamiltonian $\hat{H}_0$ for our calculation. The eigenstates of $\hat{H}_0$ include plane waves arising from the second term, impinging on bound states, arising from the first term. Explicit expressions for the interactions appearing in (A1) and their physical significance are as follows.

(a) *Two-particle scattering.* The interaction for two-particle scattering is given by

$$
\langle \mathbf{r}_i \mathbf{r}_j | V | \mathbf{r}'_i \mathbf{r}'_j \rangle = V_{ij}(\mathbf{r}_i, \mathbf{r}_j) \delta(\mathbf{r}_i - \mathbf{r}'_i) \delta(\mathbf{r}_j - \mathbf{r}'_j) - (1 - \delta_{ij,13}) \sum_{\mu_\alpha} \epsilon^{\alpha}_{\mu_\alpha} \Delta^{\alpha}_{\mu_\alpha}(\mathbf{r}_i, \mathbf{r}_j; \mathbf{r}'_i, \mathbf{r}'_j) \,. \qquad \text{(A2)}
$$

The second term in (A2) expresses the subtraction of the bound-state part of the interaction from the total interaction to give the remaining "scattering" interaction. (In this equation $\Delta^{\alpha}_{\mu_\alpha}(\mathbf{r}_i, \mathbf{r}_j; \mathbf{r}'_i, \mathbf{r}'_j) = \psi^{\alpha}_{\mu_\alpha}(\mathbf{r}_i, \mathbf{r}_j) [\psi^{\alpha}_{\mu_\alpha}(\mathbf{r}'_i, \mathbf{r}'_j)]^*$.) Note that it is zero for the pair (13) which is assumed not to form a bound state.

(b) *Nonreactive scattering of $\bar{\alpha}$ from the bound states of α.* Due to the $(\alpha_1 \rightleftarrows \alpha_2)$ asymmetry of the transformation in (3.4a), this interaction is not symmetric for the two arrangement channels:

$$
\langle \mu_{12} \mathbf{r}_3 | V | \nu_{12} \mathbf{r}'_3 \rangle = \int d\mathbf{r}_1\, d\mathbf{r}_2 [\psi^{(12)}_{\mu_{12}}(\mathbf{r}_1, \mathbf{r}_2)]^* [V_{13}(\mathbf{r}_1, \mathbf{r}_3) + V_{23}(\mathbf{r}_2, \mathbf{r}_3)] \psi_{\nu_{12}}(\mathbf{r}_1, \mathbf{r}_2) \delta(\mathbf{r}_3 - \mathbf{r}'_3) \qquad \text{(A3a)}
$$

and

$$
\begin{aligned}
\langle \mu_{23}\mathbf{r}_1|V|\nu_{23}\mathbf{r}_1'\rangle = &\int d\mathbf{r}_2 d\mathbf{r}_3[\psi^{(23)}_{\mu_{23}}(\mathbf{r}_2,\mathbf{r}_3)]^*[V_{12}(\mathbf{r}_1,\mathbf{r}_2)+V_{13}(\mathbf{r}_1,\mathbf{r}_3)]\psi^{(23)}_{\nu_{23}}(\mathbf{r}_2,\mathbf{r}_3)\delta(\mathbf{r}_1-\mathbf{r}_1')\\
&-\sum_{\lambda_{12}}\int d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_2'[\psi^{(23)}_{\mu_{23}}(\mathbf{r}_2,\mathbf{r}_3)]^*[V_{13}(\mathbf{r}_1,\mathbf{r}_3)+V_{13}(\mathbf{r}_1',\mathbf{r}_3)+V_{23}(\mathbf{r}_2,\mathbf{r}_3)+V_{23}(\mathbf{r}_2',\mathbf{r}_3)+\epsilon^{(12)}_{\lambda_{12}}]\\
&\qquad\times\Delta^{(12)}_{\lambda_{12}}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2')\psi^{(23)}_{\nu_{23}}(\mathbf{r}_2',\mathbf{r}_3)\\
&+\int d\mathbf{r}_2 d\mathbf{r}_3 d\mathbf{r}_2' d\mathbf{r}_1'' d\mathbf{r}_2''[\psi^{(23)}_{\mu_{23}}(\mathbf{r}_2,\mathbf{r}_3)]^*\Delta^{(12)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1'',\mathbf{r}_2'')\\
&\qquad\times[V_{13}(\mathbf{r}_1'',\mathbf{r}_3)+V_{23}(\mathbf{r}_2'',\mathbf{r}_3)]\Delta^{(12)}(\mathbf{r}_1'',\mathbf{r}_2'';\mathbf{r}_1',\mathbf{r}_2')\psi^{(23)}_{\mu_{23}}(\mathbf{r}_2',\mathbf{r}_3)\,.
\end{aligned}\tag{A3b}
$$

(c) *Formation and breakup of bound states.* In this case also the interaction is different for pairs (12) and (23):

$$
\begin{aligned}
\langle \mu_{12}\mathbf{r}_3|V|\mathbf{r}_1'\mathbf{r}_2'\mathbf{r}_3'\rangle = &\int d\mathbf{r}_1 d\mathbf{r}_2[\psi^{(12)}_{\mu_{12}}(\mathbf{r}_1,\mathbf{r}_2)]^*[V_{13}(\mathbf{r}_1,\mathbf{r}_3)+V_{23}(\mathbf{r}_2,\mathbf{r}_3)]\\
&\qquad\times[\delta(\mathbf{r}_1-\mathbf{r}_1')\delta(\mathbf{r}_2-\mathbf{r}_2')-\Delta^{(12)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2')]\delta(\mathbf{r}_3-\mathbf{r}_3')\\
&+\int d\mathbf{r}_2 d\mathbf{r}_1'' d\mathbf{r}_2''[\psi^{(12)}_{\mu_{12}}(\mathbf{r}_1'',\mathbf{r}_2'')]^*[V_{13}(\mathbf{r}_1'',\mathbf{r}_3)+V_{23}(\mathbf{r}_2'',\mathbf{r}_3)]\\
&\qquad\times[\Delta^{(12)}(\mathbf{r}_1'',\mathbf{r}_2'';\mathbf{r}_1',\mathbf{r}_2)-\delta(\mathbf{r}_1'-\mathbf{r}_1'')\delta(\mathbf{r}_2'-\mathbf{r}_2'')]\Delta^{(23)}(\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_2',\mathbf{r}_3')
\end{aligned}\tag{A4a}
$$

and

$$
\begin{aligned}
\langle \mu_{23}\mathbf{r}_1|V|\mathbf{r}_2'\mathbf{r}_3'\mathbf{r}_1'\rangle = &\int d\mathbf{r}_2 d\mathbf{r}_3[\psi^{(23)}_{\mu_{23}}(\mathbf{r}_2,\mathbf{r}_3)]^*[V_{12}(\mathbf{r}_1,\mathbf{r}_2)+V_{13}(\mathbf{r}_1,\mathbf{r}_3)]\\
&\qquad\times[\delta(\mathbf{r}_2-\mathbf{r}_2')\delta(\mathbf{r}_3-\mathbf{r}_3')-\Delta^{(23)}(\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_2',\mathbf{r}_3')]\delta(\mathbf{r}_1-\mathbf{r}_1')\\
&-\sum_{\nu_{12}}\int d\mathbf{r}_2[\psi^{(23)}_{\mu_{23}}(\mathbf{r}_2,\mathbf{r}_3')]^*[V_{13}(\mathbf{r}_1,\mathbf{r}_3')+V_{23}(\mathbf{r}_2,\mathbf{r}_3')+V_{13}(\mathbf{r}_1',\mathbf{r}_3')+V_{23}(\mathbf{r}_2',\mathbf{r}_3')+\epsilon^{(12)}_{\nu_{12}}]\Delta^{(12)}_{\nu_{12}}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2')\\
&+\int d\mathbf{r}_2 d\mathbf{r}_1'' d\mathbf{r}_2''[\psi^{(23)}_{\mu_{23}}(\mathbf{r}_2,\mathbf{r}_3')]^*\Delta^{(12)}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1'',\mathbf{r}_2'')[V_{13}(\mathbf{r}_1'',\mathbf{r}_3')+V_{23}(\mathbf{r}_2'',\mathbf{r}_3')]\Delta^{(12)}(\mathbf{r}_1'',\mathbf{r}_2'';\mathbf{r}_1',\mathbf{r}_2')\,.
\end{aligned}\tag{A4b}
$$

(d) *Rearrangement interaction.* The interaction for breakup of (23) and formation of (12) is given by

$$
\begin{aligned}
\langle \mu_{12}\mathbf{r}_3|V|\mu_{23}\mathbf{r}_1\rangle = &\int d\mathbf{r}_2 d\mathbf{r}_1' d\mathbf{r}_2'[\psi^{(12)}_{\mu_{12}}(\mathbf{r}_1',\mathbf{r}_2')]^*[V_{13}(\mathbf{r}_1',\mathbf{r}_3')+V_{23}(\mathbf{r}_2',\mathbf{r}_3')]\\
&\qquad\times[\delta(\mathbf{r}_1-\mathbf{r}_1')\delta(\mathbf{r}_2-\mathbf{r}_2')-\Delta^{(12)}(\mathbf{r}_1',\mathbf{r}_2';\mathbf{r}_1,\mathbf{r}_2)]\psi^{(23)}_{\mu_{23}}(\mathbf{r}_2,\mathbf{r}_3)\,.
\end{aligned}\tag{A5}
$$

The interaction for the reverse process is obtained by complex conjugation.

