

## Reduced-mass Fock-Tani representations for $a^+ + (b^+c^-) \rightarrow (a^+c^-) + b^+$ and first-order results for $\{abc\} = \{ppe, epe, \mu p\mu, \mu d\mu, \text{ and } \mu t\mu\}$

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The Fock-Tani transformation in the Jacobi three→two-body reduced-mass system is carried out and the first-order  $T$  matrix is found to be identical to that for the full three-body transformation. The Fock-Tani transformation in the reduced-mass system in which particle  $b$  is fixed at the origin is found to give a first-order  $T$  matrix with an error of  $m_c/m_b$  in the initial momentum wave function. First-order differential and total cross sections are calculated for  $a^+ + (b^+c^-) \rightarrow (a^+c^-) + b^+$  where  $\{abc\} = \{ppe, epe, \mu p\mu, \mu d\mu, \text{ and } \mu t\mu\}$ .

### I. INTRODUCTION

Atomic three-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<sup>1</sup> 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 rearrangements is difficult to handle using conventional representations which have different Hamiltonians for different arrangement channels. Thus, a representation that can accurately account for various arrangements simultaneously would be of great utility.

A representation (Fock-Tani) has been developed<sup>2</sup> which does give a Hamiltonian that treats reactants, intermediate states, 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 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 Hamiltonian corresponds to an immediately identifiable and specific physical process.

All interactions are of smaller magnitude due to terms orthogonalizing continuum states to the bound states. Therefore, the Born series in Fock-Tani representation is more convergent than the Born series in Fock (or Schrödinger) representation and the reliability of first-order approximations should be improved. In fact, this improvement has been shown for resonant charge exchange in proton-hydrogen collisions by Ojha *et al.*<sup>3</sup> Good agreement is found with experimental total cross sections<sup>4</sup> at energies greater than 10 keV and over dif-

ferential angles 1 mrad and smaller at 25, 60, and 125 keV.<sup>5</sup>

The drawback of Fock-Tani representation is the difficulty in actually carrying out the transformation. 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 three-body Fock Hamiltonian<sup>3</sup> and also starting with the special case of the three→two-body Hamiltonian with an infinite-mass proton.<sup>6</sup> In this paper the latter is generalized to allow for finite masses.

In Sec. II the Fock-Tani transformation for the initial-state Jacobi reduced-mass system is found and in Sec. III this is shown to give the same first-order  $T$  matrix for charge transfer as does the full three-body case. In Appendix A the Fock-Tani transformation for the symmetrical reduced-mass system, which includes momentum-dependent cross terms, is given and is shown to have an error of order  $m_e/m_p$  in the initial asymptotic state.

In Sec. VI the Fock-Tani  $T$  matrix for charge transfer is analytically reduced to tractable numerical form, for arbitrary masses of the three particles, and in Sec. V the Fock-Tani total and differential scattering cross sections are given for reactions  $a^+ + (b^+c^-) \rightarrow (a^+c^-) + b^+$ , where  $\{abc\} = \{ppe, epe, \mu p\mu, \mu d\mu, \text{ and } \mu t\mu\}$ . Comparisons are made with the results of other theories and, for  $\{abc\} = \{ppe\}$ , experiments. Section VI is a discussion of the reduced-mass Fock-Tani approach and its applicability to the four-body problem.

### II. THE INITIAL-STATE VERSION OF THE FOCK-TANI HAMILTONIAN

The initial-state version of the (second-quantized) Fock Hamiltonian in the Jacobi center-of-mass system is

$$\hat{H}_{Fi} = \int d\mathbf{R} \hat{a}^\dagger(\mathbf{R}) T_a(\mathbf{R}) \hat{a}(\mathbf{R}) + \int d\mathbf{r} \hat{e}^\dagger(\mathbf{r}) H_e(\mathbf{r}) \hat{e}(\mathbf{r}) \\ + \int d\mathbf{R} d\mathbf{r} \hat{a}^\dagger(\mathbf{R}) \hat{e}^\dagger(\mathbf{r}) [V_{ae}(\mathbf{R}, \mathbf{r}) + V_{ab}(\mathbf{R}, \mathbf{r})] \\ \times \hat{e}(\mathbf{r}) \hat{a}(\mathbf{R}), \quad (1)$$

where

$$H_e(\mathbf{r}) = T_e(\mathbf{r}) - \frac{Z_b}{r}, \quad (2)$$

$$T_a(\mathbf{R}) = -\frac{1}{2M}\nabla_{\mathbf{R}}^2, \quad T_e(\mathbf{r}) = -\frac{1}{2m}\nabla_{\mathbf{r}}^2, \quad (3)$$

$$V_{ae}(\mathbf{R}, \mathbf{r}) = -\frac{Z_a}{|\mathbf{R} - \gamma\mathbf{r}|}, \quad V_{ab}(\mathbf{R}, \mathbf{r}) = \frac{Z_a Z_b}{|\mathbf{R} + \lambda\mathbf{r}|}, \quad (4)$$

$$\gamma = \frac{m_b}{m_b + m_e}, \quad \lambda = \frac{m_e}{m_b + m_e}, \quad (5)$$

and where the three-body reduced mass accounting for the motion of the projectile  $a$ , at coordinate  $\mathbf{R}$ , relative to the center of mass of ( $be$ ) is

$$M = \frac{m_a(m_b + m_e)}{m_a + m_b + m_e}, \quad (6)$$

and the two-body reduced mass accounting for the bound-state internal motion, with relative vector  $\mathbf{r}$ , is

$$m = \frac{m_b m_e}{m_b + m_e}. \quad (7)$$

The notation convention will be that  $\mathbf{R} = (\mathbf{R}_a, \sigma_a)$ , where  $\sigma$  is the spin of the particle, and  $\int d\mathbf{R} = \sum_{\sigma} \int d\mathbf{R}_a$ , except where stated otherwise. A similar convention is used for  $r$ . It is assumed the charge of  $e$  is  $-1$  but the mass is arbitrary (although labeled “ $e$ ”, it may be a negative muon). Atomic units ( $\hbar = m_{\text{electron}} = e = 1$ ) are used throughout.

The Fock creation operators for initial- and final-state bound species are

$$\hat{E}_{\nu}^{\dagger} = \int d\mathbf{r} u_{\nu}^E(\mathbf{r}) \hat{e}^{\dagger}(\mathbf{r}) \quad (8)$$

and

$$\hat{A}_{\mu}^{\dagger} = \int d\mathbf{R} d\mathbf{r} \phi_{\mu}^A(\mathbf{R}, \mathbf{r}) \hat{a}^{\dagger}(\mathbf{R}) \hat{e}^{\dagger}(\mathbf{r}), \quad (9)$$

respectively. However, the coordinates for the latter bound-state orbital must be transformed from the natural (final-state) set  $\{R_f, r_f\}$ , to the set  $\{R, r\}$ . The author has previously shown<sup>7</sup> that the initial- to final-state coordinate relations are

$$\mathbf{R}_f = \zeta\mathbf{R} + \iota\mathbf{r}, \quad \mathbf{r}_f = \gamma\mathbf{r} - \mathbf{R}, \quad (10)$$

and

$$\mathbf{R} = \lambda\mathbf{R}_f - \iota\mathbf{r}_f, \quad \mathbf{r} = \zeta\mathbf{r}_f + \mathbf{R}_f, \quad (11)$$

where

$$\zeta = \frac{m_a}{m_a + m_e}, \quad \eta = \frac{m_e}{m_a + m_e}, \quad (12)$$

and

$$\iota = \zeta\lambda + \eta. \quad (13)$$

Then the final-state wave function is

$$\begin{aligned} \phi_{\mu}^A(\mathbf{R}, \mathbf{r}) &= (2\pi)^{-3/2} e^{i\mathbf{k}\cdot\mathbf{R}_f} u_{\nu}^A(\mathbf{r}_f) \\ &= (2\pi)^{-3/2} e^{i\mathbf{k}\cdot(\zeta\mathbf{R} + \iota\mathbf{r})} u_{\nu}^A(\gamma\mathbf{r} - \mathbf{R}), \end{aligned} \quad (14)$$

where  $\mu = \{\mathbf{k}, \nu\}$ . In Ref. 6 it was stated that the  $u$ 's

could be either free or perturbed orbitals, but perturbed orbitals in (8) would require an  $R$  dependence also,<sup>8</sup> which would eliminate the reduction in difficulty of finding the Fock-Tani transformation in a reduced-mass system.

The  $e$  and  $a$  fields satisfy the standard anticommutation relations

$$\begin{aligned} \{\hat{e}(r), \hat{e}^{\dagger}(r')\} &= \delta(\mathbf{r} - \mathbf{r}') = \delta(\mathbf{r}_e - \mathbf{r}'_e) \delta_{\sigma\sigma'}, \\ \{\hat{a}(\mathbf{R}), \hat{a}^{\dagger}(\mathbf{R}')\} &= \delta(\mathbf{R} - \mathbf{R}'), \\ \{\hat{e}(\mathbf{r})\hat{e}(\mathbf{r}')\} &= \{\hat{a}(\mathbf{R}), \hat{a}(\mathbf{R}')\} \\ &= \{\hat{e}(\mathbf{r}), \hat{a}(\mathbf{R})\} = \{\hat{e}(\mathbf{r}), \hat{a}^{\dagger}(\mathbf{R})\} = 0, \end{aligned} \quad (15)$$

whereas the bound-state fields satisfy extremely complicated (anti) commutation relations with the free particles and among themselves.<sup>6</sup> For this reason a transformation to a new representation in which all of the fields satisfy elementary (anti) commutation relations is done.

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  $\hat{\epsilon}_{\nu}^{\dagger}$  and  $\hat{\alpha}_{\nu}^{\dagger}$  as representing the composite states of the bound, reduced-mass electron, and the electron bound to particle  $a$ , respectively. They are to be kinematically independent of the free particle states so that the commutation ( $[,]$ ) and anticommutation ( $\{, \}$ ) relations involving the “ideal” composite states are

$$\begin{aligned} \{\hat{\epsilon}_{\mu}, \hat{\epsilon}_{\nu}^{\dagger}\} &= [\hat{\alpha}_{\mu}, \hat{\alpha}_{\nu}^{\dagger}] = \delta_{\mu\nu}, \\ \{\hat{\epsilon}_{\mu}, \hat{\epsilon}_{\nu}\} &= \{\hat{\epsilon}_{\mu}, \hat{e}^{(\dagger)}(\mathbf{y})\} = \{\hat{\epsilon}_{\mu}, \hat{a}^{(\dagger)}(\mathbf{x})\} = 0, \\ [\hat{\alpha}_{\mu}, \hat{\alpha}_{\nu}] &= [\hat{\alpha}_{\mu}, \hat{e}^{(\dagger)}(\mathbf{y})] = [\hat{\alpha}_{\mu}, \hat{a}^{(\dagger)}(\mathbf{x})] = [\hat{\alpha}_{\mu}, \hat{\epsilon}_{\nu}^{(\dagger)}] = 0, \end{aligned} \quad (16)$$

where the quantum numbers, and hence the Kronecker deltas, include spin indices. Initially these ideal composites have no physical content on the subspace  $I_0$ ,

$$\hat{N}_{\beta} | \rangle = 0 \quad \text{if } | \rangle \text{ is in } I_0, \quad (17)$$

where the number operator is

$$\hat{N}_{\beta} = \sum_{\nu} \hat{\beta}_{\nu}^{\dagger} \hat{\beta}_{\nu} \quad (18)$$

and where a generic notation,  $\beta$  equal to either  $\alpha$  or  $\epsilon$ , has been introduced for compactness.

