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## Multiple-Scattering Expansions for Nonrelativistic Three-Body Collision Problems. VI. Differential and Total Cross Section for Electron-Transfer Rearrangement Collisions\*

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Differential and total cross sections for electron-transfer rearrangement collisions are calculated in the first-order Faddeev-Watson multiple-scattering approximation for a number of three-body atomic systems. For the ( $p^+$ , H) system, it is shown that the inclusion of the pure  $p^+-p^+$  interaction to all orders (including the contributions coming from the on-shell Coulomb cuts) cancels only part of the effect given by the bare  $p^+-p^+$  interaction so that the present electron-transfer cross section lies in between the Brinkman-Kramers and Jackson-Schiff cross sections and asymptotically approaches the Jackson-Schiff cross section from above in the high-energy limit (where the nonrelativistic approximation is no longer expected to be valid). The knock-out contributions to the electron-transfer amplitude at large angles are particularly important for the equal-mass resonant ( $e^+$ ,  $e^-e^+$ ) electron-transfer collision. Owing to the  $e^+-e^+$  knock-out contribution, the total ( $e^+$ ,  $e^-e^+$ ) electron-transfer cross section exhibits an  $E^{-3}$  energy dependence in the high-energy limit.

### I. INTRODUCTION

Three-body electron-transfer processes such as

$$p^+ + H \rightarrow H + p^+, \quad (1.1a)$$

$$e^+ + (e^- e^+) \rightarrow (e^+ e^-) + e^+, \quad (1.1b)$$

$$e^+ + H \rightarrow (e^+ e^-) + p^+, \quad (1.1c)$$

$$p^+ + (e^- \mu^+) \rightarrow H + \mu^+ \quad (1.1d)$$

are among the simplest types of rearrangement collision processes. The high-energy behavior of such processes has, however, not yet been adequately understood.<sup>1</sup> The purpose of the present work is to investigate the high-energy behavior of these processes in the first-order Faddeev-Watson multiple-scattering approximation.

One of the difficulties encountered in the past concerns the role of the repulsive pair interaction  $V_2$  [such as the  $p^+-p^+$  interaction in the ( $p^+$ , H) system, for example] in the high-energy behavior of electron-transfer collisions. It is clear that the repulsive interaction may contribute to the electron-transfer amplitude through knock-out collisions

which are peaked in the backward direction. Depending on the particle masses of the system, the knock-out contribution to the electron-transfer amplitude may not always be significant in the energy domain of validity of the nonrelativistic approximation. The repulsive pair interaction may also contribute to the electron-transfer probability through nonclassical behavior. The importance of the nonclassical behavior in the high-energy region depends also on the particle masses of the system. Owing to the large proton-electron mass ratio, one may argue that the ( $p^+$ , H) collision should follow a classical description in the high-energy region. Consequently, the repulsive pair interaction in the ( $p^+$ , H) system (i.e., the  $p^+-p^+$  interaction) merely defines the classical trajectory and introduces a phase factor in the amplitude so that it should not effectively contribute to the ( $p^+$ , H) electron-transfer probability.<sup>2,3</sup>

Using arguments based on the above classical picture, Brinkman and Kramers<sup>3</sup> (BK) neglected the bare  $p^+-p^+$  interaction in their treatment of the ( $p^+$ , H) electron-transfer collision in the first-order

Born approximation. This was, however, questioned later by Bates and Dalgarno<sup>4</sup> and by Jackson and Schiff<sup>5</sup> (JS). The latter have shown that not only is this interaction not negligible, but that it has the same energy dependence ( $E^{-6}$ ) at high energies as the rest of the first-order Born term (i. e., the bare electron-proton interaction). The inclusion of the bare  $p^+ - p^+$  interaction reduces the BK cross section at all energies, and by a factor of 0.661 in the high-energy limit.

These results spurred investigation of higher-order terms in the Born series for the ( $p^+$ , H) electron-transfer collision. Drisko<sup>6</sup> found that part of the second-order Born term cancels the first-order term and the remainder gives rise to an  $E^{-5.5}$  energy dependence for the cross section in the high-energy limit. Thus, the second-order Born approximation does not converge to the first-order Born approximation in the high-energy limit. Mapleton<sup>7</sup> also investigated the second-order Born term and found agreement with Drisko's result for small-angle scattering. However, he was unable to determine whether the second-order Born term yields a convergent amplitude when all the intermediate states are summed over.

According to the first-order Faddeev-Watson multiple-scattering (FWMS) approximation,<sup>1,8</sup> the repulsive pair interaction is not simply given by the bare Coulomb potential. Instead it is given by the off-shell Coulomb  $T$  matrix. It is not unreasonable to expect that the effect of the bare  $p^+ - p^+$  interaction in the ( $p^+$ , H) electron-transfer collision would be reduced in the high-energy limit if the off-shell Coulomb  $T$  matrix for the  $p^+ - p^+$  interaction is taken into consideration. By going into the complex plane, it can be shown<sup>9</sup> that in the first-order FWMS approximation the additional amplitude (due to the pure repulsive interaction to all orders) consists of contributions coming from (a) the asymptotic two-body poles in the initial and final bound-state wave functions, (b) the intermediate two-body antibound-state poles, and (c) the branch-point singularities in the off-shell  $T$  matrix for the repulsive interaction.

Owing to the long range of the Coulomb interaction, the two-body off-shell Coulomb  $T$  matrix in the plane-wave representation has cuts on the initial and final half of the energy shell<sup>10-13</sup> in addition to the normal continuum (unitarity) cut. These on-shell Coulomb cuts are important for the electron-transfer amplitude in the high-energy limit, since in this limit the off-shell contributions coming from the intermediate antibound-state poles and the continuum cut are small in comparison with the on-shell contributions. Thus, in the first-order FWMS approximation the dominate contributions due the repulsive interaction are coming from the asymptotic bound-state poles (which are the on-shell

contribution) and the on-shell Coulomb cuts in the high-energy limit.

There are arguments as to whether the on-shell Coulomb cuts are physical<sup>14</sup> and whether the contribution coming from the on-shell cuts should be included in the calculation of the electron-transfer amplitude. If the on-shell-cut contributions are neglected, the electron-transfer cross section in the first-order FWMS approximation approaches the Brinkman-Kramers cross section.<sup>15-17</sup> However, the appearance of the cuts on the energy shell is a consequence of the absence of the long-range Coulomb distortion in the plane-wave momentum representation. The convenience of adopting a representation in which the free Green's function is diagonal is obtained at the expense of having the on-shell Coulomb cuts. Thus, these cuts are a part of the package deal of the plane-wave momentum representation for the Coulomb interaction adopted in our work and should therefore be included in the calculation of the electron-transfer amplitude.<sup>9,15</sup> In the present work, we have included all the contributions in our calculation.