(e) *Three-particle scattering.* The interaction for three-particle scattering is given by

$$
\begin{aligned}
\langle \mathbf{r}_1\mathbf{r}_2\mathbf{r}_3|V|\mathbf{r}_1'\mathbf{r}_2'\mathbf{r}_3'\rangle = &-\sum_{\alpha}\Delta^{\alpha}(\mathbf{r}_i,\mathbf{r}_j;\mathbf{r}_i',\mathbf{r}_j')[V_{i\alpha}(\mathbf{r}_i,\mathbf{r}_\alpha)+V_{j\alpha}(\mathbf{r}_j,\mathbf{r}_\alpha)+V_{i\alpha}(\mathbf{r}_i',\mathbf{r}_\alpha')+V_{j\alpha}(\mathbf{r}_j',\mathbf{r}_\alpha')]\delta(\mathbf{r}_\alpha-\mathbf{r}_\alpha')\\
&+\sum_{\alpha}\int d\mathbf{r}_i'' d\mathbf{r}_j''\Delta^{\alpha}(\mathbf{r}_i,\mathbf{r}_j;\mathbf{r}_i'',\mathbf{r}_j'')[V_{i\alpha}(\mathbf{r}_i'',\mathbf{r}_\alpha)+V_{j\alpha}(\mathbf{r}_j'',\mathbf{r}_\alpha)]\Delta^{\alpha}(\mathbf{r}_i'',\mathbf{r}_j'';\mathbf{r}_i',\mathbf{r}_j')\delta(\mathbf{r}_\alpha-\mathbf{r}_\alpha')\\
&+\sum_{\mu_{12}}\int d\mathbf{r}_2'' d\mathbf{r}_3''[V_{13}(\mathbf{r}_1,\mathbf{r}_3'')+V_{23}(\mathbf{r}_2'',\mathbf{r}_3'')+V_{13}(\mathbf{r}_1',\mathbf{r}_3'')+V_{23}(\mathbf{r}_2',\mathbf{r}_3'')+\epsilon^{(12)}_{\mu_{12}}]\\
&\qquad\times[\delta(\mathbf{r}_3-\mathbf{r}_3'')\Delta^{(12)}_{\mu_{12}}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2'')\Delta^{\alpha_2}(\mathbf{r}_2'',\mathbf{r}_3'';\mathbf{r}_2',\mathbf{r}_3')+\delta(\mathbf{r}_3'-\mathbf{r}_3'')\Delta^{\alpha_2}(\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_2'',\mathbf{r}_3'')\Delta^{(12)}_{\mu_{12}}(\mathbf{r}_1,\mathbf{r}_2'';\mathbf{r}_1',\mathbf{r}_2')]\\
&-\int d\mathbf{r}_2'' d\mathbf{r}_1''' d\mathbf{r}_2'''\Delta^{\alpha_1}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1'''\mathbf{r}_2''')[V_{13}(\mathbf{r}_1''',\mathbf{r}_3)+V_{23}(\mathbf{r}_2''',\mathbf{r}_3)]\Delta^{\alpha_1}(\mathbf{r}_1''',\mathbf{r}_2''';\mathbf{r}_1',\mathbf{r}_2'')\Delta^{\alpha_2}(\mathbf{r}_2'',\mathbf{r}_3;\mathbf{r}_2',\mathbf{r}_3')\\
&-\int d\mathbf{r}_2'' d\mathbf{r}_1''' d\mathbf{r}_2'''\Delta^{\alpha_2}(\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_2'',\mathbf{r}_3')\Delta^{\alpha_1}(\mathbf{r}_1,\mathbf{r}_2'';\mathbf{r}_1''',\mathbf{r}_2''')[V_{13}(\mathbf{r}_1''',\mathbf{r}_3')+V_{23}(\mathbf{r}_2''',\mathbf{r}_3')]\Delta^{\alpha_1}(\mathbf{r}_1''',\mathbf{r}_2''';\mathbf{r}_1',\mathbf{r}_2')\\
&-\sum_{\mu_{12}}\int d\mathbf{r}_2'' d\mathbf{r}_3'' d\mathbf{r}_2'''\Delta^{\alpha_2}(\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_2'',\mathbf{r}_3'')\\
&\qquad\times[V_{13}(\mathbf{r}_1,\mathbf{r}_3'')+V_{23}(\mathbf{r}_2,\mathbf{r}_3'')+V_{13}(\mathbf{r}_1',\mathbf{r}_3'')+V_{23}(\mathbf{r}_2''',\mathbf{r}_3'')+\epsilon^{(12)}_{\mu_{12}}]
\end{aligned}
$$

$$\times \Delta^{(12)}_{\mu_{12}}(\mathbf{r}_1,\mathbf{r}_2;\mathbf{r}_1',\mathbf{r}_2''')\Delta^{\alpha_2}(\mathbf{r}_2''',\mathbf{r}_3'';\mathbf{r}_2',\mathbf{r}_3')$$

$$+\int d\mathbf{r}_2''d\mathbf{r}_3''d\mathbf{r}_1''d\mathbf{r}_2'''d\mathbf{r}_2''''\Delta^{\alpha_2}(\mathbf{r}_2,\mathbf{r}_3;\mathbf{r}_2'',\mathbf{r}_3'')\Delta^{\alpha_1}(\mathbf{r}_1,\mathbf{r}_2'';\mathbf{r}_1''',\mathbf{r}_2''')$$

$$\times[V_{13}(\mathbf{r}_1''',\mathbf{r}_3'')+V_{23}(\mathbf{r}_2'''',\mathbf{r}_3'')]\Delta^{\alpha_2}(\mathbf{r}_2'''',\mathbf{r}_3'';\mathbf{r}_2',\mathbf{r}_3')\ . \qquad \text{(A6)}$$

APPENDIX B: ASSORTED ANALYTICAL INTEGRALS IN THE EVALUATION OF THE ORTHOGONALITY CORRECTION

For specific final and intermediate states, the integral in (5.7) is evaluated by a spherical harmonic expansion of the plane wave. The result for the $1s$ final state and the $1s$, $2s$, and $2p$ intermediate states is as follows:

$$I_{1s,1s}(\mathbf{p}+\mathbf{q}_2)=\frac{32\sqrt{\pi}}{(4+|\mathbf{p}+\mathbf{q}_2|^2)^2}Y_{00}(\Omega_{\mathbf{p}+\mathbf{q}_2})\ , \qquad \text{(B1a)}$$

$$I_{1s,2s}(\mathbf{p}+\mathbf{q}_2)=\frac{512\sqrt{2\pi}\,|\mathbf{p}+\mathbf{q}_2|^2}{(q+4|\mathbf{p}+\mathbf{q}_2|^2)^3}Y_{00}(\Omega_{\mathbf{p}+\mathbf{q}_2}) \qquad \text{(B1b)}$$

and

$$I_{1s,2pm}(\mathbf{p}+\mathbf{q}_2)=-i\frac{256\sqrt{6\pi}\,|\mathbf{p}+\mathbf{q}_2|}{(9+4|\mathbf{p}+\mathbf{q}_2|^2)^3}Y_{1m}(\Omega_{\mathbf{p}+\mathbf{q}_2})\ . \qquad \text{(B1c)}$$