One then transforms the physics on the enlarged space  $I$  from the subspace  $I_0$  to the subspace  $I_c$  on which these ideal<sup>6</sup> composite operators represent the physical composite states and the fields  $\hat{a}^{\dagger}(\mathbf{R})$  and  $\hat{e}^{\dagger}(\mathbf{r})$  are the continuum states that will not have enough interaction energy for binding.

The Hamiltonian is transformed by means of the unitary operator<sup>6</sup>

$$\hat{U} = \hat{U}_A \hat{U}_E, \quad (19)$$

where

$$\hat{U}_A = \exp \left[ \frac{\pi}{2} \hat{F}_\alpha \right], \quad \hat{F}_\alpha = \sum_{\nu} (\hat{A}^{\dagger} \hat{\alpha}_{\nu} - \hat{\alpha}_{\nu}^{\dagger} \hat{A}_{\nu}) \quad (19a)$$

and

$$\hat{U}_E = \exp \left[ \frac{\pi}{2} \hat{F}_E \right], \quad \hat{F}_E = \sum_{\nu} (\hat{E}_{\nu}^{\dagger} \hat{\epsilon}_{\nu} - \hat{\epsilon}_{\nu}^{\dagger} \hat{E}_{\nu}). \quad (19b)$$

Then the Fock-Tani Hamiltonian is given by

$$\hat{H} = \hat{U}^{-1} \hat{H}_F \hat{U} = \hat{U}_E^{-1} (\hat{U}_A^{-1} \hat{H}_F \hat{U}_A) \hat{U}_E = \hat{H}_0 + \hat{V}, \quad (20)$$

and the states are transformed as

$$|v\alpha\rangle = \hat{\alpha}_{\nu}^{\dagger} |0\rangle \equiv \hat{U}_A^{-1} \hat{A}_{\nu}^{\dagger} |0\rangle$$

and

$$|v\epsilon\rangle = \hat{\epsilon}_{\nu}^{\dagger} |0\rangle \equiv \hat{U}_E^{-1} \hat{E}_{\nu}^{\dagger} |0\rangle. \quad (21)$$

The ordering of the  $U$ 's is critical since they do not commute in general.<sup>2</sup> For the opposite ordering, the second equation of (21) is violated unless  $a$  and  $b$  are identical particles, in which case the ordering gives the post-prior discrepancy familiar in scattering theory.<sup>9</sup>

The mechanics of the transformation are given in detail in Gilbert<sup>10</sup> [who has the opposite sign for all terms due to his sign in the equivalent of (19a) and (19b)] and in Girardeau.<sup>6</sup> The explicit result below, differs somewhat from Girardeau's Eqs. (34)–(42).<sup>11</sup> The rightmost  $y$ 's in the second and fourth matrix elements in his Eq. (41), which should be  $y'$  and  $y_2$ , respectively, are given correctly in (B5) below. The  $\alpha^{\dagger}\alpha$  matrix elements ( $\psi^{\dagger}\psi$  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  $E_{\mu}$  in the unperturbed Hamiltonian  $H_0$ , is not renormalized as in his Eq. (38), and the lack of terms of the same parity in  $V$  is indicated below by a prime on the summation sign. Finally, the mass denominator of  $T_a$  in  $H_0$  is  $M$  rather than  $\mu_a$ , of (A3), and the second term in  $V$  of Girardeau's Eq. (34) does not appear in (23) [the physical content of this term appears in the additional term in (B9) below].

As in Girardeau, the eigenvalue equations

$$H_e(\mathbf{r}) u_{\nu}^E(\mathbf{r}) = E_{\nu} u_{\nu}^E(\mathbf{r}) \quad (22)$$

and

$$[T_a(\mathbf{R}) + T_e(\mathbf{r}) + V_{ae}(\mathbf{R}, \mathbf{r})] \phi_{\mu}^A(\mathbf{R}, \mathbf{r}) = \mathcal{E}_{\mu} \phi_{\mu}^A(\mathbf{R}, \mathbf{r}) \quad (23)$$

are used to simplify matrix elements.

The resulting Fock-Tani Hamiltonian is given by

$$\begin{aligned} \hat{H}_0 = & \sum_{\nu} E_{\nu} \hat{\epsilon}_{\nu}^{\dagger} \hat{\epsilon}_{\nu} + \sum_{\mu} \mathcal{E}_{\mu} \hat{\alpha}_{\mu}^{\dagger} \hat{\alpha}_{\mu} + \int d\mathbf{r} \hat{e}^{\dagger}(\mathbf{r}) \hat{T}_e(\mathbf{r}) \hat{e}(\mathbf{r}) \\ & + \int d\mathbf{R} \hat{a}^{\dagger}(\mathbf{R}) T_a(\mathbf{R}) \hat{a}(\mathbf{R}) \end{aligned} \quad (24)$$

and

$$\begin{aligned} \hat{V} = & \int d\mathbf{r} d\mathbf{r}' \hat{e}^{\dagger}(\mathbf{r})(\mathbf{r} | V_e | \mathbf{r}') \hat{e}(\mathbf{r}') + \sum_{\mu} \sum_{\gamma} \hat{\alpha}_{\mu}^{\dagger}(\mu | V_b | \gamma) \hat{\alpha}_{\gamma} \\ & + \sum_{\mu} \int d\mathbf{R} d\mathbf{r} [\hat{\alpha}_{\mu}^{\dagger}(\mu | V_b | \mathbf{R}, \mathbf{r}) \hat{e}(\mathbf{r}) \hat{a}(\mathbf{R}) + \text{H.c.}] + \sum_{\mu} \sum_{\nu} \int d\mathbf{R} [\hat{\alpha}_{\mu}^{\dagger}(\mu | V_b | \mathbf{R}, \nu) \hat{\epsilon}_{\nu} \hat{a}(\mathbf{R}) + \text{H.c.}] \\ & + \int d\mathbf{R} d\mathbf{r} d\mathbf{r}' \hat{a}^{\dagger}(\mathbf{R}) \hat{e}^{\dagger}(\mathbf{r})(\mathbf{R}, \mathbf{r} | H_{ae} | \mathbf{R}', \mathbf{r}') \hat{e}(\mathbf{r}') \hat{a}(\mathbf{R}') \\ & + \sum_{\nu} \int d\mathbf{R} d\mathbf{r} d\mathbf{r}' [\hat{a}^{\dagger}(\mathbf{R}) \hat{e}^{\dagger}(\mathbf{r})(\mathbf{R}, \mathbf{r} | H_{ae} | \mathbf{R}', \nu) \hat{\epsilon}_{\nu} \hat{a}(\mathbf{R}') + \text{H.c.}] \\ & + \sum_{\nu} \sum_{\tau} \int d\mathbf{R} d\mathbf{R}' \hat{a}^{\dagger}(\mathbf{R}) \hat{\epsilon}_{\nu}^{\dagger}(\mathbf{R}, \nu | H_{ae} | \mathbf{R}', \tau) \hat{\epsilon}_{\tau} \hat{a}(\mathbf{R}'), \end{aligned} \quad (25)$$

where H.c. denotes Hermitian conjugate. The matrix elements are given in Appendix B.

### III. COMPARISON TO THE THREE-BODY FOCK-TANI HAMILTONIAN

The asymptotic states for the charge-transfer reaction

$$a^+ + (b^+ e^-) \rightarrow (a^+ e^-) + b^+ \quad (26)$$

are

$$|\phi_i\rangle = (2\pi)^{-3/2} \int d\mathbf{R} \exp(i\mathbf{k}_i \cdot \mathbf{R}) \hat{a}^{\dagger}(\mathbf{R}) \hat{\epsilon}_{\rho}^{\dagger} |0\rangle, \quad (27)$$

with energy eigenvalue

$$\mathcal{E}_i = \frac{k_i^2}{2M} + E_{\rho}, \quad (28)$$

and

$$\langle \phi_f | = \langle 0 | \hat{\alpha}_{\mu}, \quad (29)$$

with energy eigenvalue

$$\mathcal{E}_{\mu} = \frac{k_f^2}{2M_f} + E_{\nu}. \quad (30)$$

The final-state three-body reduced mass  $M_f$  is given by interchanging  $a$  and  $b$  in (6). Note that (27) is a specific asymptotic state so that there is no sum over spin implied in the integral.

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

$$T_{fi}^1 = \langle \phi_f | \hat{V} | \phi_i \rangle = T_{fi}^{1B} + T_{fi}^{1O}, \quad (31)$$

where, from (25) and Appendix B,

$$\begin{aligned} T_{fi}^{1B} = & (2\pi)^{-3/2} \int d\mathbf{R} d\mathbf{r} \phi_{\mu}^{A*}(\mathbf{R}, \mathbf{r}) \left[ \frac{Z_a Z_b}{|\mathbf{R} + \lambda \mathbf{r}|} - \frac{Z_b}{r} \right] \\ & \times u_{\rho}^E(\mathbf{r}) \exp(i\mathbf{k}_i \cdot \mathbf{R}) \end{aligned} \quad (32)$$

and

$$T_{fi}^{1O} = -(2\pi)^{-2/3} \int d\mathbf{R} d\mathbf{r} d\mathbf{R}' d\mathbf{r}' \phi_{\mu}^{A*}(\mathbf{R}', \mathbf{r}') \left[ \frac{Z_a Z_b}{|\mathbf{R}' + \lambda \mathbf{r}'|} - \frac{Z_b}{r'} \right] \Delta^A(\mathbf{R}', \mathbf{r}'; \mathbf{R}, \mathbf{r}) u_{\rho}^E(\mathbf{r}) \exp(i\mathbf{k}_i \cdot \mathbf{R}), \quad (33)$$

Because (27) and (29) are specific asymptotic states, and because the Kronecker deltas in (16) include spin quantum numbers, the integrals over unprimed variables in (32) and (33) have no implied sum over spin. Also, because  $\Delta$  is diagonal in spin<sup>6</sup> there is a no sum over spin in the integrals over primed variables in (33). Therefore, all subsequent integrals have no implied sum over spin.