In Sec. II, a resume of the Faddeev-Watson multiple-scattering expansion for rearrangement collision is given. Application of the FWMS expansion to the electron-transfer rearrangement collision process is then carried out in the first-order approximation. Our results are presented in Sec. III together with a comparison with results obtained in the Born approximation. Concluding remarks with a brief review of the various investigations of the higher-order FWMS terms are given in Sec. IV.

## II. FIRST-ORDER MULTIPLE-SCATTERING APPROXIMATION

The Faddeev-Watson multiple-scattering expansion for rearrangement collisions has been investigated in some detail in Papers II and III. In this section we recall only the necessary equations which are used in the present application.

The transition amplitude for the rearrangement collision

$$1 + (2, 3) \rightarrow (1, 2) + 3 \quad (2.1)$$

takes the form [Eq. (II 2.13) or Eq. (III 2.4)]

$$\begin{aligned} & \langle \psi_f^{(3)} | T_r | \psi_i^{(1)} \rangle \\ &= (2\pi)^3 \int d\vec{p}_3 d\vec{q}_3 d\vec{p}'_1 d\vec{q}'_1 \chi_f^{(3)*}(\vec{p}_3) \chi_i^{(1)}(\vec{p}'_1) \delta(\vec{q}_3 - \vec{k}_f) \\ & \quad \times \delta(\vec{k}_i - \vec{q}'_1) \langle \vec{p}_3 \vec{q}_3 | T_r | \vec{p}'_1 \vec{q}'_1 \rangle, \quad (2.2) \end{aligned}$$

where the  $\chi_f^{(i)}$  are the two-body bound-state wave functions for  $i$ th pair of particles with quantum numbers collectively denoted by  $f$ . The mass-scaled momentum variables ( $\vec{p}_i, \vec{q}_i$ ) are defined

by Eqs. (II 2.7). The energy conservation relation in terms of the mass-scaled asymptotic momenta,  $\vec{k}_i$  and  $\vec{k}_f$ , of the incident and outgoing particles with respect to their corresponding two-body subsystems is given by the equation

$$E = \kappa_f^2 + \epsilon_f^{(3)} = \kappa_i^2 + \epsilon_i^{(1)}, \quad (2.3)$$

where  $E$  is the total energy of the system and  $\epsilon_f^{(i)}$  are the two-body bound-state energies for the  $i$ th pair of particles.

The Faddeev-Watson multiple-scattering expansion for the rearrangement collision operator  $T_r$  takes the form [see Eq. (I 2.31)]

$$T_r = V_1 + T_2 + T_1 G_0 T_3 + T_1 G_0 T_2 + T_2 G_0 T_3 + \dots, \quad (2.4)$$

with

$$\frac{d\sigma_r}{d\Omega} = \frac{\mu_3^{3/2} \mu_1^{1/2}}{4\pi^2} \left( \frac{\kappa_f}{\kappa_i} \right) \left| [(2\mu_{23})(2\mu_{12})]^{3/4} \left( \frac{\langle \psi_f^{(3)} | V_1 | \psi_i^{(1)} \rangle}{(2\mu_{23})(2\mu_1)^{3/2}} + \frac{\langle \psi_f^{(3)} | T_2 | \psi_i^{(1)} \rangle}{(2\mu_{13})(2\mu_2)^{3/2}} + \dots \right) \right|^2, \quad (2.8)$$

with

$$\mu_{ij} = \frac{m_i m_j}{m_i + m_j}, \quad \mu_i = \frac{m_i (m_i + m_k)}{(m_i + m_j + m_k)}, \quad (2.9)$$

and where  $m_1$ ,  $m_2$ , and  $m_3$  are the masses of the three particles.

The Born term  $\langle \psi_f^{(3)} | V_1 | \psi_i^{(1)} \rangle$  can be evaluated analytically for a transition between any initial and final two-body states of a three-body system with arbitrary masses.<sup>18</sup> For a transition between ground states we have simply

$$\langle \psi_{1s}^{(3)} | V_1 | \psi_{1s}^{(1)} \rangle = \frac{32\pi Z_1 \beta_{31}^3 (-\epsilon_1^{(3)})^{5/4} (-\epsilon_1^{(1)})^{3/4}}{[\beta_{31}^2 \kappa_5^2 - \beta_{31}^2 \epsilon_1^{(3)}]^2 [\beta_{31}^2 \kappa_4^2 - \beta_{31}^2 \epsilon_1^{(1)}]}, \quad (2.10)$$

with

$$\vec{k}_4 = (\alpha_{31} \vec{k}_i + \vec{k}_f) / \beta_{31}, \quad (2.11)$$

$$\vec{k}_5 = (\vec{k}_i + \alpha_{31} \vec{k}_f) / \beta_{31}, \quad (2.12)$$

$$T_i = V_i + V_i G_0 T_i, \quad (2.5)$$

where  $V_i$  is the two-body Coulomb potential  $V_{jk}$ ,  $G_0$  is the Green's function for the three-body system in the absence of interaction, and  $T_i$  is the two-body  $T$  matrix in the presence of a spectator particle " $i$ ." The corresponding Born expansion for  $T_r$  is

$$T_r^B = \mathbf{U}_f + \mathbf{U}_f G_0 \mathbf{U}_i + \mathbf{U}_f G_0 \mathbf{U}_i G_0 \mathbf{U}_i + \dots, \quad (2.6)$$

with

$$\mathbf{U}_f = V_1 + V_2, \quad \mathbf{U}_i = V_2 + V_3, \quad (2.7)$$

where the superscript  $B$  on  $T_r$  denotes the Born expansion.

When the Faddeev-Watson expansion is utilized, the differential rearrangement cross section may be written as<sup>17</sup>

$$\alpha_{ij}^2 = \frac{m_i m_j}{(m_i + m_k)(m_j + m_k)}, \quad \beta_{ij}^2 = 1 - \alpha_{ij}^2, \quad (2.13)$$

where  $Z_i$  is the product of the charges of particles  $j$  and  $k$ .