In Eq. (5.6) the integral of the initial-state wave function over the coordinate ϕ_p, for the $1s$ initial state ($\beta=1s$), is explicitly written as

$$I\equiv\int_0^{2\pi}d\phi_p\Phi_\beta\left[\frac{m_1+m_2}{m_1}(\mathbf{p}+m\,\mathbf{k}_i)\right]$$

$$=\frac{2\sqrt{2}}{\pi}\left[\frac{m_1}{m_1+m_2}\right]^4$$

$$\times\int_0^{2\pi}d\phi_p\left[\left[\frac{m_1}{m_1+m_2}\right]^2+p^2+2\,m\,\mathbf{p}\cdot\mathbf{k}_i+m^2k_i^2\right]^{-2}. \qquad \text{(B2)}$$

The only ϕ_p dependence of the integrand comes from the $\mathbf{p}\cdot\mathbf{k}_i$ term which is expanded in terms of trigonometric functions of angles ϕ_p, θ_p, and θ_{k_i} with reference to Fig. 3. Noting that the integrand is of the form $(A+B\cos\phi_p)^{-2}$, where

$$A=\left[\frac{m_1}{m_1+m_2}\right]^2+p^2+2\,m\,pk_i\cos\theta_p\cos\theta_{k_i}+m^2k_i^2 \qquad \text{(B3a)}$$

and

$$B=2\,m\,pk_i\sin\theta_p\sin\theta_{k_i}\ , \qquad \text{(B3b)}$$

the integral is evaluated analytically[22] to give

$$I=4\sqrt{2}\left[\frac{m_1}{m_1+m_2}\right]^4\frac{A}{(A^2-B^2)^{3/2}}\ . \qquad \text{(B4)}$$

The angle θ_{k_i} in Eq. (B3) is related to the scattering angle θ_{if} once again with reference to Fig. 3.