Substituting (14) into (32) and changing variables to

$$\mathbf{r}' = \gamma \mathbf{r} - \mathbf{R}, \quad (34)$$

gives

$$T_{fi}^{1B} = (2\pi)^{-3} \int d\mathbf{r}' d\mathbf{r} e^{-i\mathbf{C} \cdot \mathbf{r}'} u_{\nu}^{A*}(\mathbf{r}') \times \left[ \frac{Z_a Z_b}{|\mathbf{r} - \mathbf{r}'|} - \frac{Z_b}{r} \right] u_{\rho}^E(\mathbf{r}) e^{i\mathbf{B} \cdot \mathbf{r}}, \quad (35)$$

where  $\mu = \{k_f, \nu\}$  and

$$\mathbf{C} = \mathbf{k}_i - \zeta \mathbf{k}_f, \quad \mathbf{B} = \gamma \mathbf{k}_i - \mathbf{k}_f, \quad (36)$$

which is the result of Ojha *et al.*<sup>3</sup>

For the orthogonalization term (33), change variables to

$$\mathbf{R} = \gamma \mathbf{r}_3 - \iota \mathbf{r}_1, \quad \mathbf{r} = \mathbf{r}_3 + \zeta \mathbf{r}_1, \quad (37)$$

for both primed and unprimed variables. Then the final-state wave function (14) becomes simply

$$\phi_{\mu}^A(\mathbf{R}, \mathbf{r}) = (2\pi)^{-3/2} e^{i\mathbf{k}_f \cdot \mathbf{r}_3} u_{\nu}^A(\mathbf{r}_1). \quad (38)$$

Integration over the momentum variables in the corresponding bound-state kernel (B13) gives

$$\Delta^A(\mathbf{R}', \mathbf{r}'; \mathbf{R}, \mathbf{r}) = \delta(\mathbf{r}'_3 - \mathbf{r}_3) \sum_{\tau} u_{\tau}^A(\mathbf{r}') u_{\tau}^{A*}(\mathbf{r}_1), \quad (39)$$

so that (33) becomes

$$T_{fi}^{1O} = -(2\pi)^{-3} \sum_{\tau} \int d\mathbf{r}_1 d\mathbf{r}_3 d\mathbf{r}'_1 e^{+i\mathbf{B} \cdot \mathbf{r}_3} u_{\nu}^{A*}(\mathbf{r}'_1) \times u_{\tau}^A(\mathbf{r}'_1) u_{\tau}^{A*}(\mathbf{r}_1) \times \left[ \frac{Z_a Z_b}{|\mathbf{r}_3 - \eta \mathbf{r}'_1|} - \frac{Z_b}{|\mathbf{r}_3 + \zeta \mathbf{r}'_1|} \right] \times u_{\rho}^E(\mathbf{r}_3 + \zeta \mathbf{r}_1) e^{-i\mathbf{k}_i \cdot \mathbf{r}_1}, \quad (40)$$

where  $\mathbf{B}$ , given in (36), equal  $-\mathbf{q}_1$  in Eq. (4.8a) of Ojha *et al.*,<sup>3</sup> and  $\iota$ , given in (13), equals  $\mathbf{m}$  of their Eq. (4.8b). Therefore, the Fock-Tani transformation of the (initial-state) Jacobi three→two-body reduced-mass Fock Hamiltonian (1) gives a matrix element for charge transfer (35)

and (40) that is entirely equivalent to that given by the Fock-Tani transformation of the full three-body Hamiltonian of Ojha *et al.* In Appendix A it is shown that the same is not true of matrix elements of the Fock-Tani transformation of the symmetrical three→two-body reduced-mass equivalent to (1).

#### IV. ANALYTIC REDUCTION OF MATRIX ELEMENTS

Equations (35) and (40) can be analytically reduced to forms allowing numerical integration. Apart from a factor of  $2\pi$ , which is absorbed in the definition of the differential cross section for rearrangement,

$$\frac{d\sigma}{d\Omega}(\theta\phi) = (2\pi)^4 M_i M_f \frac{k_f}{k_i} |T_{fi}|^2 \quad (41)$$

[where the reduced masses for the initial and final states are given by (6) and an identical relation with  $a$  and  $b$  interchanged, respectively, and where the  $k$ 's are center-of-mass momenta],<sup>12</sup> (35) equals the post form of the first-Born term found by Jackson and Schiff<sup>9</sup> [their Eqs. (12) and (8')]. The second term in (35) is the Brinkman-Kramers<sup>13</sup> (BK) term given explicitly by

$$T_{fi}^{\text{BK}} = - \left[ \frac{\mathbf{B}^2}{2m_i} - E_{\rho} \right] u_{\rho}^E(\mathbf{B}) u_{\nu}^{A*}(\mathbf{C}), \quad (42)$$

where  $m_i = 1/a_0$  is the two-body reduced mass in (7). (Note that Jackson and Schiff set  $-E_{\rho} = \epsilon$ .)

Using the normalization convention

$$f(\mathbf{k}) = (2\pi)^{-3/2} \int d\mathbf{w} e^{-i\mathbf{k} \cdot \mathbf{w}} f(\mathbf{w}), \quad (43)$$

the hydrogenic 1s momentum wave function is

$$u_{1s}(\mathbf{p}) = \frac{2\sqrt{2}}{\pi} P_0^{5/2} \frac{1}{(P_0^2 + p^2)^2}. \quad (44)$$

For ease of notation define

$$\beta = P_0^E = Z_b/a_0^E \quad \text{and} \quad \alpha = P_0^A = Z_a/a_0^A, \quad (45)$$

where  $a_0$  is the initial- or final-state Bohr radius. With the normalizations in (41) and (43) the 1s-1s BK term becomes

$$T_{1s,1s}^{\text{BK}} = - \frac{4\beta^{3/2}\alpha^{5/2}}{\pi^2(\beta^2 + B^2)(\alpha^2 + C^2)^2}. \quad (46)$$

The first term in (35), for  $\rho = \nu = 1s$ , is given by Eq. (II.3) of Jackson and Schiff,<sup>9</sup> but with the expression for  $\Delta$  generalized to allow  $\beta \neq \alpha$  and with the normalizations in (41) and (43),

$$T_{1s,1s}^{\text{JS1}} = 4/\pi^2 \int_0^1 dx x(1-x) \left[ \frac{2}{\Delta^3(\Delta - q^2)^{1/2}} + \frac{1}{\Delta^2(\Delta - q^2)^{3/2}} + \frac{3/4}{\Delta(\Delta - q^2)^{5/2}} \right], \quad (47)$$

where

$$\Delta = \beta^2 + x(\alpha^2 - \beta^2 + C^2) + (1-x)B^2 \quad (48)$$

and

$$\mathbf{q} = x\mathbf{C} + (1-x)\mathbf{B} . \quad (49)$$

In calculating the cross sections for  $p^+ + \text{H} \rightarrow \text{H} + p^+$ , Ojha *et al.*<sup>3</sup> note that if  $\eta$  is small then the denominator of the first term in (40) can be approximated by  $r_3$ , allowing the  $r_1'$  integral to be done. The resulting expression is the negative of the first term of (32) rewritten by changing variables to  $r_1$  and  $r_3$  and neglecting  $\eta$ . This cancellation fulfills, at first order, Wick's expectation<sup>9</sup> that the internuclear potential should make a negligible contribution to the exact  $T$  matrix.

For the reaction  $e^+ + \text{H} \rightarrow \text{Ps} + p^+$ ,  $\eta$  cannot be neglected because  $m_a = m_e$ . But because of the similarity of the form of the two terms in (40), the analytical reduction of the first term follows exactly the procedure Ojha *et al.*<sup>3</sup> used for the second term. 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 together, and they differ in sign for even  $l$ , so that they cancel. The generalization of their result [their Eq. (5.10)] is

$$T_{\tau \leftarrow 1s}^{10} = Z_a Z_b T_{\tau \leftarrow 1s}^0(-m_e/m_a) - Z_b T_{\tau \leftarrow 1s}^0(1) , \quad (50)$$

where

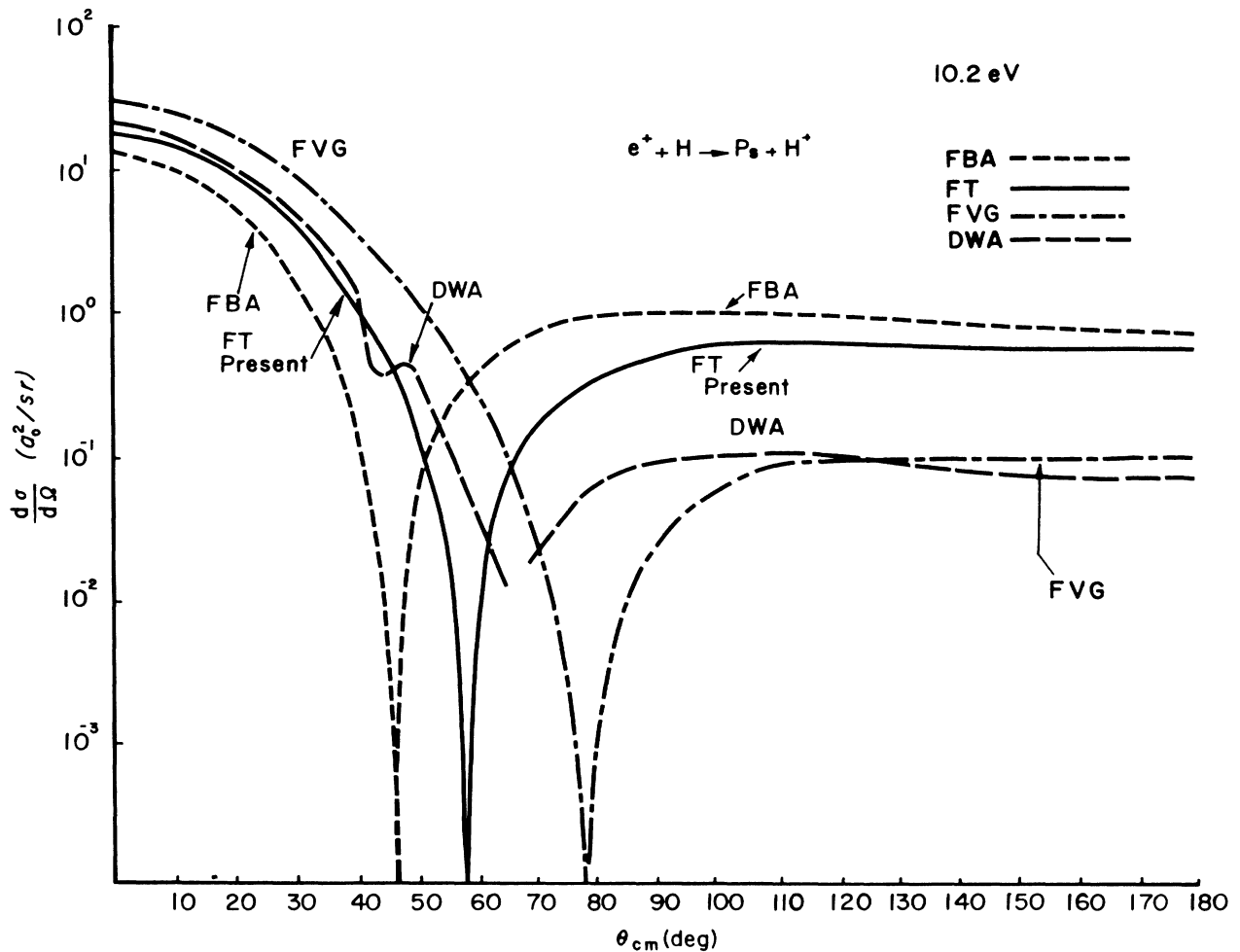


FIG. 1. Differential cross section for positronium formation at 10.2 eV. The short-dashed curve is the FBA, the long-dashed curve is the DWA of Mandel *et al.* (Ref. 16), the dot-dashed curve is the Fock-Tani result of Ficocelli Varracchio and Girardeau (Ref. 15) (FVG), and the solid curve is the present Fock-Tani result.