The Born term  $\langle \psi_f^{(3)} | V_2 | \psi_i^{(1)} \rangle$  can also be evaluated analytically for a transition between ground states of a three-body system with arbitrary masses. We have (see Appendix)

$$\begin{aligned} \langle \psi_{1s}^{(3)} | V_2 | \psi_{1s}^{(1)} \rangle \\ = \frac{32\pi Z_2 \beta_{12}^2 (-\epsilon_1^{(3)})^{5/4} (-\epsilon_1^{(1)})^{5/4}}{\beta_{23}^4 \beta_{31}^2} I_{1s}(\kappa_i, \kappa_f, \hat{k}_i \cdot \hat{k}_f), \end{aligned} \quad (2.14)$$

where  $I_{1s}(\kappa_i, \kappa_f, \hat{k}_i \cdot \hat{k}_f)$ , which is defined in Appendix, takes on different forms according to the particle masses of the system. The sum of Eqs. (2.10) and (2.14) gives the Born amplitude for an electron-transfer collision between ground states. The Jackson-Schiff cross section then takes the form for arbitrary masses:

$$\frac{d\sigma_r^B}{d\Omega} = \frac{\mu_3^{3/2} \mu_{12}^{3/2}}{16\pi^2 \mu_{23} \mu_1^{5/2}} \left( \frac{\kappa_f}{\kappa_i} \right) \left| \langle \psi_{1s}^{(3)} | V_1 | \psi_{1s}^{(1)} \rangle + \left( \frac{\mu_{23} \mu_1^{3/2}}{\mu_{13} \mu_2^{3/2}} \right) \langle \psi_{1s}^{(3)} | V_2 | \psi_{1s}^{(1)} \rangle \right|^2. \quad (2.15)$$

The Brinkman-Kramers cross section can be obtained from Eq. (2.15) with the  $V_2$  term dropped.

The electron-transfer cross section between ground states in the first-order FWMS approximation takes the form

$$\frac{d\sigma_r^{(1)}}{d\Omega} = \frac{\mu_3^{3/2} \mu_{12}^{3/2}}{16\pi^2 \mu_{23} \mu_1^{5/2}} \left( \frac{\kappa_f}{\kappa_i} \right) \left| \langle \psi_{1s}^{(3)} | V_1 | \psi_{1s}^{(1)} \rangle + \left( \frac{\mu_{23} \mu_1^{3/2}}{\mu_{13} \mu_2^{3/2}} \right) \langle \psi_{1s}^{(3)} | T_2 | \psi_{1s}^{(1)} \rangle \right|^2. \quad (2.16)$$

The matrix element  $\langle \psi_{1s}^{(3)} | T_2 | \psi_{1s}^{(1)} \rangle$  may be written as [see Eqs. (III 3. 14) and (III 3. 15)]

$$\langle \psi_{1s}^{(3)} | T_2 | \psi_{1s}^{(1)} \rangle = (16 Z_2 \beta_{12}^3 / \pi \beta_{31}^2 \beta_{23}^4) (-\epsilon_1^{(1)})^{5/4} (-\epsilon_1^{(3)})^{5/4} \int d\hat{u}_2 I^{(2)}(\hat{u}_2), \quad (2.17)$$

with

$$I^{(2)}(\hat{u}_2) = 2 \int_0^\infty \frac{du_2 \tau_2(\vec{u}_2)}{[(u_2 - u_1^{(+)})(u_2 - u_1^{(-)})(u_2 - u_2^{(+)})(u_2 - u_2^{(-)})]^2}, \quad (2.18)$$

$$\tau_2(\vec{u}_2) = \frac{2\pi^2}{Z_2 e^2} \left( \frac{\beta_{31}}{\beta_{12}} \right)^2 |u_2|^2 T_2(\vec{K}_1, \vec{K}_2; E - K_3^2 + i\eta), \quad (2.19)$$

where  $u_1^{(\pm)}$ ,  $u_2^{(\pm)}$ , and  $T_2(\vec{K}_1, \vec{K}_2, E - K_3^2 + i\eta)$  are defined in Eqs. (III 3. 2) to (III 3. 13).

In Paper III, the integral  $I^{(2)}(\hat{u}_2)$  along the positive real axis was investigated in detail by converting it into an integral around the various singularities of the integrand lying in the upper half of the  $u_2$  plane. It was shown that the integral consists of contributions coming from (a) the asymptotic two-body poles in the initial and final bound-state wave functions, (b) the intermediate two-body anti-bound-state poles, and (c) the branch-point singularities associated both with the continuum (unitarity) cut and the on-shell Coulomb cuts in the off-shell  $T_2$  matrix. The detailed expressions for the asymptotic bound-state-pole contribution [see Eq. (III B6) or Eq. (II 3. 27)] and the intermediate anti-bound-state-pole contribution [see Eq. (III 3. 44)] as well as the integral of discontinuity along the unitarity cut [see Eqs. (III 3. 35) and (III 3. 40)] were derived in Paper III.

Calculations are carried out using these expressions.<sup>15</sup> As expected the dominant contribution in the high-energy limit comes from the asymptotic bound-state poles which are the on-shell contributions. The off-shell contributions coming from the intermediate antibound-state poles and the continuum cut are negligible in the high-energy limit. The contributions coming from the on-shell Coulomb cuts on the initial and final half of the energy shell are also important. To include the on-shell-cut contribution, we found it convenient to go back to the integral  $I^{(2)}(\hat{u}_2)$  along the positive real axis.

To evaluate the integral  $I^{(2)}(\hat{u}_2)$  along the real axis, we make use of the analytic expression for  $\tau_2$  [see Eqs. (III 2. 23), (III 2. 25), and (III 2. 26)]:

$$\tau_2 = \tau_2^A + \tau_2^B, \quad (2.20)$$

$$\tau_2^A = 1 - \frac{1}{(1 + \epsilon_2)^{1/2}} \left( 1 + \sum_{\lambda=1}^{\infty} \frac{2\nu_2^2}{\lambda^2 + \nu_2^2} [t_2^{(+)}]^\lambda \right), \quad (2.21)$$

$$\tau_2^B = \frac{2\pi\nu_2}{e^{2\pi\nu_2} - 1} \frac{[t_2^{(+)}]^{-i\nu_2}}{(1 + \epsilon_2)^{1/2}}, \quad (2.22)$$

with

$$t_2^{(+)} = (1 + 2/\epsilon_2) - (2/\epsilon_2)(1 + \epsilon_2)^{1/2}, \quad (2.23)$$

$$\nu_2 = i \frac{Z_2 e^2}{\beta_{23}} \left( \frac{\mu_{31}}{2} \right)^{1/2} [(u_2 - u_3^{(+)})(u_2 - u_3^{(-)})]^{-1/2}, \quad (2.24)$$

$$\epsilon_2 = - \frac{(u_2 - u_1^{(+)})(u_2 - u_1^{(-)})(u_2 - u_2^{(+)})(u_2 - u_2^{(-)})}{\beta_{31}^2 |u_2|^2 (u_2 - u_3^{(+)})(u_2 - u_3^{(-)})}, \quad (2.25)$$

and where  $u_1^{(\pm)}$ ,  $u_2^{(\pm)}$ , and  $u_3^{(\pm)}$  are defined in Eqs. (III 3. 11)–(III 3. 13).