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APPENDIX B

THE PROGRAMS

The total cross section main program is on page 193.

```
C        THIS PROGRAM CALCULATES THE DIFFERENTIAL CROSS SECTION FOR CHARGE
C        TRANSFER IN BORN APPROXIMATION BASED ON THE FOCK-TANI HAMILTONIAN
C        FOR THE GENERAL CASE P+(TE)->(PE)+T, WHERE P, E, AND T ARE BARE
C        CHARGES OF MASS PMASS, EMASS, AND TMASS AND "(..)" IS AN ATOM.
C
C        ORTHOGONALIZATION TERMS THROUGH 3D ARE INCLUDED

C        ALL FOURIER TRANSFORMS CONTAIN A GENERAL BOHR RADIUS
C
C        THE J.D. JACKSON AND H. SCHIFF (PHYS. REV. 89,359 (1953) TERM
C        IS CALCULATED BY THEIR EQ. II.3, BUT WITH C**2 IN THE RELATION
C        FOR DEL REPLACED BY 1/AOI**2 - 1/AOF**2 +C**2 TO PROPERLY
C        ACCOUNT FOR THE BOHR RADII IN II.1. THE RESULT IS IDENTICAL TO
C        THAT GIVEN IN
C        H.S.W. MASSEY AND C.B.O. MOHR, PROC. PHYS. SOC. A67, 695(1954)
C        ONLY WITH THE POSITION VECTOR OF THE INCIDENT PARTICLE
C        IN THE INITIAL MOMENTUM EIGENSTATE RELATIVE TO THE ATOMIC
C        C.M RATHER THAN THE NUCLEUS.
C
C        16 POINT GAUSSIAN INTEGRATION IS USED THROUGHOUT
C
C        UNLESS OTHERWISE SPECIFIED, ATOMIC UNITS ARE USED
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/CONSTS/PI,SQRT2
      COMMON/IO/IREAD,IWRITE
      COMMON/MASSES/EMASS,TMASS,PMASS,AOE,AOPE
      COMMON/RANGE/ PLOW,PHIGH,DP
      COMMON/SCAT/RKIAU,RTHETA,RATKFI
      DATA IREAD,IWRITE/5,21/
      DATA PI,SQRT2/3.141592654,1.414213562/
C
      WRITE(IWRITE,100)
C
C     READ THE ELECTRON MASS AND THE MASSES OF THE TARGET AND PROJECTILE
C     NUCLEI.
C
         WRITE(IREAD,101)
      READ(IREAD,110) EMASS,TMASS,PMASS
      WRITE(IWRITE,120) EMASS,TMASS,PMASS
C
C     READ THE INCIDENT ENERGY IN KEV, CONVERT TO ATOMIC UNITS AND
C     CALCULATE THE KINETIC ENERGY OF RELATIVE MOTION AND
C     CORRESPONDING INITIAL MOMENTUM
C
         WRITE (IREAD,102)
      READ(IREAD,110) EIKEV
      EIAU=EIKEV*1000.0/27.21183
      RMASS=PMASS*(TMASS+EMASS)/(PMASS+TMASS+EMASS)
        RMUI=RMASS
        RMUF=TMASS*(PMASS+EMASS)/(PMASS+TMASS+EMASS)
      REAU=(RMASS/PMASS)*EIAU

      RKIAU=(2.0*RMASS*REAU)**0.50
C
        EMU=EMASS*TMASS/(EMASS+TMASS)
        PMU=PMASS*TMASS/(PMASS+TMASS)
        PEMU=EMASS*PMASS/(PMASS+EMASS)
C
C          THE CONTRIBUTIONS FROM THE TWO TERMS IN THE POTENTIAL CAN BE
C          CALCULATED USING THE SAME FUNCTION, BUT WITH A SLIGHTLY
C          DIFFERENT ARGUMENT:
C

        C1=-EMASS/PMASS
C                FOR THE T-P COULOMB POTETIAL TERM
        C2=1.
C                FOR THE E-T TERM.
```

```
C
C               THE BOHR RADII ARE
        AOE=1./EMU
        AOPE=1./PEMU
C       IN GENERAL WE HAVE FROM CONSERVATION OF ENERGY
C
        RKFAU=DSQRT(RMUF*(RKIAU*RKIAU/RMUI-EMU+PEMU))
        RATKFI=RKFAU/RKIAU
C
      WRITE(IWRITE,130) EIKEV,EIAU,REAU,RKIAU,RKFAU
C
C     READ AND WRITE THE RANGE OF ANGLES AND INCREMENTS (IN MILLIRADS OF
C     ARC) OVER WHICH THE DIFFERENTIAL CROSS SECTION IS REQUIRED
C
          WRITE(IREAD,103)
      READ (IREAD,110) THETAL,THETAH,DTHETA
      WRITE (IWRITE,140) THETAL,THETAH,DTHETA
C
C     READ THE RANGE OF THE INTEGRATION VARIABLE P (MOMENTUM) OVER WHICH
C     THE NUMERICAL INTEGRATION MUST BE PERFORMED
C
          WRITE(IREAD,104)
      READ(IREAD,110) PLOW,PHIGH,DP
      WRITE (IWRITE,155) PLOW,PHIGH,DP
C
C     BEGIN COMPUTATION
C
      ACONS=(RKFAU/RKIAU)*RMUF*RMUI*((2.0*PI)**4)
      THETA=THETAL
C
   10 CONTINUE
        DEGETA=THETA*.180/PI
      WRITE (IWRITE,150) THETA,DEGETA
C
C     CONVERT THETA TO RADIANS
C
      RTHETA=THETA/1000.00
C
C     CALCULATE THE CORRESPONDING ANGLE IN LAB FRAME
C
        RHO=(PMASS+EMASS)/(TMASS+EMASS)/RATKFI
C
C
      TERM=DCOS(RTHETA)
      TERM=(TERM+RHO)/((1.0+(2.0*RHO*TERM)+(RHO*RHO))**0.50)
      RPHI=DBLE(ACOS(SNGL(TERM)))
      PHI=(RPHI*1000.00)
        DPHI=RPHI*180./PI
      WRITE(IWRITE,190) PHI,DPHI
C
C     Q2 = MAGNITUDE OF EFFECTIVE MOMENTUM TRANSFER
C
      AMUP=RATKFI*PMASS/(EMASS+PMASS)
      B=2.0*AMUP*DCOS(RTHETA)
        C=AMUP*AMUP
        Q=1.-B+C
      Q2=RKIAU*DSQRT(Q)
      WRITE(IWRITE,170) Q2
C
      CALL TMAT1B(Q2,TRM1BA,TRM1BB)
        TERM1B=TRM1BA-TRM1BB
C               THE MINUS DUE TO THE COULOMB POTETIAL P-E
C
        N=1
        L=0
        CALL ORTH(N,L,C1,T101)
```

```
        CALL ORTH(N,L,C2,T102)
        TERM1S=T101-T102
C
      N=2
        CALL ORTH(N,L,C1,T201)
        CALL ORTH(N,L,C2,T202)
        TERM2S=T201-T202
      L=1
        CALL ORTH(N,L,C1,T211)
        CALL ORTH(N,L,C2,T212)
        TERM2P=T211-T212
C
      N=3
      L=0
        CALL ORTH(N,L,C1,T301)
        CALL ORTH(N,L,C2,T302)
        TERM3S=T301-T302
      L=1
        CALL ORTH(N,L,C1,T311)
        CALL ORTH(N,L,C2,T312)
        TERM3P=T311-T312
      L=2
        CALL ORTH(N,L,C1,T321)
        CALL ORTH(N,L,C2,T322)
        TERM3D=T321-T322
C
      WRITE(IWRITE,180) TRM1BA,TRM1BB,TERM1B
        WRITE(IWRITE,181) T101,T102,TERM1S
        WRITE(IWRITE,182) T201,T202,TERM2S
        WRITE(IWRITE,183) T211,T212,TERM2P
        WRITE(IWRITE,184) T301,T302,TERM3S
        WRITE(IWRITE,185) T311,T312,TERM3P
        WRITE(IWRITE,186) T321,T322,TERM3D
C
C     DIFFERENTIAL CROSS SECTION IN VARIOUS APPROXIMATIONS
C

      DCS1B=ACONS*(TERM1B*TERM1B)
      TMAT=TERM1B+TERM1S
        DCS1=ACONS*(TMAT*TMAT)
        TMAT=TMAT+TERM2S+TERM2P
      DCS2=ACONS*(TMAT*TMAT)
      TMAT=TMAT+TERM3S+TERM3P+TERM3D
        DCS3=ACONS*TMAT*TMAT
C
C       CONVERT FROM AO**2 TO CM**2
C
        AOS=2.8002829*10.**(-17.)
C
        DCA1B=AOS*DCS1B
        DCA1=AOS*DCS1
        DCA2=AOS*DCS2
        DCA3=AOS*DCS3
C
      WRITE(IWRITE,200)
      WRITE (IWRITE,160) DCS1B,DCA1B,DCS1,DCA1,DCS2,DCA2,DCS3,DCA3
C
C     CONVERT TO THE LAB FRAME
C
      TERM=DCOS(RTHETA)
      FACTOR=(1.0+(2.0*RHO*TERM)+(RHO*RHO))**1.50
      FACTOR=FACTOR/DABS(1.0+(RHO*TERM))
      DCS1B=FACTOR*DCS1B
        DCS1=FACTOR*DCS1
      DCS2=FACTOR*DCS2
      DCS3=FACTOR*DCS3
C
```

```
C         CONVERT FROM AO**2 TO CM**2
C
          DCA1B=AOS*DCS1B
          DCA1=AOS*DCS1
          DCA2=AOS*DCS2
          DCA3=AOS*DCS3
C