$$T_{Ns, k_f \leftarrow 1s, k_i}^O(s) = -\frac{\xi^3}{\sqrt{2\pi^3}} \sum_{n,l} (2l+1) \int dp d\theta \sin\theta \frac{p^2}{|\mathbf{p}+\mathbf{C}|} R_{nl}^A(p) \times I_{Ns, nl} [ |s(\mathbf{p}+\mathbf{C})| ] P_l \left[ \frac{s\mathbf{p}\cdot(\mathbf{p}+\mathbf{C})}{p |s(\mathbf{p}+\mathbf{C})|} \right] \frac{A}{(A^2 - D^2)^{3/2}}, \quad (51)$$

where  $[(2\pi)^{3/2}$  times] the radial part of the Fourier transforms of the product of the first six pairs of one-center hydrogenic orbitals are

$$I_{1s, 1s}(p) = \frac{32\sqrt{\pi}}{[4+(p/P_0)^2]^2}, \quad (52)$$

$$I_{1s, 2s}(p) = \frac{512\sqrt{2\pi}(p/P_0)^2}{[9+4(p/P_0)^2]^3}, \quad (53)$$

$$I_{1s, 2p}(p) = \frac{-i 256\sqrt{6\pi}(p/P_0)}{[9+4(p/P_0)^2]^3}, \quad (54)$$

$$I_{1s, 3s}(p) = \frac{864\sqrt{3\pi}[16(p/P_0)^2+27(p/P_0)^4]}{[16+9(p/P_0)^2]^4}, \quad (55)$$

$$I_{1s, 3s}(p) = \frac{-i 576\sqrt{6\pi}(p/P_0)[16+27(p/P_0)^2]}{[16+9(p/P_0)^2]^4}, \quad (56)$$

and

$$I_{1s, 3d}(p) = \frac{-13824\sqrt{30\pi}(p/P_0)^2}{5[16+9(p/P_0)^2]^4}. \quad (57)$$

$R$  is the final-state radial hydrogenic wave function,

$$A = \xi^2 + p^2 + 2ipk_i \cos\theta_p \cos\theta_{k_i} + i^2 k_i^2, \quad (58)$$

and

$$D = 2ipk_i \sin\theta_p \sin\theta_{k_i}. \quad (59)$$

## V. DIFFERENTIAL AND TOTAL CROSS SECTIONS

A general-mass computer program for the differential and total scattering cross sections for reaction (26) was written using the forms (46), (47), and (50) for the Fock-

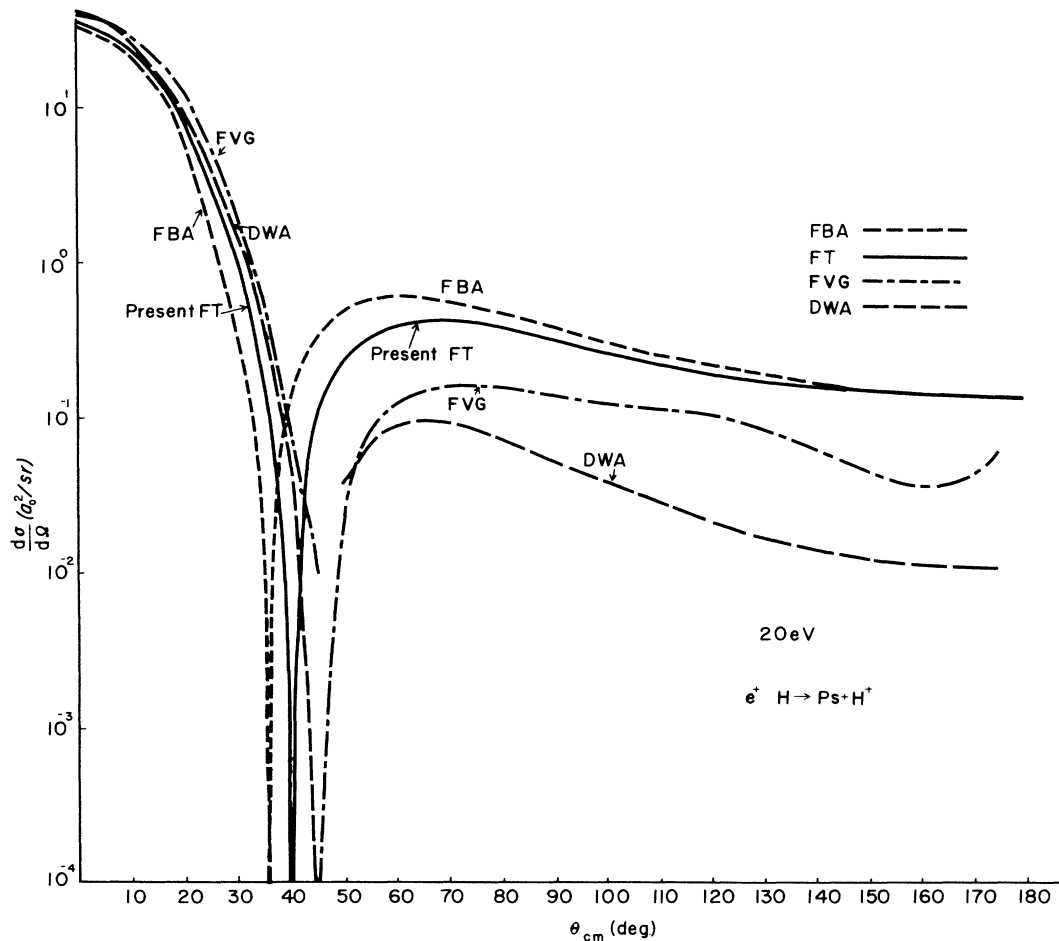
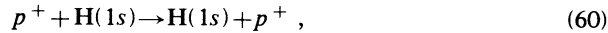


FIG. 2. Differential cross section for positronium formation at 20 eV. The curves are labeled as in Fig. 1.

Tani  $T$  matrix. The integrations were done numerically using 16-point Gaussian quadrature. The upper limit of the  $p$  integration and the number of subregions were varied until a consistent result was found. This program was run for  $(abc) = \{(ppe), (epe), (\mu p\mu), (\mu d\mu), \text{ and } (\mu t\mu)\}$ .

#### A. Results for the proton-hydrogen initial state

To check the approximation made in Ojha *et al.*<sup>3</sup> in which the internuclear potential was neglected for the reaction



the present program was run with and without such contributions. The latter reproduces the result of Ojha *et al.* to order  $1/m_{\text{prot}}$ . 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%. At an incident (c.m.) energy of 25 keV, the differential cross section of the former was found to be 12% larger than the latter at 0 mrad and 18% smaller at 3 mrad. Also inclusion removes the slight oscillations

found in Ojha *et al.* in this region (see their Fig. 4). Good agreement with the experimental result of Martin *et al.*<sup>5</sup> exists for angles within 1 mrad of the forward direction at 25, 60, and 125 keV in either case.

At 25 keV the total cross section excluding  $p$ - $p$  terms is 18% smaller than when these terms are included. In contrast, the Brinkman-Krammers<sup>13</sup> result, which excludes the  $p$ - $p$  term, is 1000% larger than the first-order Jackson and Schiff total cross section, which includes this term.<sup>9</sup> Thus the orthogonalization corrections inherent in the Fock-Tani representation, in addition to giving a first-order total cross section that agrees with experimental results of McClure<sup>4</sup> for energies greater than 10 keV, produces agreement at first order between experiment and Wick's expectation<sup>9</sup> that the internuclear potential should play a negligible role in exact calculations of this process. It is interesting to note that Bates<sup>14</sup> predicted in 1958 that accounting for orthogonalization would give such a resolution.

A check on the inclusion of the  $3s$ ,  $3p$ , and  $3d$  orthogonalization terms gives a difference of order 1%. At 25 keV the differential cross section including these terms was 1% smaller at 0 mrad and 3% larger at 3 mrad. The

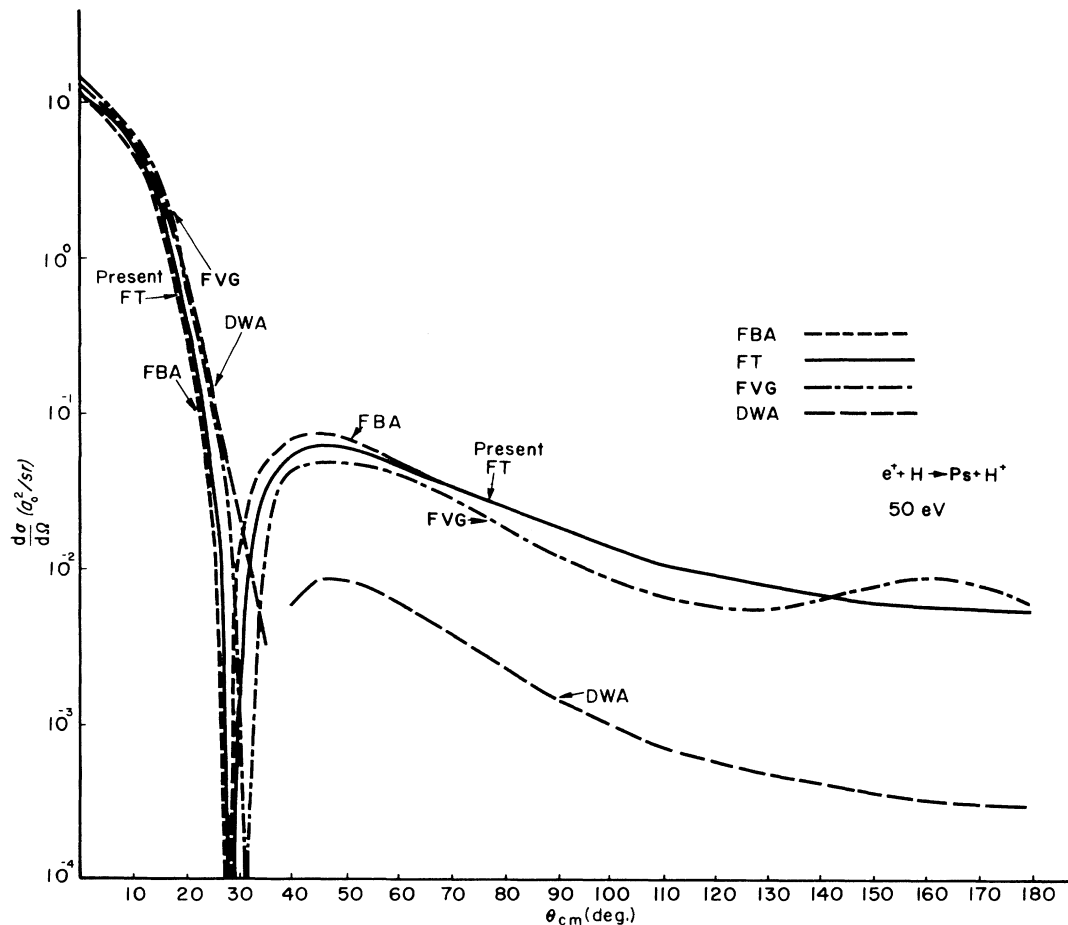
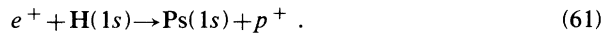


FIG. 3. Differential cross section for positronium formation at 50 eV. The curves are labeled as in Fig. 1.

total cross section including these terms was 0.3% smaller.