When integrating along the real axis, we also take  $\eta \rightarrow 0^+$  limit in  $T_2$ . Because the off-shell Coulomb  $T$  matrix  $T \equiv T(\vec{p}, \vec{p}'; k^2)$  does not approach a well-defined limit as  $p \rightarrow k$  or  $p' \rightarrow k$  on the energy shell, care must be exercised in examining the different regions from which the on-shell limit may be approached for the  $k^2 > 0$  case.<sup>10,12,13</sup> There are four such regions

$$\begin{aligned} p > k \text{ and } p' > k, & \text{ region I} \\ p > k > p', & \text{ region II} \\ p < k \text{ and } p' < k, & \text{ region III} \\ p < k < p', & \text{ region IV} \end{aligned} \quad (2.26)$$

It can be easily shown<sup>9,19</sup> that the quantity  $t_2^{(\pm)}$  in these four regions takes on the following different forms in the limit of  $\eta \rightarrow 0^+$ :

$$t_2^{(\pm)} = |t_2^{(\pm)}| \times \begin{cases} e^{2i\pi} & \text{for region I} \\ e^{i\pi} & \text{for regions II and IV} \\ e^0 & \text{for regions III} \end{cases} \quad (2.27)$$

These phase relations must be explicitly considered in carrying out the integration along the positive real axis.

### III. APPLICATION TO ELECTRON-TRANSFER REARRANGEMENT COLLISIONS

Applications of the first-order FWMS approximation ( $V_1 + T_2$  terms) of Sec. II to the electron-transfer rearrangement collisions are carried out for a number of three-body systems [see Eqs. (1. 1a)–(1. 1d)]. The results so obtained are compared with the BK approximation ( $V_1$  term only) and the JS approximation ( $V_1 + V_2$  terms, or the first-order Born approximation) for each process.

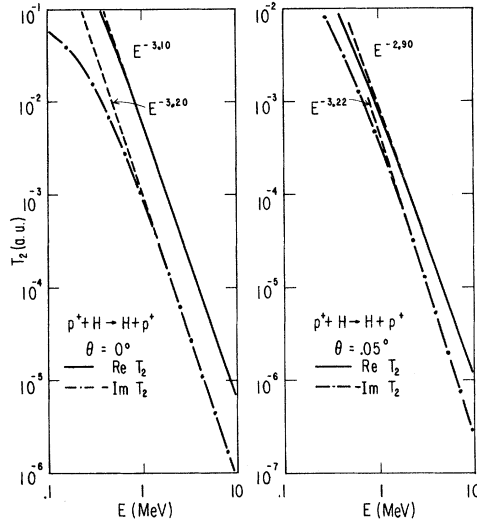


FIG. 1. Real (solid lines) and imaginary (dot-dashed lines) parts of the matrix element  $\langle \psi_1^{(3)} | T_2 | \psi_1^{(1)} \rangle$  (denoted by  $T_2$ ) in a.u. as a function of the laboratory energy of the projectile in MeV for the  $(p^+, H)$  electron-transfer rearrangement collision at two fixed center-of-mass scattering angles. The dashed lines are tangent to their respective curves at the high energy end of the curve and have the indicated energy dependence.

#### A. $p^+ + H \rightarrow H + p^+$

In the light of the controversy regarding the role of the  $p^+ - p^+$  interaction in the  $(p^+, H)$  electron-transfer collision, it is instructive to examine the energy dependence of the  $\langle \psi_1^{(3)} | T_2 | \psi_1^{(1)} \rangle$  matrix ele-

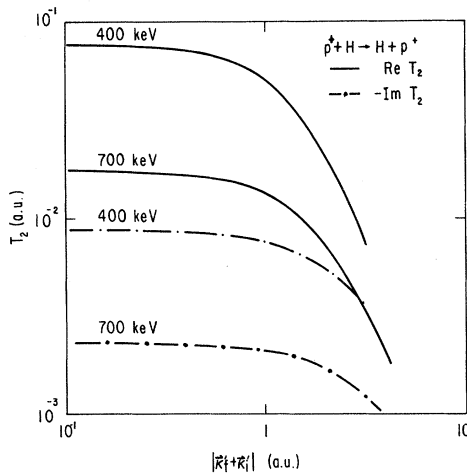


FIG. 2. Real (solid lines) and imaginary (dot-dashed lines) parts of the matrix element  $\langle \psi_1^{(3)} | T_2 | \psi_1^{(1)} \rangle$  (denoted by  $T_2$ ) as a function of the center-of-mass momentum transfer  $|\vec{k}_f + \vec{k}_i|$  for the  $(p^+, H)$  electron-transfer rearrangement collision at two fixed laboratory energies. Atomic units are used except where specified.

ment. This is shown in Fig. 1 ( $\langle \psi_1^{(3)} | T_2 | \psi_1^{(1)} \rangle$  is denoted simply by  $T_2$ ) for two fixed scattering angles. Owing to the large  $p^+ - e^-$  mass ratio, the electron pickup amplitude decreases rapidly with increasing angle as shown in Fig. 2. Thus, the energy dependence of  $\langle \psi_1^{(3)} | T_2 | \psi_1^{(1)} \rangle$  is given essentially by small-angle collisions. In our calculation, the contributions coming from the on-shell Coulomb cuts are included so that  $\langle \psi_1^{(3)} | T_2 | \psi_1^{(1)} \rangle$  does not exhibit an  $E^{-7/2}$  energy dependence. The  $E^{-7/2}$  energy dependence which was predicted<sup>16,17</sup> previously based only on the contributions coming from the asymptotic bound-state poles was obtained when the on-shell-cut contributions were neglected. In the plane-wave representation, it is incorrect to neglect the on-shell-cut contributions.<sup>9,15</sup>

The scattering-angle and energy dependences of the  $(p^+, H)$  electron-transfer differential cross section are given in Figs. 3 and 4, respectively. For comparison we have included in these figures the results obtained in the two Born approximations. It is seen that the JS cross section goes through zero at a small forward angle where an exact cancellation of the bare  $e^- - p^+$  and  $p^+ - p^+$  contributions occurs.<sup>20</sup> This cancellation does not appear in the first-order FWMS approximation as a result of the pure  $p^+ - p^+$  interaction being allowed to interact to all orders.

We have found that at high energies the differential  $(p^+, H)$  electron-transfer cross section in the first-order FWMS approximation (denoted by CK)

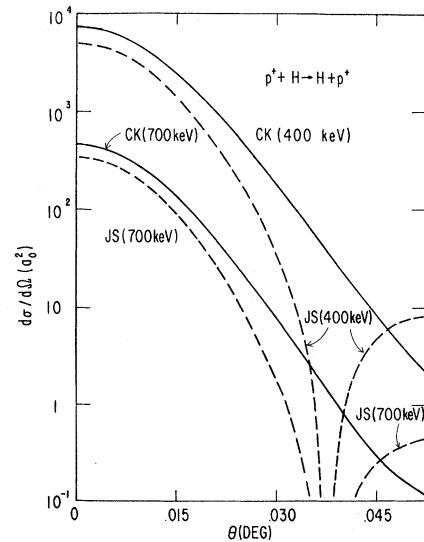


FIG. 3. Comparison of the Jackson-Schiff (JS) and the first-order FWMS (CK) approximations to the differential  $(p^+, H)$  electron-transfer cross section in a.u. as a function of the center-of-mass scattering angle at two fixed laboratory energies (in keV).