        WRITE(IWRITE,210)
        WRITE (IWRITE,160) DCS1B,DCA1B,DCS1,DCA1,DCS2,DCA2,DCS3,DCA3
C
          WRITE(5,90) THETA
        THETA=THETA+DTHETA
        IF (THETA.LE.THETAH) GO TO 10
C
        STOP
C
C       FORMAT STATEMENTS
C
   90 FORMAT(1X,E12.5)
  100 FORMAT(/2X,'FOCK-TANI DIFFERENTIAL CROSS SECTION'//)
  101   FORMAT(1X,'INPUT IN F10.5'/'  EMASS--> TARGMASS> PROJMASS>(AU)')
  102   FORMAT(1X,' KINETIC ENERGY (INCIDENT IN KEV)')
  103   FORMAT(1X,' THETAMIN> THETAMAX> INCREMENT (ANGLES IN MRAD)')
  104   FORMAT(1X,' LOWERLIM> UPPERLIM> STEPSIZE> (OF P-INTEGRAL)')
  110 FORMAT(8F10.5)
  120 FORMAT(/2X,'ELECTRON MASS        = ',E12.5,' A.U.'
     1       /2X,'TARGET MASS          = ',E12.5,' A.U.'
     2       /2X,'PROJECTILE MASS      = ',E12.5,' A.U.'/)
  130 FORMAT(/2X,'INCIDENT KINETIC ENERGY                = ',E12.5,' KEV '
     1       /2X,'                                       = ',E12.5,' A.U.'
     2       /2X,'KINETIC ENERGY OF RELATIVE MOTION      = ',E12.5,' A.U.'
     3       /2X,'INITIAL MOMENTUM                       = ',E12.5,' A.U.'
     4       /2X,'FINAL MOMENTUM                         = ',E12.5,' A.U.'/)
  140 FORMAT(/2X,'MINIMUM VALUE OF THETA = ',E12.5,' MRADS'
     1       /2X,'MAXIMUM VALUE OF THETA = ',E12.5,' MRADS'
     2       /2X,'INCREMENT              = ',E12.5,' MRADS'/)
  150 FORMAT(/2X,'THETA (CM)  = ',E12.5,' MRADS     ',E12.5,' DEGREES'/)
  155 FORMAT(/2X,'PLOW = ',E12.5,' PHIGH = ',E12.5,' DP = ',E12.5)
  160 FORMAT(//2X,'FIRST BORN APPROX.                            = ',E12.5
     1,5X,E12.5
     2        /2X,'                      + (N=1)                 = ',E12.5
     1,5X,E12.5
     4        /2X,'                               + (N=2)        = ',E12.5
     1,5X,E12.5
     3        /2X,'                                        + (N=3) = ',E12.5
     1,5X,E12.5/)
  170 FORMAT(/2X,'EFFECTIVE TRANSFERRED MOMENTUM = ',E12.5,' A.U.')
  180 FORMAT(//2X,'TERM1B = (',E12.5,' - ',E12.5,') =',E12.5)
  181 FORMAT(/2X,'TERM1S = (',E12.5,' - ',E12.5,') =',E12.5)
  182 FORMAT(/2X,'TERM2S = (',E12.5,' - ',E12.5,') =',E12.5)
  183 FORMAT(2X,'TERM2P = (',E12.5,' - ',E12.5,') =',E12.5)
  184 FORMAT(/2X,'TERM3S = (',E12.5,' - ',E12.5,') =',E12.5)
  185 FORMAT(2X,'TERM3P = (',E12.5,' - ',E12.5,') =',E12.5)
  186 FORMAT(2X,'TERM3D = (',E12.5,' - ',E12.5,') =',E12.5)
  190 FORMAT(/2X,'PHI (LAB) =',E12.5,' MRADS     ',E12.5,' DEGREES')
  200 FORMAT(//2X,'CM DIFFERENTIAL CROSS SECTION ',
     1'              (AO**2/SRAD)        (CM**2/SRAD)')
  210 FORMAT(//2X,'LAB DIFFERENTIAL CROSS SECTION ',
     1'             (AO**2/SRAD)        (CM**2/SRAD)')
       END
C

        SUBROUTINE TMAT1B(Q2,SUMA,SUMB)
C
C       THIS SUBROUTINE CALCULATES THE FIRST BORN APPROXIMATION
C         USING THE FORMULA II.3 IN J.D. JACKSON AND H. SCHIFF, PHS.
C         REV. 89,359 (1953) SLIGHTLY MODIFIED TO ACCOUNT FOR DIFFERENT
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C       BOHR RADII. IN THE EXPRESSION FOR DEL, C**2 IS REPLACED BY
C       AOF**2 - AOI**2 + C**2 . ALSO WE USE THE OVERALL COEFFICIENT
C       FROM THE POSITRONIUM CASE QUOTED IN
C       VARRACHIO AND M.D. GIRARDEAU, J.PHYS.B 16:(1983)1097
C       (WHICH ERRONEOUSLY HAS 2 RATHER THAN 8 AS THE COEFFICIENT OF
C       THE LAST TERM) BECAUSE OF THE NORMALIZATION CONVENTION OF
C       THE MOMENTUM EIGENSTATES.THE INTEGRAL IS DONE USING A 16
C       POINT GAUSSIAN QUADRATURE FORMULA
C               NOTE THAT MASSEY & MOHR APPROXIMATED THE INITIAL
C               C.M. COORDINATE IN THE MOMENTUM EIGENSTATE BY
C               THE PROJ. MASS . WE HAVE USED THE GENERAL C.M.
C               THE RESULTS OF THIS PROGRAM MATCH M&M MODIFIED IN
C               THIS WAY.
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/CONSTS/PI,SQRT2
                COMMON/SCAT/AK,RTHETA,RATKFI
                COMMON/IO/IREAD,IWRITE
      COMMON/GAUSS/ABSC(8),WEIGHT(8)
        COMMON/MASSES/EMASS,TMASS,PMASS,AOE,AOPE
        COMMON/BORN/AS,US,AK1S,AK2S,AK1DK2
C
C               CALCULATE CONSTANTS FOR BOTH TERMS
C
        ZT=PMASS/(EMASS+PMASS)
        GA=TMASS/(EMASS+TMASS)
        RATSQ=RATKFI*RATKFI
        RATCOS=RATKFI*DCOS(RTHETA)
        AK1=AK*DSQRT(1.-2.*ZT*RATCOS+ZT*ZT*RATSQ)
        AK2=AK*DSQRT(GA*GA-2.*GA*RATCOS+RATSQ)
C               NOTE THAT MASSEY & MOHR HAVE SET GA=1 IN INITIAL
C               MOMENTUM EIGENSTATE (OR TMASS--> INFINITY)
        AK1DK2=AK*AK*(GA-(1.+GA*ZT)*RATCOS+ZT*RATSQ)
        AS=1./AOE/AOE
        US=1./AOPE/AOPE
        ACONS=(1./AOE/AOPE)**2.5
C               NOTE THESE THREE ASSUME Z=1 IN NUMERATOR
        AK1S=AK1*AK1
        AK2S=AK2*AK2
        SK1MK2=AK1S-2.*AK1DK2+AK2S
C
C
C
C               PERFORM FIRST TERM INTEGRATION
C
      XLOW=0.0
      XHIGH=1.0
      A1=(XHIGH-XLOW)/2.0
      A2=(XHIGH+XLOW)/2.0
      SUMA=0.0
C
      DO 45 I=1,8
      X1=A2-(A1*ABSC(I))
      X2=A2+(A1*ABSC(I))
      CALL B1INT(X1,TERM1)
      CALL B1INT(X2,TERM2)
      SUMA=SUMA+(WEIGHT(I)*(TERM1+TERM2))
   45 CONTINUE
      SUMA=A1*SUMA*ACONS*4./PI/PI
C
C               NOW CALCULATE THE SECOND TERM
        D1=AS+AK2S
        D2=US+AK1S
        SUMB=4.*AOE/D1/D2/D2
        SUMB=SUMB*ACONS/PI/PI
C
C               NOTE THE MINUS SIGN IS IN MAIN PROGRAM
```

```
C
      RETURN

      END
C
      SUBROUTINE B1INT(X,TERM)
C
C     THIS SUBROUTINE CALCULATES THE INTEGRAND OF THE FIRST TERM OF THE
C     FIRST BORN APPROXIMATION
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/MASSES/EMASS,TMASS,PMASS,AOE,AOPE
      COMMON/SCAT/AK,RTHETA,RATKFI
        COMMON/BORN/AS,US,AK1S,AK2S,AK1DK2
C               THE LATTER ARE CALCULATED IN SUBROUTINE TMAT1B
C
C     EMASS = ELECTRON MASS      PMASS = PROJECTILE MASS
C     AK    = MOMENTUM           RTHETA = SCATTERING ANGLE IN RADIANS
C
C
        DEL=AS+(US-AS+AK1S)*X+(1.-X)*AK2S
        DS=DEL*DEL
        DC=DS*DEL
C
        XS=X*X
        QS=XS*AK1S+(1.-2.*X+XS)*AK2S+2.*(X-XS)*AK1DK2
        B=DEL-QS
        BOH=DSQRT(B)
        BTH=BOH*B
        BFH=BTH*B
C
        TERM=2./DC/BOH+1./DS/BTH+.75/DEL/BFH
      TERM=X*(1.0-X)*TERM
C
      RETURN
      END
C
      SUBROUTINE ORTH(N,L,C,TERM)
C