### B. Results for the positron-hydrogen initial state

The present program was also run for the reaction



The differential cross sections at energies of 10.2, 20, 50, and 100 eV are given in Figs. 1–4, respectively. Figure 5 shows the forward scattering cross section over this range of energies. A comparison is made between the first-Born result (FBA), the present first-order Fock-Tani result (FT), which contains higher-order contributions, and that of Ficocelli Varracchio and Girardeau (FVG),<sup>15</sup> and the distorted-wave approximation (DWA) of Mandal *et al.*<sup>16</sup>

The present result and that of Ficocelli Varracchio, and Girardeau do not agree. The results given in Ojha *et al.*<sup>3</sup> for reaction (58) were calculated by three independent methods. In addition to the method outlined by Ojha

*et al.*, the quantity  $\lambda$  of (32) can be set to zero for energies less than 5 keV. Analytic integration is then possible and was done for  $\tau$  from 1s to 3d. In the third method, a program containing a solution for the  $I$ 's of (51) for arbitrary quantum numbers, in the  $\lambda=0$  approximation, gave numerical results that matched the other two. Because the present program is capable of reproducing these results it is also likely to give the correct Fock-Tani result for (61).

Equations (24) and (27) in Ficocelli Varracchio and Girardeau<sup>15</sup> 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 altering the present program to use the incorrect coefficients does not reproduce their result. In any case, Ficocelli Varracchio has assured me that the computer program he used has the correct coefficients 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 Figs. 2 and 3. In the 100–180-deg region their results show oscillations characteristic of convergence problems.

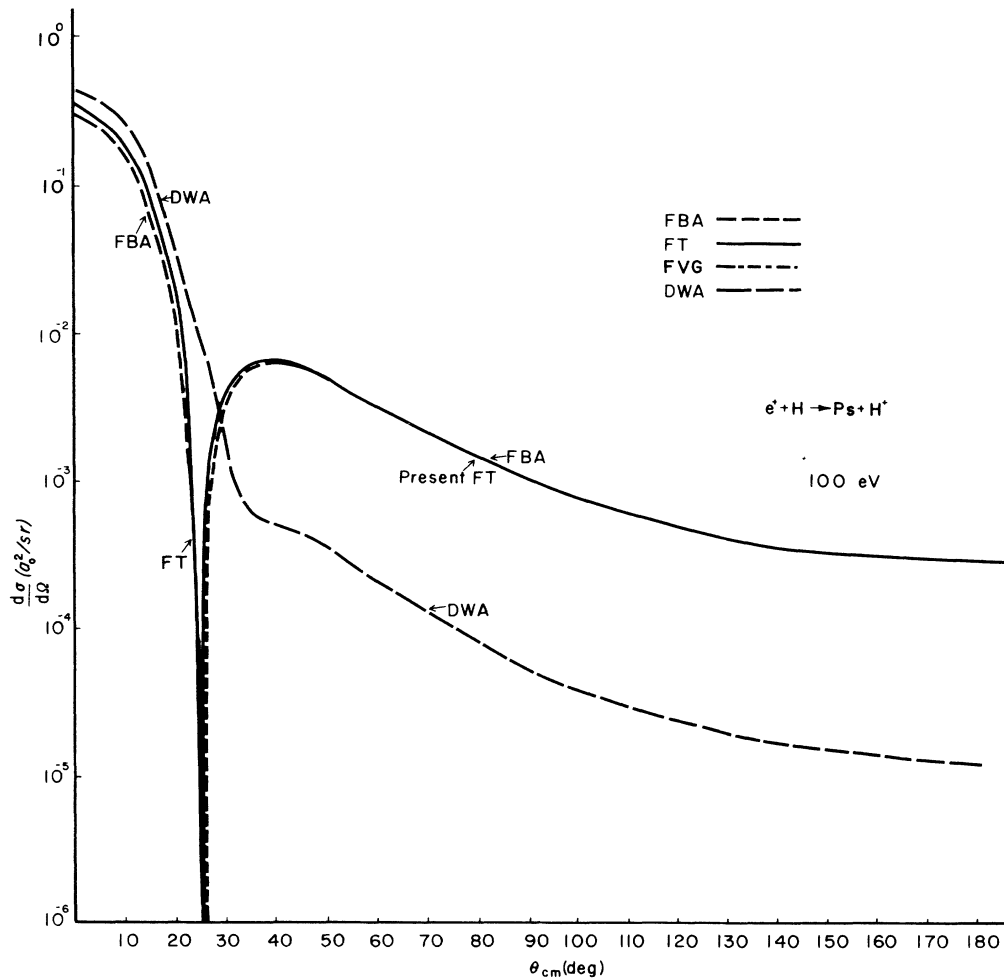


FIG. 4. Differential cross section for positronium formation at 100 eV. The curves are labeled as in Fig. 1.



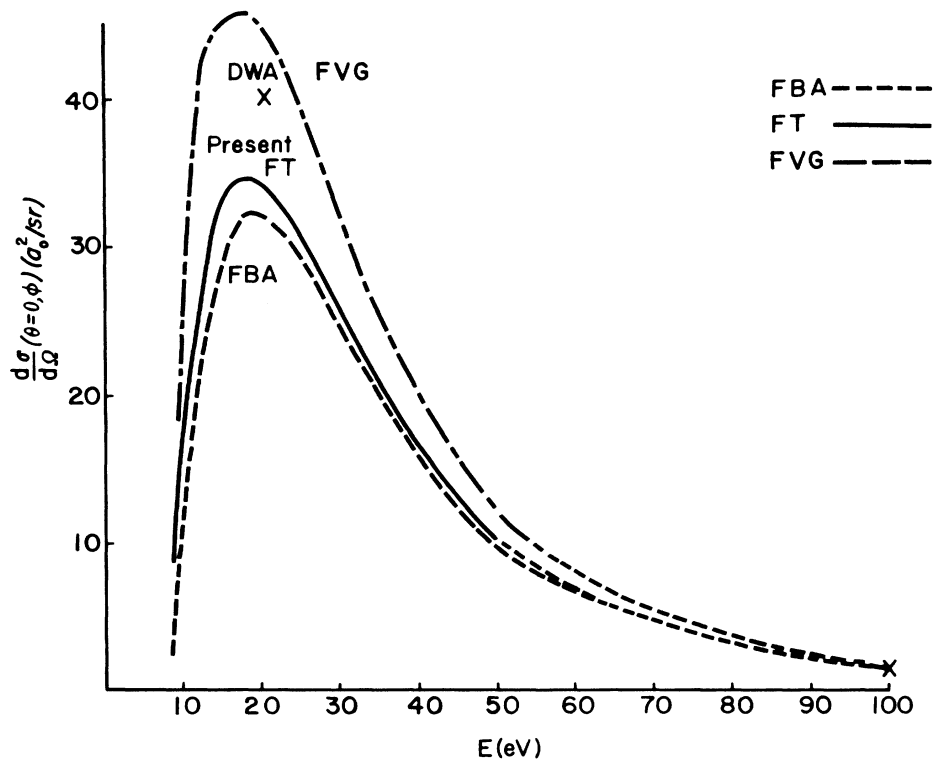


FIG. 5. Forward scattering for positronium formation. The short-dashed curve is the FBA, the  $\times$ 's are the DWA of Mandal *et al.* (Ref. 16), the dot-dashed curve is the Fock-Tani result of Ficocelli Varracchio and Girardeau (Ref. 15) (FVG), and the solid curve is the present Fock-Tani result.

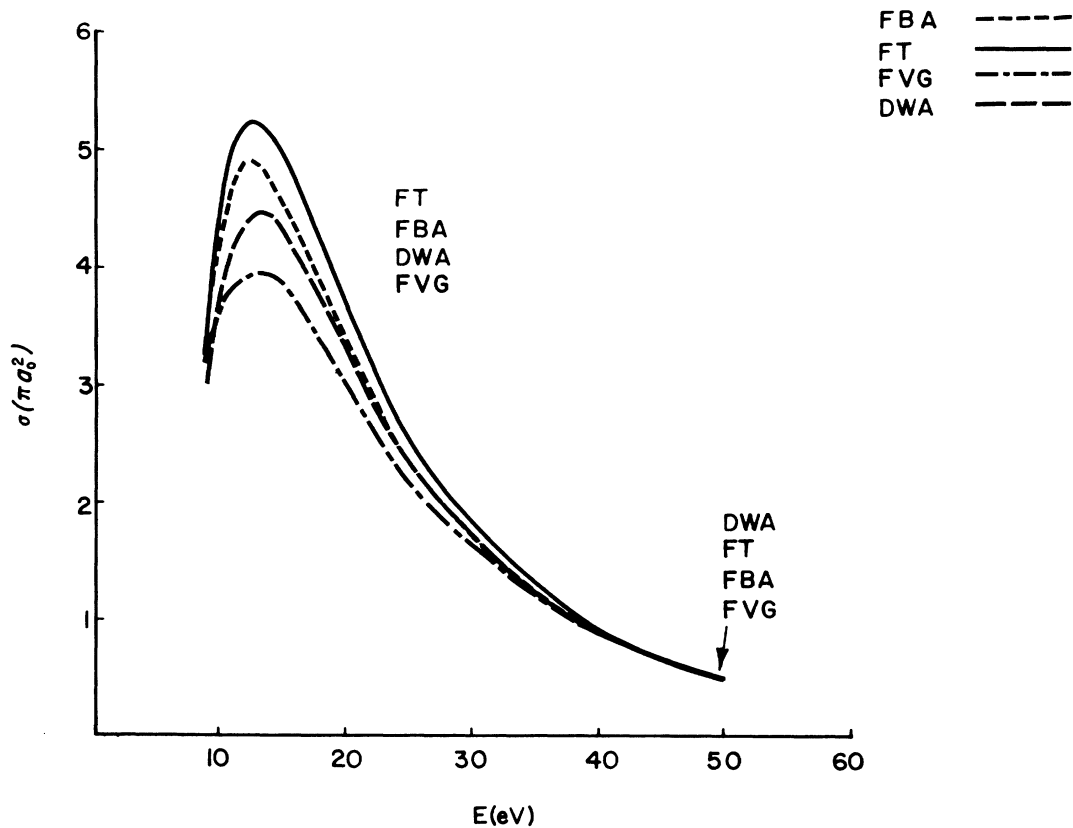


FIG. 6. Total cross section for positronium formation. The curves are labeled in Fig. 1.

The present Fock-Tani calculation for the total cross section, Fig. 6, gives a larger result than does the FBA, whereas the result of Ficocelli Varracchio and Girardeau is less than the FBA. In examining the differential cross sections it might appear that the present result should fall between their result and the FBA. But this is an illusion resulting from relative magnitude compression due to the logarithmic scale. The present result was confirmed by separately integrating the partial cross sections for the angles where the FT cross section is greater than the FBA cross section, and less than the FBA cross section, and for the transition region, and then adding these three.

A comparison of the FT differential cross sections with the DWA results of Mandal *et al.*<sup>16</sup> and with the FBA (Figs. 1–5) shows the FT to be intermediate between the latter two. The first-order Fock-Tani  $T$  matrix contains more physics than the nonorthogonal 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 momentum eigenstates of the full Hamiltonian (20) should contain in the interaction region. Therefore, it is not surprising that the Fock-Tani result is intermediate between the first-Born and distorted-wave approximations.

Because of averaging, the FT total cross section (Fig. 6) does not lie between the FBA and the DWA, but is larger than the FBA by about the same amount as the DWA is smaller than the FBA.

As a final note, the addition of the  $3p$  orthogonalization

term results in changes of order 0.1%. The  $3s$  orthogonality corrections to each of the two potential terms are of the same order as the  $2p$  corrections, but since the  $s$ -state terms cancel each other they do not contribute.