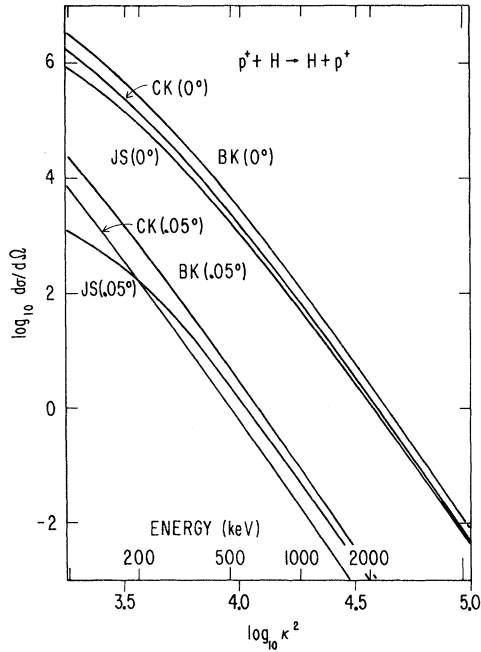


FIG. 4. Comparison of the Brinkman-Kramers (BK), Jackson-Schiff (JS), and the first-order FWMS (CK) approximations to the differential ( $p^+$ , H) electron-transfer cross section as a function of the center-of-mass energy of the projectile (the corresponding laboratory energy is also given) at two fixed center-of-mass scattering angles. Atomic units are used except where specified.

approaches the JS differential cross section from above at forward angles (Fig. 4). This is generally true for all the four systems we have investigated. As the scattering angle increases, the CK cross section gradually crosses the JS cross section and then lies below it. Since the major contribution to the total cross section comes from the forward peak (and backward peak if the knock-out collision is significant), the total CK cross section is found to approach the JS cross section from above in the high-energy region where the nonrelativistic approximation is no longer expected to be valid.

The inclusion of the pure  $p^+ - p^+$  interaction to all orders thus shifts the cross section back from the JS cross section towards the BK cross section (Fig. 5), but asymptotically ( $E > 2$  MeV) it returns to the JS cross section (Fig. 4). The total cross section shown in Fig. 5 agrees with that obtained independently by Shastry *et al.*<sup>21</sup> to two or more significant figures. These results imply that, in the high-energy limit, the pure  $p^+ - p^+$  interaction still provides a significant contribution to the electron-transfer cross section in comparison with the contribution coming from the bare  $e^- - p^+$  interaction. This then reopens the question whether the leading term for the electron-transfer amplitude is given by the bare  $e^- - p^+$  interaction and whether

the classical argument that the  $p^+ - p^+$  interaction should not effectively contribute to the ( $p^+$ , H) electron-transfer probability is valid.

At high energies, it is possible to distinguish the fast proton from the atomic proton in the ( $p^+$ , H) system for small-angle scattering. In our analysis we did not take into consideration the interference from the direct-scattering collision. It can be shown that this interference is small. The  $p^+ - p^+$  knock-out contribution to the electron-transfer amplitude is not appreciable in the energy region of the validity of the nonrelativistic approximation. The backward peaking of the  $p^+ - p^+$  knock-out contribution discussed by Mapleton<sup>7</sup> is found in the JS differential cross section at high energies.

#### B. $e^+ + (e^- e^+) \rightarrow (e^+ e^-) + e^+$

The important difference between the resonant ( $e^+$ ,  $e^- e^+$ ) and ( $p^+$ , H) electron-transfer processes lies in the masses. The ( $e^+$ ,  $e^- e^+$ ) system is an equal-mass system without any mass disparity. Consequently, we expect the  $e^+ - e^+$  interaction to contribute to the electron-transfer probability.

The energy and scattering-angle dependences of the ( $e^+$ ,  $e^- e^+$ ) differential electron-transfer cross section are shown in Figs. 6 and 7, respectively. From Fig. 6, it is seen that at forward angles the CK differential cross section again approaches the JS differential cross section from above. This remains true even at substantially large scattering angles. Then, gradually the  $e^+ - e^+$  knock-out contribution becomes important and the CK differential

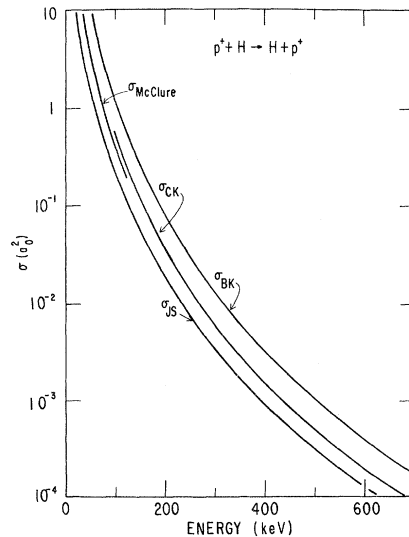


FIG. 5. Comparison of the Brinkman-Kramers (BK), Jackson-Schiff (JS), and the first-order FWMS (CK) approximations to the total ( $p^+$ , H) electron-transfer cross section with experimental results [W. McClure, Phys. Rev. 148, 47 (1966)] in a.u. as a function of the laboratory energy of the projectile in keV.

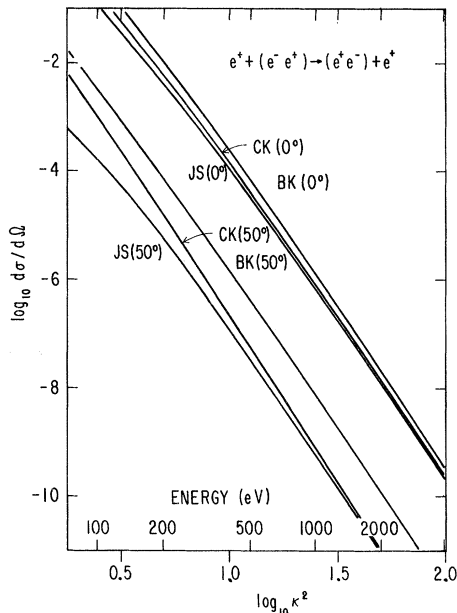


FIG. 6. Comparison of the Brinkman-Kramers (BK), Jackson-Schiff (JS), and the first-order FWMS (CK) approximations to the differential  $(e^+, e^-e^+)$  electron-transfer cross section as a function of the center-of-mass energy of the projectile (the corresponding laboratory energy is also given) at two fixed center-of-mass scattering angles. Atomic units are used except where specified.

cross section lies below the JS cross section. Figure 7 shows that for the  $(e^+, e^-e^+)$  system both the CK and JS differential cross sections have a dip. The JS differential cross section dips to zero at an angle which is, however, considerably larger than the corresponding angle for the  $(p^+, H)$  system (see Fig. 3). In this case, after returning from the dip, both the CK and JS cross sections begin to increase steadily to  $\theta = 180^\circ$ . This indicates that the  $e^+e^-e^+$  knock-out contribution to the  $(e^+, e^-e^+)$  differential electron-transfer cross section is considerable.