C     THIS SUBROUTINE CALCULATES THE  ORTHOGONALIZATION CORRECTION
C     FOR THE INTERMEDIATE STATE (N,L), BY NUMERICAL INTEGRATION.
C     A TWO DIMENSIONAL INTEGRAL IS EVALUATED USING 16 POINT GAUSSIAN
C     QUADRATURE.
C
C     INPUT           N = PRINCIPAL QUANTUM # OF THE INTERMEDIATE STATE
C                     L = ANGULAR MOMENTUM OF THE INTERMEDIATE STATE
C                     C = -EMASS/PMASS  FOR THE T-P  COULOMB TERM
C                     C = 1 FOR THE E-T TERM.
C
C     OUTPUT       TERM = ORTHOGONALIZATION INTEGRAL
C
C     THE PROGRAM CAN CURRENTLY HANDLE 1S TO 3D INTERMEDIATE STATES
C
C

      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
C
      COMMON/CONSTS/PI,SQRT2
      COMMON/GAUSS/ABSC(8),WEIGHT(8)
      COMMON/MASSES/EMASS,TMASS,PMASS,AOE,AOPE
      COMMON/RANGE/PLOW,PHIGH,DP
C
      DATA   ABSC/0.095012509837637,0.281603550779258,0.458016777657227,
     1            0.617876244402643,0.755404408355003,0.865631202387831,
     2            0.944575023073232,0.989400934991649/
      DATA WEIGHT/0.189450610455068,0.182603415044923,0.169156519395002,
     1            0.149595988816576,0.124628971255533,0.095158511682492,
```

```
     2           0.062253523938647,0.027152459411754/
C
C     FIRST CALCULATE THE OVERALL MULTIPLICATIVE CONSTANT
C
      AMUP=PMASS/(PMASS+EMASS)
        ACONS=-(2.*L+1.)*(AOPE**1.5)*(AMUP/PI)**3./(AOE)**2.5
C
C       THE ABOVE GIVEN BY A GENERALIZED VERSION OF OJHA ET. AL.'S
C       EQ. 5.10 EXCEPT THAT 1/SQRT2 HAS BEEN MULTIPLIED INTO EACH
C       COEFFICIENT BELOW. THE ABOVE EQ. IS GIVEN BY MULTIPLYING THE
C       FOLLOWING FACTORS: AOPE**1.5 FROM RNLSTAR(P) (NOTE OJHA HAS
C       DEFINED THIS AS JUST RNL(P)). AOE**1.5 FROM FOURIER TRANSFORM
C       OF INITIAL W.F.. (AMUP/AOE)**4 FROM PHI INTEGRATION. (1/AMUP)**3
C       FACTORED OUT OF DELTA(P1-...) . AMUP**2 FROM OPERATING WITH
C       DELTA(P2-AMUP(P+Q2)) ON 1/P2**2 OF OJHA EQ. 5.5 .
C
      TERM=0.0
C
C     AN INDEX II IS DEFINED SUCH THAT II = 1,2,3,4..... CORRESPONDS TO
C     1S,2S,2P,3S..... INTERMEDIATE STATES
C
      II=((N*(N-1))/2)+L+1
      IF (II.LE.0.OR.II.GE.7) RETURN
      GO TO (10,20,30,40,50,60) II
C
   10 CONTINUE
C     1S INTERMEDIATE STATE
C
        ACONS=ACONS*4.*32.
C
C       1/SRQT2*(4*SQRT2/SQRTPI)*(32*SRQTPI)
C          ^           ^               ^
C
C       OVERALL      R1SSTAR       I1S,1S    COEFFICIENTS
C
        GO TO 70
C
   20 CONTINUE
C     2S INTERMEDIATE STATE
C
        ACONS=ACONS*32.*512.
C
C       1/SQRT2*(32./SQRTPI)*(512.*SQRT2*SQRTPI)
C
        GO TO 70
C
   30 CONTINUE
C     2P INTERMEDIATE STATE
C
      ACONS=ACONS*128.*256.
C
C       1/SQRT2*(I*128/SQRT(3PI))*((-I)*SQRT2*SQRT(3PI)*256)
C
      GO TO 70
C
   40 CONTINUE
C     3S INTERMEDIATE STATE
C
        ACONS=ACONS*180.*864.
C
C       1/SQRT2*(180*SQRT2/SQRT(3PI))*(864*SQRT(3PI))
C
        GO TO 70
C
   50 CONTINUE
C     3P INTERMEDIATE STATE
C
        ACONS=ACONS*864.*576.
```

```
C
C       1/SQRT2*(I*864/SQRT(3PI))*((-I)*SQRT2*SQRT(3PI)*576)
C
        GO TO 70
C
   60 CONTINUE
C     3D INTERMEDIATE STATE
C
        ACONS=ACONS*5184.*2764.8
C
C     1/SQRT2*(I**2*5184*SQRT2/SQRT(30PI))*((-I)**2*13824*SQRT(30PI)/5)
C
        GO TO 70
C
C       ALL CONVERGE HERE (UNLESS INOPERATIVE)
   70 CONTINUE
C
C     NOW THE NUMERICAL INTEGRATION
C
      TERM=0.0
      PA=PLOW
   80 CONTINUE
      PB=PA+DP

      A1=(PB-PA)/2.0
      A2=(PB+PA)/2.0
C
      SUM=0.0
      DO 90 I=1,8
      P1=A2-(A1*ABSC(I))
      P2=A2+(A1*ABSC(I))
      CALL PINT(N,L,C,P1,TERM1)
      CALL PINT(N,L,C,P2,TERM2)
      SUM=SUM+(WEIGHT(I)*(TERM1+TERM2))
   90 CONTINUE
      SUM=A1*SUM
      TERM=TERM+SUM
C
      PA=PB
      IF (PA.LE.PHIGH) GO TO 80
C
      TERM=ACONS*TERM
C
      RETURN
      END
C
      SUBROUTINE PINT(N,L,C,P,TERM)
C
C     THIS SUBROUTINE CALCULATES THE INTEGRAND IN THE  ORTHOGONALIZATION
C     TERM FOR GIVEN VALUES OF THE INTEGRATION VARIABLE P (MOMENTUM).
C     NUMERICAL INTEGRATION OVER THETA COORDINATE IS REQUIRED. SIXTEEN POINT
C     GAUSSIAN QUADRATURE IS USED.
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
                COMMON/CONSTS/PI,SQRT2
      COMMON/GAUSS/ABSC(8),WEIGHT(8)
        COMMON/MASSES/EMASS,TMASS,PMASS,AOE,AOPE
C
C     FIRST CALCULATE THE PART WHICH DOES NOT REQUIRE INTEGRATION OVER
C     THETA, CONSISTING OF THE MOMENTUM FUNCTIONS IN RNLSTAR OF
C       OJHA ET. AL. EQ 5.10 (RNL IN HIS NOTATION)
C
      ACONS=P*P
C       THE VOLUME ELEMENT
        AP=AOPE*P
C       AOPE IS FINAL STATE BOHR RADIUS
        APS=AP*AP
```

```
      TERM=0.0
      II=((N*(N-1))/2)+L+1
C
C     SEE COMMENT IN SUBROUTINE ORTH FOR AN EXPLANATION OF INDEX II. THE
C     PROGRAM CAN CURRENTLY HANDLE 1S TO 3D INTERMEDIATE STATES ONLY.
C
      IF (II.LE.0.OR.II.GE.7) RETURN
      GO TO (10,20,30,40,50,60) II
C
   10 CONTINUE
C     1S INTERMEDIATE STATE
C
        DR1S=1.+APS
        ACONS=ACONS/DR1S/DR1S
        GO TO 70
C
   20 CONTINUE
C     2S INTERMEDIATE STATE
C
        DR2S=1.+4.*APS
        ACONS=ACONS*(4.*APS-1.)/DR2S/DR2S/DR2S
        GO TO 70
C
   30 CONTINUE
C     2P INTERMEDIATE STATE
C
        DR2P=1.+4.*APS
      ACONS=ACONS*AP/DR2P/DR2P/DR2P
      GO TO 70
C
   40 CONTINUE
C     3S INTERMEDIATE STATE
C
        DR3S=1.+9.*APS
        ACONS=ACONS*(81.*APS*APS-30.*APS+1.)/DR3S/DR3S/DR3S/DR3S
        GO TO 70
C
   50 CONTINUE
C     3P INTERMEDIATE STATE
C
        DR3=1.+9.*APS
        ACONS=ACONS*AP*(9.*APS-1.)/DR3/DR3/DR3/DR3
        GO TO 70
C
   60 CONTINUE
C     3D INTERMEDIATE STATE
C
        DR3=1.+9.*APS
        ACONS=ACONS*APS/DR3/DR3/DR3/DR3
        GO TO 70
C
C       ALL CONVERGE HERE (UNLESS INOPERATIVE)
   70 CONTINUE
C
C     INTEGRATION VARIABLE X=COS(THETAP) GOES FROM -1.0 TO 1.0
C
      XLOW=-1.0
      XHIGH=1.0
      A1=(XHIGH-XLOW)/2.0
      A2=(XHIGH+XLOW)/2.0
C
      SUM=0.0
      DO 80 I=1,8
      X1=A2-(A1*ABSC(I))
      X2=A2+(A1*ABSC(I))
      CALL XINT(N,L,C,P,X1,TERM1)
      CALL XINT(N,L,C,P,X2,TERM2)
```

```
      SUM=SUM+(WEIGHT(I)*(TERM1+TERM2))
   80 CONTINUE
      SUM=A1*SUM
C
      TERM=ACONS*SUM
C
      RETURN
      END
C
      SUBROUTINE XINT(N,L,C,P,X,TERM)
C