### C. $(\mu^+\mu^-)$ from muonic hydrogen, deuterium, and tritium

A parallel to the formation of positronium, a bound state of an electron, and its antiparticle, is the formation of the bound state  $(\mu^+\mu^-)$ . This has been given the name “mu-muonium” because the more consistent name muonium was used in the naming of the  $(\mu^+e^-)$  bound state.<sup>17</sup> The muon is a fermion [with mass  $m_\mu = 206.76859(29)m_e$  (Ref. 18)] so that no hadronic interactions obscure the tests of electromagnetic interactions involving muons and electrons. Recently Conti *et al.*<sup>19</sup> have proposed using one-photon transitions in positronium as a test of CPT invariance, a test that could be applied to mu-muonium. 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).<sup>20</sup> But because the Bohr radii for mu-muonium ( $0.00967265a_0$ ), muonic hydrogen [ $(\mu^-p^+)$ ,  $0.00538094a_0$ ], muonic deuterium [ $(\mu^-d^+)$ ,  $0.00510877a_0$ ], and muonic tritium [ $(\mu^-dt^+)$ ,  $0.00501824a_0$ ] (Ref. 21) are so much smaller than that for muonium ( $0.99518605a_0$ ), one would expect QED effects to be much larger.

Muonic-hydrogen isotopes are also of importance in ca-

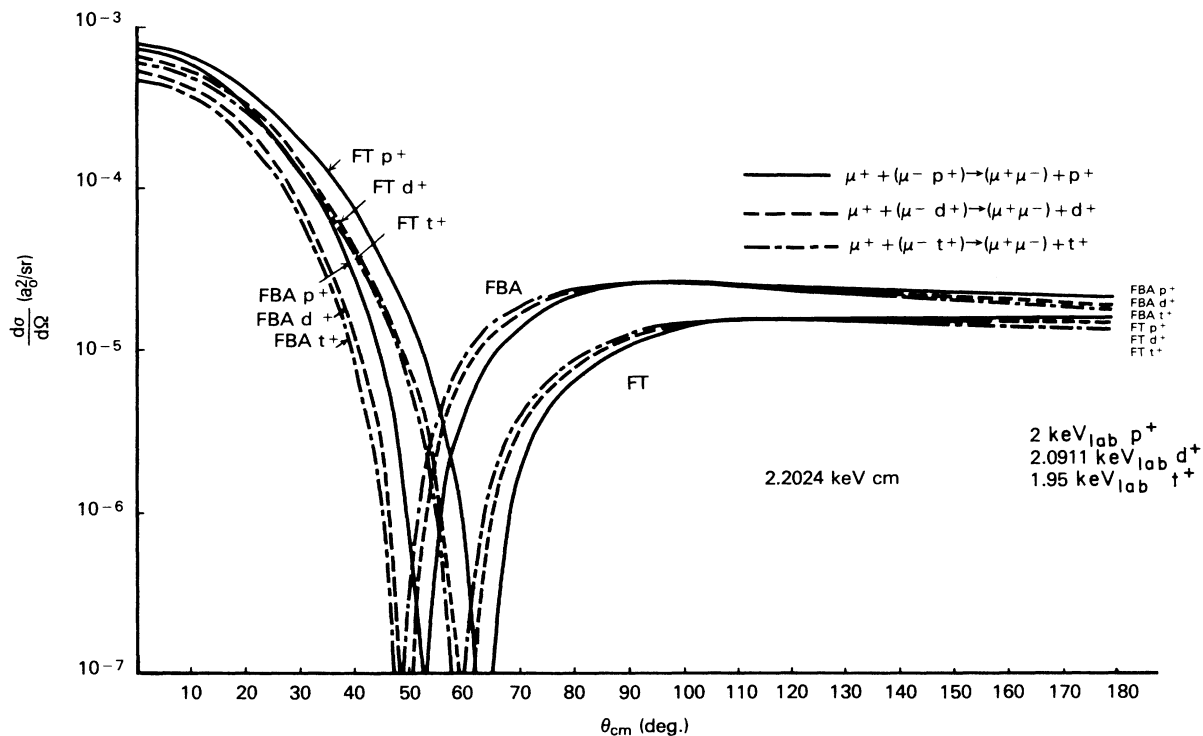


FIG. 7. Differential cross section for muonium formation at 2.2024 keV. The solid, dashed, and dot-dashed curves are for muonic hydrogen, muonic deuterium, and muonic tritium, respectively. Both first-order Born and Fock-Tani results are shown.

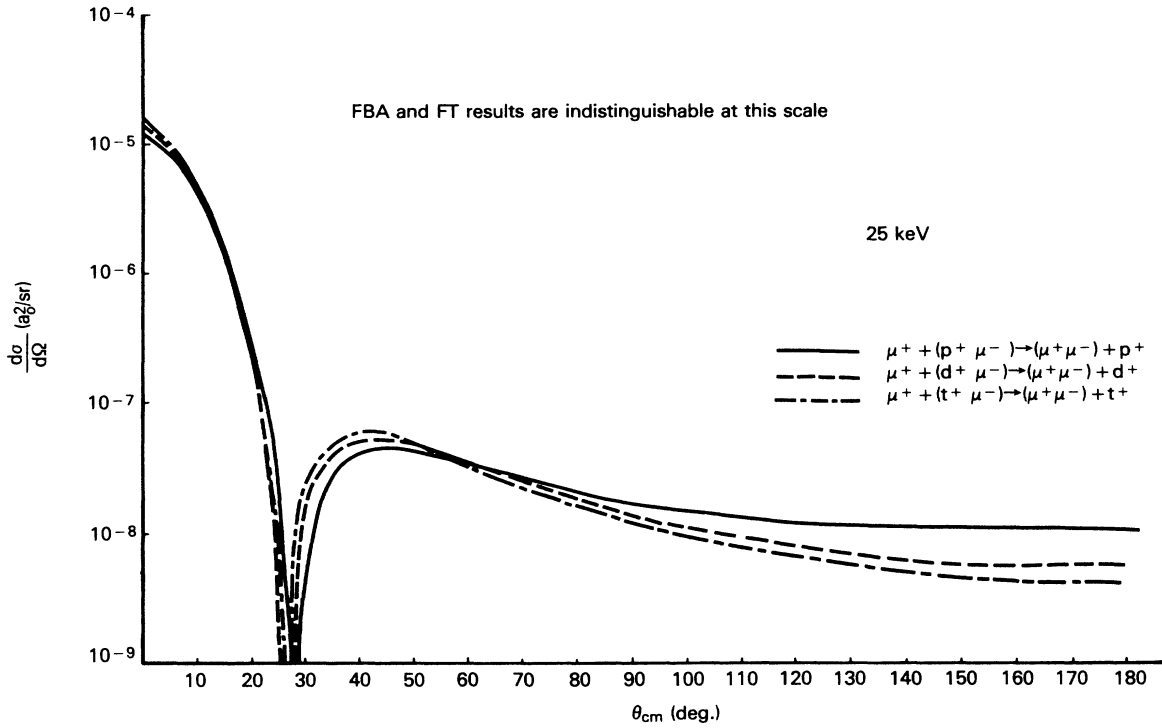
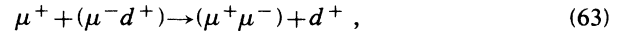
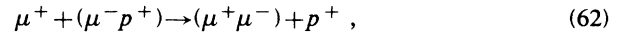


FIG. 8. Differential cross section for mu-muonium formation at 25 keV. The curves are labeled as in Fig. 7.

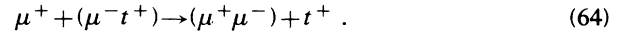
talyzed fusion, again because of the small Bohr radius. One of the most interesting processes from the standpoint of a theory, such as Fock-Tani, that gives an exact accounting of composite states is the initial formation of  $(d\mu)$ , subsequent formation of  $(d\mu d)^+$ , followed rapidly by nuclear fusion. The muon is then free ( $f \approx 87\%$ ) to catalyze another fusion.<sup>22</sup> Charge-transfer cross sections involving the  $(ped)^+$  intermediate state have been studied in Fock-Tani representation by Hsu.<sup>23</sup> 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, protons, deuterons, and tri-

tons, but for the present consider only the formation of muonium from muonic-hydrogen isotopes by charge transfer,



and



Figures 7 and 8 show the differential cross sections for these processes at c.m. energies of 2.2024 and 25 keV, respectively, in first-order Born and Fock-Tani approxi-

TABLE I. Total cross sections for reaction (74). The notation  $1.234[-5]$  means  $1.234 \times 10^{-5}$ .

Lab energy of projectile	FBA	FT (units of $\pi a_0^2$ )	DWBA (Ref. 27)	CTMC <sup>a</sup>
1.121 90	1.090[-10]	1.608[-7]		
1.130 00	9.928[-7]	1.285[-5]	1.47[-10]	
1.200 00	2.445[-5]	5.234[-5]	4.80[-5]	
1.700 00	1.617[-4]	1.772[-3]	1.79[-4]	
2.000 00	1.768[-4]	1.869[-4]	1.89[-4]	
2.400 00	1.670[-4]	1.738[-4]	1.75[-4]	4.0[-5]
3.600 00	1.046[-4]	1.085[-4]	1.09[-4]	3.8[-5]
5.000 00	5.667[-5]	5.890[-5]		
6.000 00	3.745[-5]	3.893[-5]		
7.000 00	2.538[-5]	2.638[-5]	2.79[-5]	1.8[-5]
10.000 00	9.057[-6]	9.402[-6]		
20.000 00	7.506[-7]	7.878[-7]	9.76[-7]	4.8[-7]
100.000 00	3.467[-10] <sup>b</sup>	3.471[-10]	6.02[-10]	

<sup>a</sup>Estimated from graph (Ref. 25).

<sup>b</sup>The value given by Ma *et al.* (Ref. 24) is  $3.48[-10]$ .

TABLE II. Total cross sections for reactions (74), (75), and (76). The notation  $1.234[-5]$  means  $1.234 \times 10^{-5}$ .

Lab energy of projectile	Muonic hydrogen FT	Muonic deuterium		Muonic tritium	
		FBA	FT	FBA	FT
		(units of $\pi a_0^2$ )			
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]		

mations. The former cross section is near the energy of the maximum in the total cross section for (61),  $2 \text{ keV}_{\text{lab}}$ . A comparison to the FBA and FT graphs in Fig. 1, the differential cross section at an energy near the positronium formation cross section maximum  $10.2 \text{ eV}$ , shows many similarities. Likewise, a comparison of the muonium differential cross section at about ten times the formation maximum  $25 \text{ keV}$ , and the corresponding positronium differential cross section at about ten times the formation maximum  $100 \text{ eV}$  (Fig. 4), shows similarities in overall shape. This correspondence is not surprising considering the mass-scaling property demonstrated for the FBA total cross sections by Ma *et al.*<sup>24</sup> and by Ohsaki *et al.*<sup>25</sup> using a classical trajectory Monte Carlo (CTMC) method.

Table I compares the present first-order Fock-Tani and first-Born approximation total cross section to the first-order distorted-wave approximation of Ma *et al.*,<sup>24</sup> and to the CTMC of Ohsaki *et al.*<sup>25</sup> (The present FBA agrees with the result of Ma *et al.* except at  $1.13 \text{ keV}$ . This may be 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  $7 \text{ keV}$ , the range spanning the maximum in the cross section. This is much better agreement than for the positronium case (Fig. 6), perhaps due to a somewhat different choice of distorting potentials.