The  $e^+e^-e^+$  knock-out effect shows up most significantly in Fig. 8 for the total cross section for the  $(e^+, e^-e^+)$  equal-mass system where the cross section has an  $E^{-3}$  energy dependence in the high-energy limit rather than the  $E^{-6}$  energy dependence exhibited by the other systems that we have investigated. The BK approximation which does not account for the  $e^+e^-e^+$  interaction still predicts an  $E^{-6}$  energy dependence. The total electron-transfer cross section again lies between the JS and BK cross sections at intermediate energies. In this case, it is the BK cross section which lies below the CK cross section. At these high energies, we have neglected the exchange effect between the incident and target positrons.

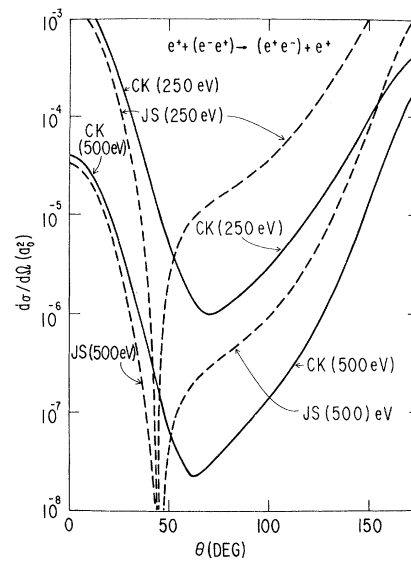


FIG. 7. Comparison of the Jackson-Schiff (JS) and the first-order FWMS (CK) approximations to the differential  $(e^+, e^-e^+)$  electron-transfer cross section in a.u. as a function of the center-of-mass scattering angle at two fixed laboratory energies (in keV).

### C. $e^+ + H \rightarrow (e^+e^-) + p^+$

The nonresonant  $(e^+, H)$  electron-transfer process has no identical particles. Unlike the two previous

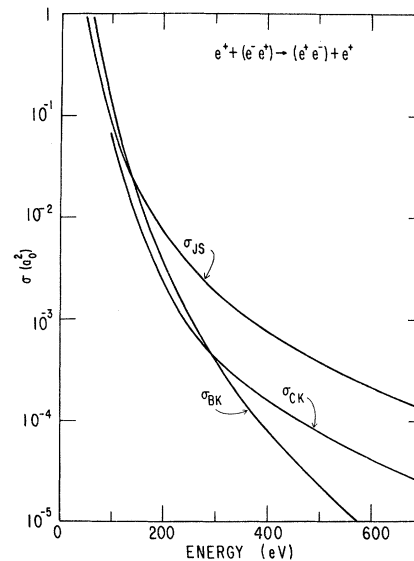


FIG. 8. Comparison of the Brinkman-Kramers (BK), Jackson-Schiff (JS), and the first-order FWMS (CK) approximations to the total  $(e^+, e^-e^+)$  electron-transfer cross section in a.u. as a function of the laboratory energy of the projectile in eV.

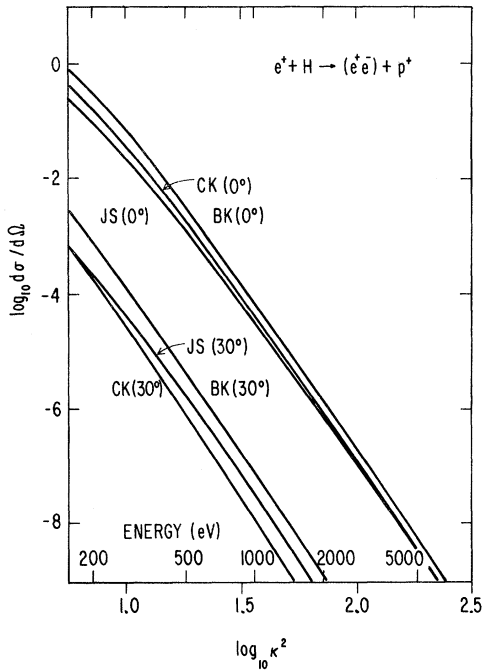


FIG. 9. Comparison of the Brinkman-Kramers (BK), Jackson-Schiff (JS), and the first-order FWMS (CK) approximations to the differential ( $e^+$ , H) electron-transfer cross section as a function of the center-of-mass energy of the projectile (the corresponding laboratory energy is also given) at two fixed center-of-mass scattering angles. Atomic units are used except where specified.

cases, the repulsive interaction in the ( $e^+$ , H) system involves particles with a large mass disparity. Consequently, the  $e^+p^+$  knock-out collision will not be significant in the nonrelativistic energy region of our interest. We also expect that the differential cross section will be less sharply peaked in the forward direction than in the ( $p^+$ , H) case. This can be seen from Figs. 9 and 10 where the energy and scattering-angle dependences of the differential electron-transfer cross section are displayed, respectively.

From Fig. 9, it is seen that in the high-energy limit the CK differential cross section again approaches the JS differential cross section from above at forward angles. It then crosses and lies below the JS cross section at large angles in the high-energy limit. The angle at which the JS differential cross section dips to zero is much larger than that for the ( $p^+$ , H) system but smaller than that for the ( $e^+$ ,  $e^-e^+$ ) system. The total electron-transfer cross section lies between the BK and JS cross sections (see Fig. 11). Numerically, the CK total cross section is closer to the JS cross section for the ( $e^+$ , H) system than it is for the other three systems that we have investigated.

#### D. $p^+ + (e^- \mu^+) \rightarrow H + \mu^+$

Finally, we present the results for the nonresonant ( $p^+$ ,  $e^- \mu^+$ ) electron-transfer processes. This system consists of three different mass particles. At high energies, the particle identity is not of importance so that one would not expect that the ( $p^+$ ,  $e^- \mu^+$ ) system would differ appreciably from the ( $p^+$ , H) system since the mass of  $\mu^+$  and  $p^+$  are of the same order. This mass difference should, however, be noticeable in the differential electron-transfer cross section shown in Figs. 12 and 13. For the ( $p^+$ ,  $e^- \mu^+$ ) system, the differential cross section is not as sharply peaked in the forward direction as that for the ( $p^+$ , H) system. The energy dependence of the differential and total ( $p^+$ ,  $e^- \mu^+$ ) electron-transfer cross sections which are displayed in Figs. 13 and 14 is similar to that for the ( $p^+$ , H) system.