C     THIS SUBROUTINE CALCULATES THE INTEGRAND IN AN INTEGRAL OVER THETA
C     (WE ACTUALLY USE A TRANSFORMED VARIABLE X=COS(THETAP)) WHICH ARISES
C     IN THE NUMERICAL EVALUATION OF THE  ORTHOGONALIZATION INTEGRAL.
C     INTEGRATION OVER PHI COORDINATE IS PERFORMED ANALYTICALLY.
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)

      COMMON/CONSTS/PI,SQRT2
      COMMON/GAUSS/ABSC(8),WEIGHT(8)
      COMMON/MASSES/EMASS,TMASS,PMASS,AOE,AOPE
      COMMON/SCAT/RKI,THETA,RATKFI
C
C     WE FIRST DETERMINE THE LENGTH OF THE VECTOR Q2
C
      AMUP=RATKFI*PMASS/(PMASS+EMASS)
      ACONS=1.0-(2.0*AMUP*DCOS(THETA))+(AMUP*AMUP)
      Q2=RKI*DSQRT(ACONS)
C
C     THEN THE FIRST PART OF THE INTEGRAND
C
C       EACH TERM CONSISTS OF THE PRODUCT OF 1/|P+Q2|**2=1/A1
C       WITH THE MOMENTUM FUNCTION IN I1S,NLM(P+Q2) AND THE
C       LEGENDRE POLYNOMIAL PL(A/|A|) WHERE A=C*P*(P+Q2) OF
C       OJHA ET. AL EQ 5.10 , BUT GENERALIZED TO ALLOW BOTH TERMS
C       OF THE POTENTIAL TO BE CALCULATED. THESE TERMS DIFFER ONLY
C       BY THE COEFFICIENT OF THE RELATIVE COORDINATE, C, IN THE
C       POTENTIALS 1/|R+CR|. THE A/|A| WILL ONLY BE NEGATIVE IF
C       C/|C| IS NEGATIVE SO (C/|C|)**L IS FACTORED OUT BELOW. THE
C       ONLY PLACE IT APPEARS IS FOR L=1 IN WHICH A FACTOR OF |C|
C       FROM I1S,2P MULTIPLIES IT LEAVING JUST C . FINALLY, THE
C       FOLLOWING HAVE THE DIVISION P*(P+Q2)/|P| ALREADY DONE.
C
      PP=P*P
      QQ=Q2*Q2
      A1=PP+(2.0*P*Q2*X)+QQ
      ACONS=0.
        AACCA1=AOPE*AOPE*C*C*A1
      TERM=0.0
      II=((N*(N-1))/2)+L+1
C
C     SEE COMMENT IN SUBROUTINE ORTH FOR AN EXPLANATION OF INDEX II. THIS
C     PROGRAM CAN CURRENTLY HANDLE INTERMEDIATE STATES 1S TO 3D ONLY.
C
      IF (II.LE.0.OR.II.GE.7) RETURN
      GO TO (10,20,30,40,50,60) II
C
   10 CONTINUE
C     1S INTERMEDIATE STATE
C
        DI1=4.+AACCA1
        ACONS=1./A1/DI1/DI1
        GO TO 70
C
   20 CONTINUE
C     2S INTERMEDIATE STATE
C
```

```
        DI2=9.+4.*AACCA1
        ACONS=AACCA1/A1/DI2/DI2/DI2
        GO TO 70
C
   30 CONTINUE
C     2P INTERMEDIATE STATE
C
        DI2=9.+4.*AACCA1
      ACONS=(P+Q2*X)*AOPE*C/A1/DI2/DI2/DI2
C
C       1/A1*((P+PQ2X)*(SIGN(C))/SQRT(A1))*AOPE*ABS(C)*SQRT(A1)/(")
C
      GO TO 70

   40 CONTINUE
C     3S INTERMEDIATE STATE
C
        DI3=16.+9.*AACCA1
        ACONS=(16.*AACCA1+27.*AACCA1*AACCA1)/A1/DI3/DI3/DI3/DI3
        GO TO 70
C
   50 CONTINUE
C
C     3P INTERMEDIATE STATE
C
        DI3=16.+9.*AACCA1
        ACONS=(P+Q2*X)*AOPE*C/A1/DI3/DI3/DI3/DI3
        GO TO 70
C
   60 CONTINUE
C     3D INTERMEDIATE STATE
C
        DI3=16.+9.*AACCA1
        PQ2X=P+Q2*X
        ACONS=.5*(3.*PQ2X*PQ2X/A1-1.)*AACCA1/A1/DI3/DI3/DI3/DI3
        GO TO 70
C
C       ALL CONVERGE HERE (UNLESS INOPERATIVE)
   70 CONTINUE

C
C     WE REQUIRE THE CONSTANT ANU AND SINE AND COSINE OF THE ANGLE
C     THETAK
C
      ANU=EMASS*(PMASS+EMASS+TMASS)/((PMASS+EMASS)*(TMASS+EMASS))
      AMUP=PMASS/(PMASS+EMASS)
        AMRK=AMUP*RATKFI
      Q2=DSQRT(1.0-(2.0*AMRK*DCOS(THETA))+(AMRK*AMRK))
        A1=Q2/RATKFI
      SINK=AMUP*DSIN(THETA)/A1
        COSK=DSQRT(1.-SINK*SINK)
C
C     THEN THE REST OF THE INTEGRAND
C
      A2=(AMUP*AMUP/AOE/AOE)+PP+(2.0*ANU*RKI*P*X*COSK)+((ANU*RKI)**2)
      B2=2.0*ANU*RKI*P*SINK*DSQRT(1.0-(X*X))
      FACTOR=A2/(((A2+B2)*(A2-B2))**1.50)
C
      TERM=ACONS*FACTOR
C
      RETURN
      END
```

```
C     THIS PROGRAM CALCULATES THE TOTAL CROSS SECTION FOR CHARGE
C     TRANSFER IN BORN APPROXIMATION BASED ON THE FOCK-TANI HAMILTONIAN
C     FOR THE GENERAL CASE P+(TE)->(PE)+T, WHERE P, E, AND T ARE BARE
C     CHARGES OF MASS PMASS, EMASS, AND TMASS AND "(..)" IS AN ATOM.
C
C           SEE NOTES AT BEGINNING OF DIFFERENTIAL VERSION ABOVE
C
C           USES SUBROUTINES ABOVE
C
      IMPLICIT DOUBLE PRECISION (A-H,O-Z)
      COMMON/CONSTS/PI,SQRT2
      COMMON/IO/IREAD,IWRITE
      COMMON/MASSES/EMASS,TMASS,PMASS,AOE,AOPE
      COMMON/GAUSS/ABSC(8),WEIGHT(8)
      COMMON/RANGE/ PLOW,PHIGH,DP
      COMMON/SCAT/RKIAU,RTHETA,RATKFI
      DATA IREAD,IWRITE/5,21/
      DATA PI,SQRT2/3.141592654,1.414213562/
         AOS=2.8002829*10.**(-17.)
C
      WRITE(IWRITE,100)
C
C     READ THE ELECTRON MASS AND THE MASSES OF THE TARGET AND PROJECTILE
C     NUCLEI.
C
            WRITE(IREAD,101)
      READ(IREAD,110) EMASS,TMASS,PMASS
      WRITE(IWRITE,120) EMASS,TMASS,PMASS
C
C        READ IN THE INITIAL LAB KINETIC ENERGY, CONVERT TO ATOMIC UNITS
C        AND CALCULATE THE INITIAL MOMENTUM AND C.M. KINETIC ENERGY
C
C
            WRITE (IREAD,102)
      READ(IREAD,110) REKEV
      REAU=REKEV*1000.0/27.21183
      RMASS=PMASS*(TMASS+EMASS)/(PMASS+TMASS+EMASS)
         RMUI=RMASS
         RMUF=TMASS*(PMASS+EMASS)/(PMASS+TMASS+EMASS)
      EIAU=(PMASS/RMASS)*REAU
         EIKEV=REKEV*EIAU/REAU
      RKIAU=(2.0*RMASS*REAU)**0.50
C
         EMU=EMASS*TMASS/(EMASS+TMASS)
         PMU=PMASS*TMASS/(PMASS+TMASS)
         PEMU=EMASS*PMASS/(PMASS+EMASS)
C
C                  FROM THE CENTER OF MASS DECOMPOSITION
         C1=-EMASS/PMASS
C                  FOR THE T-P COULOMB POTETIAL TERM
         C2=1.
C                  FOR THE E-T TERM.
C
C                  THE BOHR RADII ARE
         AOE=1./EMU
         AOPE=1./PEMU
C        IN GENERAL WE HAVE FROM CONSERVATION OF ENERGY
C
         RKFAU=DSQRT(RMUF*(RKIAU*RKIAU/RMUI-EMU+PEMU))
         RATKFI=RKFAU/RKIAU
C
      WRITE(IWRITE,130) REKEV,REAU,EIKEV,EIAU,RKIAU,RKFAU
C
C     READ AND WRITE THE RANGE OF ANGLES (IN MILLIRADS OF ARC) OVER WHICH
C     THE DIFFERENTIAL CROSS SECTION IS TO BE INTEGRATED
C
            WRITE(IREAD,103)
```

```
      READ (IREAD,110) THETAL,THETAM,THETAH
      WRITE(IWRITE,140) THETAL,THETAM,THETAH
C
C     READ THE RANGE OF THE INTEGRATION VARIABLE P (MOMENTUM) OVER WHICH
C     THE NUMERICAL INTEGRATION MUST BE PERFORMED
C
          WRITE(IREAD,104)
      READ(IREAD,110) PLOW,PHIGH,DP
      WRITE (IWRITE,155) PLOW,PHIGH,DP
C
C     T1 AND T2 ARE USED IN GAUSSIAN QUADRATURE
C
      T1=(THETAM-THETAL)/2.0
      T2=(THETAM+THETAL)/2.0
C     BEGIN COMPUTATION
C
      ACONS=(RKFAU/RKIAU)*RMUF*RMUI*((2.0*PI)**4)
C
C     SIXTEEN POINT GAUSSIAN QUADRATURE IS USED FOR INTEGRATING THE DIFFE-
C     RENTIAL CROSS SECTION