Table II compares the muonic-hydrogen, -deuterium,

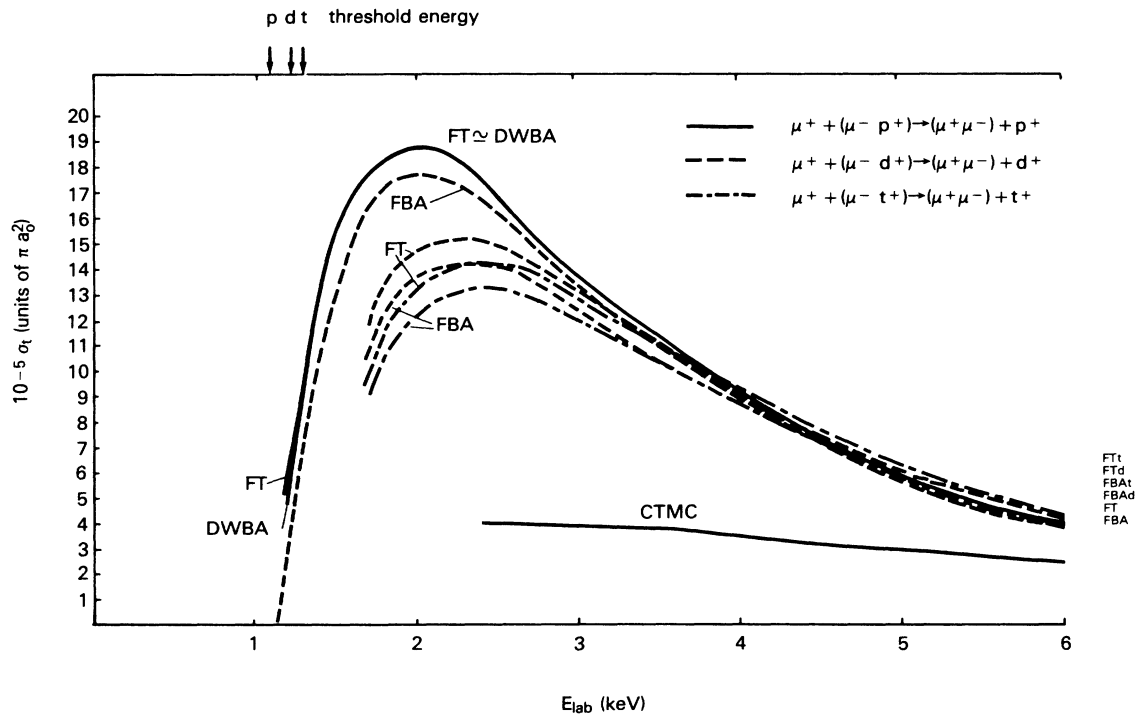


FIG. 9. Total cross section for mu-muonium formation. The curves are labeled as in Fig. 7. Note that the DWBA of Ma *et al.* (Ref. 24) for muonic hydrogen is indistinguishable from the Fock-Tani result at this scale except near threshold. The CTMC result, of Ohsaki *et al.* (Ref. 25) for muonic hydrogen is also shown.

and -tritium cases. The total cross section is fairly insensitive to variation among the heavy isotope initial states except near the threshold energies 1.1289 keV<sub>lab</sub> (1.235 544 keV<sub>c.m.</sub>) for muonic hydrogen, 1.257 29 keV<sub>lab</sub> (1.324 34 keV<sub>c.m.</sub>) for muonic deuterium, and 1.304 65 keV<sub>lab</sub> (1.351 95 keV<sub>c.m.</sub>) for muonic tritium. (Ma *et al.* quote 1.13 keV<sub>lab</sub> for the muonic hydrogen case.)

Because of the small differences in these energies there will only be small differences in the momenta of the bound muon, so that 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. 9.

## VI. DISCUSSION

The equivalence of the Fock-Tani Hamiltonians for an inertial (Jacobi) three→two-body reduced-mass system and for the full three-body system has been established. Considering that the Fock-Tani transformation for the former can be done with roughly half the work of the transformation for the latter, reduced-mass systems should be helpful in finding the Fock-Tani transformation for four-body systems. The four→three-body reduced-mass approach would allow orthogonalization to the three possible bound states with roughly one-third of the work of the full four-body transformation.

Choudhury *et al.*<sup>26</sup> have found the total cross section for the reaction



in the first-Born approximation. Because they use an approximate H<sup>-</sup> wave function, post and prior forms of the *T* matrix give different results. Girardeau's recent generalization<sup>27</sup> of the Fock-Tani approach gives a scattering theory in which the familiar post-prior discrepancy<sup>28</sup> is formally removed so that only one result is possible despite approximate wave functions.

## ACKNOWLEDGMENTS

The author would like to thank Professor Marvin Girardeau for his careful and insightful responses to questions raised throughout the course of this research. This paper is derived from part of the author's dissertation, completed in partial fulfillment of the degree of Doctor of Philosophy at the University of Oregon. This work was supported by the U.S. Office of Naval Research.

## APPENDIX A

In Sec. II the Fock-Tani transformation for the initial-state, inertial three→two-body reduced-mass coordinate system was given. For some problems it may be preferable to work in the symmetrical three→two-body reduced-mass system<sup>29</sup> in which particle *b* is fixed at the origin and the other two particles move in an accelerated frame.

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

$$\begin{aligned} \hat{H}_F = & \int d\mathbf{x} \hat{a}^\dagger(\mathbf{x}) H_a(\mathbf{x}) \hat{a}(\mathbf{x}) + \int d\mathbf{y} \hat{e}^\dagger(\mathbf{y}) H_e(\mathbf{y}) \hat{e}(\mathbf{y}) \\ & + \int d\mathbf{x} d\mathbf{y} \hat{a}^\dagger(\mathbf{x}) \hat{e}^\dagger(\mathbf{y}) [V_{ae}(\mathbf{x}, \mathbf{y}) + W_{ae}(\mathbf{x}, \mathbf{y})] \\ & \times \hat{e}(\mathbf{y}) \hat{a}(\mathbf{x}), \end{aligned} \quad (A1)$$

where the Schrödinger operators are

$$\begin{aligned} H_a(\mathbf{x}) = & T_a(\mathbf{x}) + \frac{Z_a Z_b}{x}, \quad H_e(\mathbf{y}) = T_e(\mathbf{y}) - \frac{Z_b}{y}, \\ T_a(\mathbf{x}) = & -\frac{1}{2\mu_a} \nabla_x^2, \quad T_e(\mathbf{y}) = -\frac{1}{2\mu_e} \nabla_y^2, \end{aligned} \quad (A2)$$

$$\begin{aligned} V_{ae}(\mathbf{x}, \mathbf{y}) = & -\frac{Z_a}{|\mathbf{x} - \mathbf{y}|}, \quad W_{ae}(\mathbf{x}, \mathbf{y}) = -\frac{1}{m_b} \nabla_x \cdot \nabla_y, \\ \mu_a = & \frac{m_a m_b}{m_a + m_b}, \quad \mu_e = \frac{m_e m_b}{m_e + m_b}. \end{aligned} \quad (A3)$$

Because the Schrödinger operators are spectators to the Fock-Tani transformation, one can make the replacement  $R \rightarrow x$  and  $r \rightarrow y$  in (8)–(25) and (B1)–(B13) to get the Fock-Tani Hamiltonian for this accelerated center-of-mass coordinate system, with the following exceptions.

Instead of (14), the final-state wave function is

$$\phi_\mu^A(x, y) = (2\pi)^{-3/2} e^{i\mathbf{k} \cdot (\zeta \mathbf{x} + \eta \mathbf{y})} u_\nu^A(\mathbf{y} - \mathbf{x}), \quad (A4)$$

where  $\mu = \{\mathbf{k}, \nu\}$  and where  $\zeta$  and  $\eta$  are given by (12). Eigenvalue relation (23) is replaced by

$$\begin{aligned} [T_a(\mathbf{x}) + T_e(\mathbf{y}) + V_{ae}(\mathbf{x}, \mathbf{y}) + W_{ae}(\mathbf{x}, \mathbf{y})] \phi_\mu^A(\mathbf{x}, \mathbf{y}) \\ = \mathcal{E}_\mu \phi_\mu^A(\mathbf{x}, \mathbf{y}) \end{aligned} \quad (A5)$$

[a finite mass generalization of Girardeau's Eq. (26)],<sup>6</sup> with eigenvalue given by (30). The Fock-Tani potential (25) has an additional term with a form similar to the first,

$$\begin{aligned} \hat{V} = & \int d\mathbf{y} d\mathbf{y}' \hat{e}^\dagger(\mathbf{y}) (\mathbf{y} | V_e | \mathbf{y}') \hat{e}(\mathbf{y}') + \int d\mathbf{x} \hat{a}^\dagger(\mathbf{x}) \frac{Z_a Z_b}{x} \hat{a}(\mathbf{x}) + \sum_\mu \sum_\gamma \hat{a}^\dagger_\mu(\mu | V_b | \gamma) \hat{a}_\gamma \\ & + \sum_\mu \int d\mathbf{x} d\mathbf{y} [\hat{a}^\dagger_\mu(\mu | V_b | \mathbf{x}, \mathbf{y}) \hat{e}(\mathbf{y}) \hat{a}(\mathbf{x}) + \text{H.c.}] + \dots \end{aligned} \quad (A6)$$

Matrix element (B9) is explicitly modified to be

$$(\mathbf{x}, \mathbf{y} | H_{ae} | \mathbf{x}', \mathbf{y}') = [V_{ae}(\mathbf{x}, \mathbf{y}) + W_{ae}(\mathbf{x}, \mathbf{y})] \delta(\mathbf{x} - \mathbf{x}') \delta(\mathbf{y} - \mathbf{y}') - \sum_\mu \mathcal{E}_\mu \phi_\mu^A(\mathbf{x}, \mathbf{y}) \phi_\mu^{A*}(\mathbf{x}', \mathbf{y}') + (\mathbf{x}, \mathbf{y} | V_b | \mathbf{x}', \mathbf{y}'), \quad (A7)$$

and all other matrix elements are implicitly modified by the definition of the potential arising from the Coulomb field of the charge  $Z_b$ ,

$$\Upsilon(xy) = \frac{Z_a Z_b}{x} - \frac{Z_b}{y}. \quad (\text{A8})$$

No bound state terms in the inertial potential  $W$  are included in  $H_0$  since operating on the asymptotic states with those bare terms (the matrix element excluding the orthogonalization corrections) in  $W$  that are diagonal in species (whether diagonal in label or not) gives zero.

The  $a^\dagger e^\dagger e a$  bare matrix element containing  $W$  is nonzero but still is included in  $V$  rather than  $H_0$  because 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 continuum 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.<sup>30</sup>

The initial asymptotic states for the charge-transfer reaction (26) are

$$|\phi_i\rangle = (2\pi)^{-3/2} \int d\mathbf{x} \exp(i\mathbf{k}_i \cdot \mathbf{x}) \hat{a}^\dagger(\mathbf{x}) \hat{e}_\rho^\dagger |0\rangle, \quad (\text{A9})$$

with energy eigenvalue

$$\mathcal{E}_i = \frac{k^2}{2\mu_a} + E_\rho, \quad (\text{A10})$$

and

$$\langle \phi_f | = \langle 0 | \hat{\alpha}_\mu, \quad (\text{A11})$$

with energy eigenvalue given by (30). The result in (A10) is not equal to the Schrödinger initial-state energy eigenvalue because the mass denominator is the two-body reduced mass  $\mu_a$  of (A3), rather than the three-body reduced mass (6). So (A10) differs from the correct value by a factor of  $1/m_b$ . Such an error in energy is acceptable for proton masses, but an additional error is found in the exponents of the initial momentum wave function that is not negligible for incident kinetic energies greater than 5 keV.