#### IV. CONCLUDING REMARKS

In our investigation we have found that the exact cancellation of the contributions coming from the bare attractive and repulsive interactions which causes the JS differential cross section to dip to zero at a certain scattering angle is removed in the first-order FWMS approximation. At forward angles the differential electron-transfer cross section in the first-order FWMS approximation converges to the JS differential cross section from

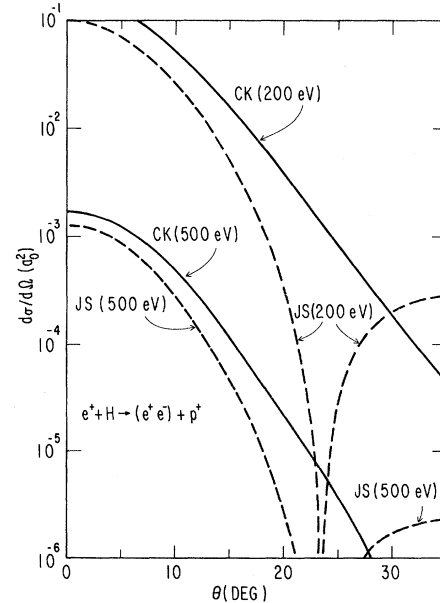


FIG. 10. Comparison of the Jackson-Schiff (JS) and the first-order FWMS (CK) approximations to the differential ( $e^+$ , H) electron-transfer cross section in a.u. as a function of the center-of-mass scattering angle at two fixed laboratory energies (in eV).



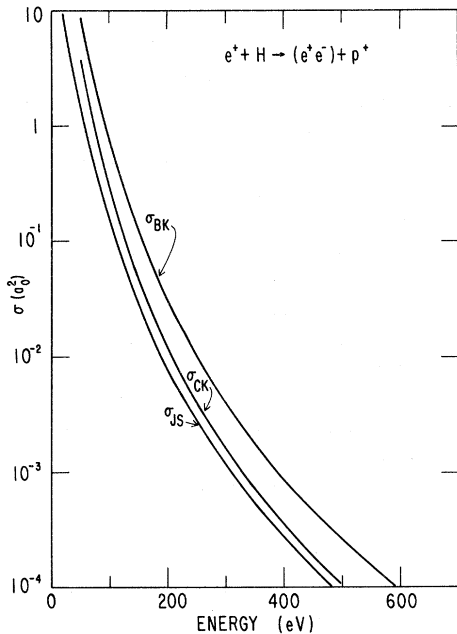


FIG. 11. Comparison of the Brinkman-Kramers (BK), Jackson-Schiff (JS), and the first-order FWMS (CK) approximations to the total  $(e^*, H)$  electron-transfer cross section in a.u. as a function of the laboratory energy of the projectile in eV.

above in the high-energy limit. This implies that, at forward angles, we have

$$\langle \psi_{1s}^{(3)} | T_2 | \psi_{1s}^{(1)} \rangle \sim \langle \psi_{1s}^{(3)} | V_2 | \psi_{1s}^{(1)} \rangle \quad (4.1)$$

in the high-energy limit. Deviation from limit (4.1) becomes significant with increasing scattering angle. The rate of deviation depends, however, on the particle masses of the system.

In the high-energy limit, the on-shell contribution dominates. We may examine limit (4.1) by putting  $T_2$  on the energy shell. From Eqs. (2.19)–(2.25) one obtains, near the energy shell,

$$T_2 \sim V_2 \left( \frac{2\pi\nu_2}{e^{2\pi\nu_2} - 1} \right) e^{-i\nu_2 \ln(\epsilon_2/4)}. \quad (4.2)$$

Since the factor  $2\pi\nu_2/(e^{2\pi\nu_2} - 1)$  approaches unity in the high-energy limit, we observe that the Coulomb  $T$  matrix approaches, in the on-shell limit, the Coulomb potential with a phase factor which contains branch-point singularities. It is the angular dependence of the contribution coming from the on-shell Coulomb cuts (associated with these branch-point singularities) which gives rise to the deviation from limit (4.1).

The total electron-transfer cross section in the first-order FWMS approximation is found to lie between the BK and JS cross section and to approach the JS cross section in the high-energy limit for all systems investigated. When the knock-out contribution becomes significant, the CK and JS cross

sections cross and lie in the reversed order above the BK cross section and the energy dependence of the cross section is changed from  $E^{-6}$  to  $E^{-3}$ . The knock-out contribution to the electron-transfer probability is significant only for the  $(e^*, e^- e^*)$  system in the energy region we have examined.

For the  $(p^*, H)$  system, the  $p^+ - p^+$  interaction when included to all orders still makes a significant contribution to the electron-transfer probability in comparison with the contribution coming from the bare  $e^- - p^+$  interaction in the first-order FWMS approximation. This then reopens the question whether the leading term for the electron-transfer amplitude is given by the bare  $e^- - p^+$  interaction and whether the classical argument, that the  $p^+ - p^+$  interaction should not effectively contribute to the  $(p^*, H)$  electron-transfer probability, is valid.

In the classical argument, one assumes that in the high-energy limit the trajectories due to the  $p^+ - p^+$  interaction lie along straight lines. Recently, concern has arisen as to whether the hyperbolic trajectory approaches rapidly to the straight-line trajectory with increasing energy. To remove this ambiguity, Geltman<sup>22</sup> proposed that the  $p^+ - p^+$  interaction be included in the unperturbed part of the problem. This then gives rise to a Coulomb wave function rather than a plane-wave function in the transition matrix elements. The results obtained in the first-order approximation agree reasonably well with our results of the first-order FWMS ap-

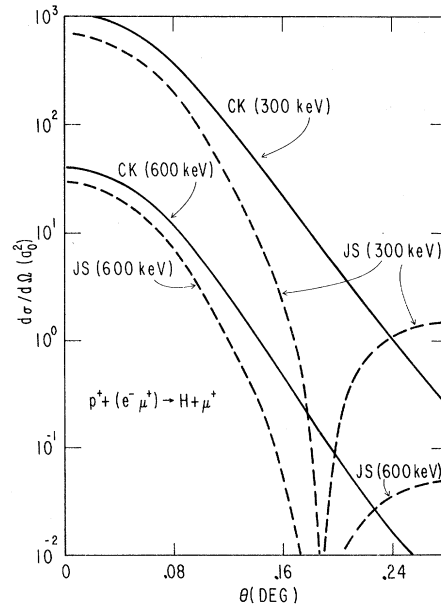


FIG. 12. Comparison of the Jackson and Schiff (JS) and the first-order FWMS (CK) approximations to the differential  $(p^*, e^- \mu^*)$  electron-transfer cross section in a.u. as a function of the center-of-mass scattering angle at two fixed laboratory energies (in keV).