C
        FLAG=0.
        SCS1B=0.
        SCS1=0.
        SCS2=0.
        SCS3=0.
        I=0
C
C       ADD CONTRIBUTIONS FROM THE FIRST SEGMENT UNLESS NULL
C
        IF(T1.EQ.0.) GO TO 15
5       CONTINUE
C
C     FIRST SET ALL TOTAL CROSS SECTIONS TO ZERO
C
      CS1B=0.0
      CS1=0.0
      CS2=0.0
      CS3=0.0
C
      DO 12 ISIGN=1,2
      ASIGN = (-1)**ISIGN
      DO 10 IGAUSS=1,8
      THETA=(ASIGN*T1*ABSC(IGAUSS))+T2
      WRITE (IWRITE,150) THETA
C
C     CONVERT THETA TO RADIANS
C
      RTHETA=THETA/1000.00
C
C
C     Q2 = MAGNITUDE OF EFFECTIVE MOMENTUM TRANSFER
C
      AMUP=RATKFI*PMASS/(EMASS+PMASS)
      B=2.0*AMUP*DCOS(RTHETA)
        C=AMUP*AMUP
        Q=1.-B+C
      Q2=RKIAU*DSQRT(Q)
      WRITE(IWRITE,170) Q2
C
      CALL TMAT1B(Q2,TRM1BA,TRM1BB)
        TERM1B=TRM1BA-TRM1BB
C               THE MINUS DUE TO THE COULOMB POTETIAL P-E
C
        N=1
        L=0
```

```
        CALL ORTH(N,L,C1,T101)
        CALL ORTH(N,L,C2,T102)
        TERM1S=T101-T102
C
      N=2
        CALL ORTH(N,L,C1,T201)
        CALL ORTH(N,L,C2,T202)
        TERM2S=T201-T202
      L=1
        CALL ORTH(N,L,C1,T211)
        CALL ORTH(N,L,C2,T212)
        TERM2P=T211-T212
C
      N=3
      L=0
        CALL ORTH(N,L,C1,T301)
        CALL ORTH(N,L,C2,T302)
        TERM3S=T301-T302
      L=1
        CALL ORTH(N,L,C1,T311)
        CALL ORTH(N,L,C2,T312)
        TERM3P=T311-T312
      L=2
        CALL ORTH(N,L,C1,T321)
        CALL ORTH(N,L,C2,T322)
        TERM3D=T321-T322
C
      WRITE(IWRITE,180) TRM1BA,TRM1BB,TERM1B
        WRITE(IWRITE,181) T101,T102,TERM1S
        WRITE(IWRITE,182) T201,T202,TERM2S
        WRITE(IWRITE,183) T211,T212,TERM2P
        WRITE(IWRITE,184) T301,T302,TERM3S
        WRITE(IWRITE,185) T311,T312,TERM3P
        WRITE(IWRITE,186) T321,T322,TERM3D
C
C     DIFFERENTIAL CROSS SECTION IN VARIOUS APPROXIMATIONS
C

      DCS1B=ACONS*(TERM1B*TERM1B)
      TMAT=TERM1B+TERM1S
        DCS1=ACONS*(TMAT*TMAT)
        TMAT=TMAT+TERM2S+TERM2P
      DCS2=ACONS*(TMAT*TMAT)
      TMAT=TMAT+TERM3S+TERM3P+TERM3D
        DCS3=ACONS*TMAT*TMAT
C
C       CONVERT FROM A0**2 TO CM**2
C
C
        DCA1B=A0S*DCS1B
        DCA1=A0S*DCS1
        DCA2=A0S*DCS2
        DCA3=A0S*DCS3
C
      WRITE(IWRITE,200)
      WRITE (IWRITE,160) DCS1B,DCA1B,DCS1,DCA1,DCS2,DCA2,DCS3,DCA3
C
C     ADD THE CONTRIBUTION TO THE TOTAL CROSS SECTION
C
      AWT=DSIN(RTHETA)*WEIGHT(IGAUSS)
      CS1B=CS1B+(AWT*DCS1B)
      CS1=CS1+(AWT*DCS1)
      CS2=CS2+(AWT*DCS2)
      CS3=CS3+(AWT*DCS3)
C
        I=I+1
        WRITE(5,9) I
```

```
9       FORMAT('+',I5,'  OUT OF 32')
C
   10 CONTINUE
12      CONTINUE
C
C     WE MUST CONVERT THE INTERVAL TO RADIANS BEFORE MULTIPLYING BY THE
C     OVERALL MULTIPLICATIVE CONSTANT. AN ADDITIONAL FACTOR OF 2.0*PI
C     COMES FROM INTEGRATION OVER THE AZIMUTHAL ANGLE.
C       FOR THE CROSS-SECTION  GIVEN IN UNITS OF PI*A.U.**2
C        WE MUST ALSO DIVIDE BY PI GIVING A NET FACTOR OF 2.
C
      T1=T1/1000.0
C
      SCS1B=2.0*T1*CS1B+SCS1B
      SCS1=2.0*T1*CS1+SCS1
      SCS2=2.0*T1*CS2+SCS2
      SCS3=2.0*T1*CS3+SCS3
C
C       NOW FOR THE SECOND SEGMENT UNLESS NULL
C
        IF(FLAG.EQ.1.) GO TO 20
15      T1=(THETAH-THETAM)/2.
        T2=(THETAH+THETAM)/2.
        FLAG=1.
        IF(T1.NE.0.) GO TO 5
20      CONTINUE
C
C       CONVERT TO CM**2
C
        SCA1B=SCS1B*PI*AOS
        SCA1=SCS1*PI*AOS
        SCA2=SCS2*PI*AOS
        SCA3=SCS3*PI*AOS
C
      WRITE(IWRITE,220)
      WRITE(IWRITE,160) SCS1B,SCA1B,SCS1,SCA1,SCS2,SCA2,SCS3,SCA3
C
      STOP
C
C     FORMAT STATEMENTS
C
   90 FORMAT(1X,E12.5)
  100 FORMAT(/2X,'FOCK-TANI DIFFERENTIAL CROSS SECTION'//)
  101   FORMAT(1X,'INPUT IN F10.5'/'  EMASS--> TARGMASS> PROJMASS>(AU)')
  102   FORMAT(1X,' KINETIC ENERGY (INCIDENT LAB IN KEV)')
  103   FORMAT(1X,' THETAMIN> THETAMID> THETAMAX> (ANGLES IN MRAD)')
  104   FORMAT(1X,' LOWERLIM> UPPERLIM> STEPSIZE> (OF P-INTEGRAL)')
  110 FORMAT(8F10.5)
  120 FORMAT(/2X,'ELECTRON MASS       = ',E12.5,' A.U.'
     1       /2X,'TARGET MASS         = ',E12.5,' A.U.'
     2       /2X,'PROJECTILE MASS     = ',E12.5,' A.U.'/)
  130 FORMAT(/2X,'INCIDENT LAB KINETIC ENERGY        = ',E12.5,' KEV '
     1       /2X,'                                   = ',E12.5,' A.U.'
     2       /2X,'C.M. INCIDENT KINETIC ENERGY       = ',E12.5,' KEV '
     1       /2X,'                                   = ',E12.5,' A.U.'
     3       /2X,'INITIAL MOMENTUM                   = ',E12.5,' A.U.'
     4       /2X,'FINAL MOMENTUM                     = ',E12.5,' A.U.'/)
  140 FORMAT(/2X,'MINIMUM VALUE OF THETA = ',E12.5,' MRADS'
     1       /2X,'MAXIMUM VALUE OF THETA = ',E12.5,' MRADS'
     2       /2X,'INCREMENT              = ',E12.5,' MRADS'/)
  150 FORMAT(/2X,'THETA (CM)  = ',E12.5,' MRADS'/)
  155 FORMAT(/2X,'PLOW = ',E12.5,' PHIGH = ',E12.5,' DP = ',E12.5)
  160 FORMAT(//2X,'FIRST BORN APPROX.                                = ',E12.5
     1,5X,E12.5
     2        /2X,'                        + (N=1)               = ',E12.5
     1,5X,E12.5
     4        /2X,'                               + (N=2)        = ',E12.5
```

```
     1,5X,E12.5
     3         /2X,'                                      + (N=3) = ',E12.5
     1,5X,E12.5/)
  170 FORMAT(/2X,'EFFECTIVE TRANSFERRED MOMENTUM = ',E12.5,' A.U.')
  180 FORMAT(//2X,'TERM1B = (',E12.5,' - ',E12.5,') =',E12.5)
  181 FORMAT(/2X,'TERM1S = (',E12.5,' - ',E12.5,') =',E12.5)
  182 FORMAT(/2X,'TERM2S = (',E12.5,' - ',E12.5,') =',E12.5)
  183 FORMAT(2X,'TERM2P = (',E12.5,' - ',E12.5,') =',E12.5)
  184 FORMAT(/2X,'TERM3S = (',E12.5,' - ',E12.5,') =',E12.5)
  185 FORMAT(2X,'TERM3P = (',E12.5,' - ',E12.5,') =',E12.5)
  186 FORMAT(2X,'TERM3D = (',E12.5,' - ',E12.5,') =',E12.5)
  190 FORMAT(/2X,'PHI (LAB) =',E12.5,' MRADS')
  200 FORMAT(//2X,'CM DIFFERENTIAL CROSS SECTION ',
     1'             (AO**2/SRAD)       (CM**2/SRAD)')
  210 FORMAT(//2X,'LAB DIFFERENTIAL CROSS SECTION ',
     1'             (AO**2/SRAD)       (CM**2/SRAD)')
220      FORMAT(//2X,'TOTAL CROSS SECTION              ',
     1'             (PI*AO**2)             (CM**2)')
      END
```

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