The first-order approximation to the  $T$  matrix for reaction (26) is

$$T_{fi}^1 = \langle \phi_f | \hat{V} | \phi_i \rangle = T_{fi}^{1B} + T_{fi}^{1O}, \quad (\text{A12})$$

where in the present case

$$T_{fi}^{1B} = (2\pi)^{-3/2} \int d\mathbf{x} d\mathbf{y} \phi_\mu^{A*}(\mathbf{x}, \mathbf{y}) \left[ \frac{Z_a Z_b}{x} - \frac{Z_b}{y} \right] \times u_\rho^E(\mathbf{y}) \exp(i\mathbf{k}_i \cdot \mathbf{x}) \quad (\text{A13})$$

and

$$T_{fi}^{1O} = -(2\pi)^{-3/2} \int d\mathbf{x} d\mathbf{y} d\mathbf{x}' d\mathbf{y}' \times \phi_\mu^{A*}(\mathbf{x}', \mathbf{y}') \left[ \frac{Z_a Z_b}{x'} - \frac{Z_b}{y'} \right] \times \Delta^A(\mathbf{x}', \mathbf{y}'; \mathbf{x}, \mathbf{y}) u_\rho^E(\mathbf{y}) \exp(i\mathbf{k}_i \cdot \mathbf{x}). \quad (\text{A14})$$

Substituting (A4) into (A13) and changing variables to

$$\mathbf{r} = \mathbf{y} - \mathbf{x} \quad (\text{A15})$$

gives

$$T_{fi}^{1B} = (2\pi)^{-3} \int d\mathbf{r} d\mathbf{y} e^{-i\mathbf{C} \cdot \mathbf{r}} u_\nu^{A*}(\mathbf{r}) \left[ \frac{Z_a Z_b}{|\mathbf{y} - \mathbf{r}|} - \frac{Z_b}{y} \right] \times u_\rho^E(\mathbf{y}) e^{i\mathbf{B}' \cdot \mathbf{y}}, \quad (\text{A16})$$

where  $\mu = \{\mathbf{k}_f, \nu\}$ ,

$$\mathbf{C} = \mathbf{k}_i - \zeta \mathbf{k}_f, \quad \mathbf{B}' = \mathbf{k}_i - \mathbf{k}_f, \quad (\text{A17})$$

and  $\zeta$  is given by (12). Equation (A16) differs from (35) only in the initial momentum vector  $\mathbf{B}'$  of (A17), which differs from  $\mathbf{B}$  of (36) to the order  $m_e/m_b$ . The first-Born result of Massey and Mohr<sup>31</sup> also contains this approximation in  $\mathbf{B}'$ , but they were calculating cross sections for electron capture from hydrogen by an incident positron of energy 6.8–100 eV. At these energies such an error is negligible. For the incident energies of order 10–100 keV appearing in Jackson and Schiff's cross sections,<sup>9</sup> those of Ojha *et al.*,<sup>3</sup> and the present calculations for resonant charge transfer in proton-hydrogen scattering,  $k_i$  is large enough that the error from such an approximation is not negligible.

Thus it is seen that, while the initial-state (inertial) three→two-body reduced-mass coordinate system leads to Fock-Tani  $T$  matrices identical to those obtained within the full three-body coordinate system, the symmetrical (accelerated) three→two-body reduced-mass coordinate system does not.

The equivalence of the post and prior forms of the first-order  $T$  matrix is well known.<sup>9</sup> It seems reasonable that a first-order  $T$  matrix derived from the nonspecialized, symmetrical reduced-mass Hamiltonian (A1) would be equivalent to those derived from the initial-state reduced-mass Hamiltonian, (1), and the corresponding final-state Hamiltonian. This equivalence must be true for the exact  $T$  matrix because of the equivalence of frames of reference. However, the Fock-Tani transformation of the initial-state Fock Hamiltonian (1) gives *both* the post form of the  $T$  matrix, with the ordering of the generators in (20), and the prior form, if the ordering in (20) is reversed. In fact one cannot even set up the reduced-mass Fock-Tani transformation from the final-state equivalent of (1) because the crucial definition of the initial bound state (8) would then include an  $R$  dependence.

The Fock-Tani transformation mixes higher-order effects into the first-order matrix elements and sequesters contributions from the Schrödinger operators into various terms that are accessible only by a specific choice of asymptotic states. It is because of this sequestering that the momentum wave function of the charge transfer asymptotic eigenstate (A9) for the symmetrical reduced-mass Hamiltonian has an error of order  $m_e/m_b$ . So if

one wishes to work in a symmetrical  $n \rightarrow (n-1)$ -body reduced-mass coordinate system, the initial Schrödinger momentum eigenstate appearing in the Fock-Tani matrix elements may need to be altered in an *ad hoc* manner to correct such errors.

## APPENDIX B

The matrix elements in (25) are, in order of appearance,

$$(\mathbf{r} | V_e | \mathbf{r}')' = -\frac{Z_b}{r} \delta(\mathbf{r}-\mathbf{r}') - \sum_{\nu} E_{\nu} u_{\nu}^E(\mathbf{r}) u_{\nu}^{E*}(\mathbf{r}'), \quad (\text{B1})$$

$$(\mu | V_b | \gamma) = \int d\mathbf{R} d\mathbf{r} \phi_{\mu}^{A*}(\mathbf{R}, r) \Upsilon(\mathbf{R}, r) \phi_{\gamma}^A(\mathbf{R}, \mathbf{r}), \quad (\text{B2})$$

$$(\mu | V_b | \mathbf{R}, \mathbf{r})'' = (\mu | V_b | \mathbf{R}, \mathbf{r})' - \int d\mathbf{r}' \Delta^E(\mathbf{r}', \mathbf{r}) (\mu | V_b | \mathbf{R}, \mathbf{r}')', \quad (\text{B3})$$

$$(\mu | V_b | \mathbf{R}, \nu)' = \int d\mathbf{r} (\mu | V_b | \mathbf{R}, \mathbf{r})' u_{\nu}^E(\mathbf{r}), \quad (\text{B4})$$

$$\begin{aligned} (\mathbf{R}, \mathbf{r} | H_{ae} | \mathbf{R}', \mathbf{r}')'' &= (\mathbf{R}, \mathbf{r} | H_{ae} | \mathbf{R}', \mathbf{r}')' - \int d\mathbf{r}_1 \Delta^E(\mathbf{r}, \mathbf{r}_1) (\mathbf{R}, \mathbf{r}_1 | H_{ae} | \mathbf{R}', \mathbf{r}')' \\ &\quad - \int d\mathbf{r}_1 (\mathbf{R}, \mathbf{r} | H_{ae} | \mathbf{R}', \mathbf{r}_1)' \Delta^E(\mathbf{r}_1, \mathbf{r}') \\ &\quad + \int d\mathbf{r}_1 d\mathbf{r}_2 \Delta^E(\mathbf{r}, \mathbf{r}_1) (\mathbf{R}, \mathbf{r}_1 | H_{ae} | \mathbf{R}', \mathbf{r}_2)' \Delta^E(\mathbf{r}_2, \mathbf{r}'), \end{aligned} \quad (\text{B5})$$

$$(\mathbf{R}, \mathbf{r} | H_{ae} | \mathbf{R}', \nu)'' = \int d\mathbf{r}' (\mathbf{R}, \mathbf{r} | H_{ae} | \mathbf{R}', \mathbf{r}')' \phi_{\nu}^E(\mathbf{r}') - \int d\mathbf{r}' d\mathbf{r}_1 \Delta^E(\mathbf{r}, \mathbf{r}_1) (\mathbf{R}, \mathbf{r}_1 | H_{ae} | \mathbf{R}', \mathbf{r}')' \phi_{\nu}^E(\mathbf{r}'), \quad (\text{B6})$$

and

$$(\mathbf{R}, \nu | H_{ae} | \mathbf{R}', \tau)' = \int d\mathbf{r} d\mathbf{r}' u_{\nu}^{E*}(\mathbf{r}) (\mathbf{R}, \mathbf{r} | H_{ae} | \mathbf{R}', \mathbf{r}')' u_{\tau}^E(\mathbf{r}'), \quad (\text{B7})$$

where

$$(\mu | V_b | \mathbf{R}, \mathbf{r})' = \phi_{\mu}^{A*}(\mathbf{R}, \mathbf{r}) \Upsilon(\mathbf{R}, r) - \int d\mathbf{R}' d\mathbf{r}' \phi_{\mu}^{A*}(\mathbf{R}', \mathbf{r}') \Upsilon(\mathbf{R}', r') \Delta^A(\mathbf{R}', \mathbf{r}'; \mathbf{R}, \mathbf{r}), \quad (\text{B8})$$

$$\begin{aligned} (\mathbf{R}, \mathbf{r} | H_{ae} | \mathbf{R}', \mathbf{r}')' &= [V_{ae}(\mathbf{R}, \mathbf{r}) + V_{ab}(\mathbf{R}, \mathbf{r})] \delta(\mathbf{R}-\mathbf{R}') \delta(\mathbf{r}-\mathbf{r}') \\ &\quad - \sum_{\mu} \mathcal{E}_{\mu} \phi_{\mu}^A(\mathbf{R}, \mathbf{r}) \phi_{\mu}^{A*}(\mathbf{R}', \mathbf{r}') + (\mathbf{R}, \mathbf{r} | V_b | \mathbf{R}', \mathbf{r}')', \end{aligned} \quad (\text{B9})$$

and

$$(\mathbf{R}, \mathbf{r} | V_b | \mathbf{R}', \mathbf{r}')' = -[\Upsilon(\mathbf{R}, r) - \Upsilon(\mathbf{R}', r')] \Delta^A(\mathbf{R}, \mathbf{r}; \mathbf{R}', \mathbf{r}') + \int d\mathbf{R}_1 d\mathbf{r}_1 \Delta^E(\mathbf{R}, \mathbf{r}; \mathbf{R}_1, \mathbf{r}_1) \Upsilon(\mathbf{R}_1, r_1) \Delta^A(\mathbf{R}_1, \mathbf{r}_1'; \mathbf{R}', \mathbf{r}'). \quad (\text{B10})$$

The potential arising from the Coloumb field of the charge  $Z_b$  is

$$\Upsilon(\mathbf{R}, r) = \frac{Z_a Z_b}{|\mathbf{R} + \lambda \mathbf{r}|} - \frac{Z_b}{r}, \quad (\text{B11})$$

and the  $\epsilon$  and  $\alpha$  bound-state kernels are, respectively,

$$\Delta^E(\mathbf{r}, \mathbf{r}') = \sum_{\nu} u_{\nu}^E(\mathbf{r}) u_{\nu}^{E*}(\mathbf{r}') \quad (\text{B12})$$

and

$$\Delta^A(\mathbf{R}, \mathbf{r}; \mathbf{R}', \mathbf{r}') = \sum_{\mu} \phi_{\mu}^A(\mathbf{R}, \mathbf{r}) \phi_{\mu}^{A*}(\mathbf{R}', \mathbf{r}'). \quad (\text{B13})$$

Girardeau<sup>6</sup> has shown that the bound-state kernels are diagonal in spin indices.

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