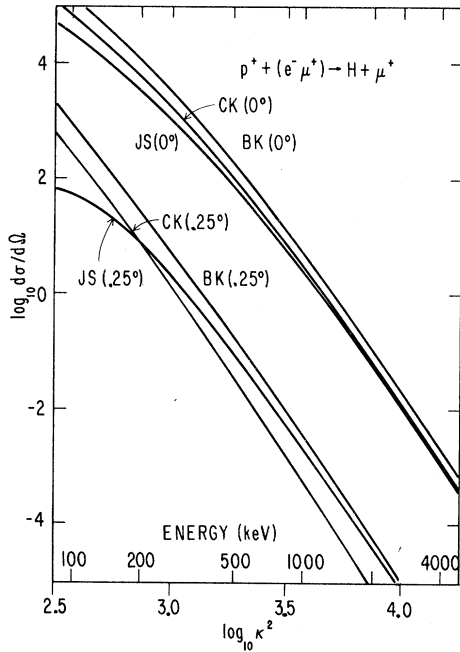


FIG. 13. Comparison of the Brinkman-Kramers (BK), Jackson-Schiff (JS), and the first-order FWMS (CK) approximations to the differential ( $p^+$ ,  $e^- \mu^+$ ) electron-transfer cross section as a function of the center-of-mass energy of the projectile (the corresponding laboratory energy is also given) at two fixed center-of-mass scattering angles. Atomic units are used except where specified

proximation at intermediate energies but disagrees in the high-energy limit.

As noted in the Introduction, it has long been questioned whether the leading term in the Born series for a rearrangement collision is given by the first-order terms. There are indications that the second-order Born terms

$$T_r^{(2,B)} = V_1 G_0 V_3 + V_1 G_0 V_2 + V_2 G_0 V_3 + V_2 G_0 V_2 \quad (4.3)$$

may be the leading terms. For the ( $p^+$ , H) system, several calculations<sup>6,7,23</sup> have shown that  $V_1 G_0 V_3$  is the leading term and gives rise to an  $E^{-11/2}$  dependence for the electron-transfer cross section. Except for the  $V_2 G_0 V_2$  term which we have already taken into consideration in the first-order FWMS approximation, all the rest of the three second-order Born terms are contained in the second-order FWMS approximation

$$T_r^{(2)} = T_1 G_0 T_3 + T_1 G_0 T_2 + T_2 G_0 T_3. \quad (4.4)$$

See Fig. 6 of Paper I for a diagrammatic interpretation of electron-flipping phenomena in the FWMS expansion for the ( $p^+$ , H) electron-transfer collision.

In view of the present results for the first-order FWMS approximation, it is therefore desirable to examine the contribution of the second-order FWMS

terms. The post-prior discrepancy introduced by the second-order terms is inconsequential to the investigation of the energy dependence of the electron-transfer cross section in the high-energy limit.

From the Faddeev equations, McCarroll and Salin<sup>24</sup> have shown that the Drisko results can be obtained. The McCarroll-Salin work was, however, disputed by Coleman.<sup>25</sup> Carpenter and Tuan<sup>26</sup> have shown that from the matrix element  $\langle \psi_{1s}^{(3)} | T_1 G_0 V_3 | \psi_{1s}^{(1)} \rangle$  the Drisko result may be obtained. However, when the complete second-order FWMS term  $\langle \psi_{1s}^{(3)} | T_1 G_0 T_3 | \psi_{1s}^{(1)} \rangle$  is considered, we found in Paper II that both the second-order Born term  $\langle \psi_{1s}^{(3)} | V_1 G_0 V_3 | \psi_{1s}^{(1)} \rangle$  considered by Drisko and the truncated second-order FWMS term  $\langle \psi_{1s}^{(3)} | T_1 G_0 V_3 | \psi_{1s}^{(1)} \rangle$  considered by Carpenter and Tuan get cancelled. In view of limit (4.1), it is conceivable that both  $\langle \psi_{1s}^{(3)} | T_1 G_0 V_3 | \psi_{1s}^{(1)} \rangle$  and  $\langle \psi_{1s}^{(3)} | T_1 G_0 T_3 | \psi_{1s}^{(1)} \rangle$  reduce to  $\langle \psi_{1s}^{(3)} | V_1 G_0 V_3 | \psi_{1s}^{(1)} \rangle$  in the high-energy limit, although the rate of approaching this limit would be different. Further investigation of the second-order FWMS terms is desirable. Experimental measurements of the total and differential electron-transfer cross sections at such high energies are needed.

#### APPENDIX: $\langle \psi_{1s}^{(3)} | V_2 | \psi_{1s}^{(1)} \rangle$ MATRIX ELEMENT

The matrix element for the bare repulsive interaction  $V_2$  can be evaluated analytically as was

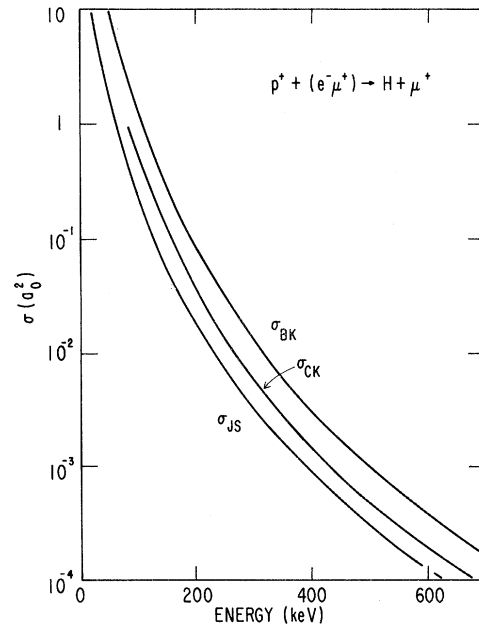


FIG. 14. Comparison of the Brinkman-Kramers (BK), Jackson-Schiff (JS), and the first-order FWMS (CK) approximations to the total ( $p^+$ ,  $e^- \mu^+$ ) electron-transfer cross section in a.u. as a function of the laboratory energy of the projectile in keV.

done by Jackson and Schiff<sup>5</sup> for the case  $m_1 = m_3$  with  $m_2$  being arbitrary. This matrix element can also be evaluated in a similar manner for the  $m_1 \neq m_3$  case with  $m_2$  being arbitrary. The results are summarized below:

$$\begin{aligned} \langle \psi_{1s}^{(3)} | V_2 | \psi_{1s}^{(1)} \rangle \\ = \frac{32\pi Z_2 \beta_{12}^3 (-\epsilon_1^{(3)})^{5/4} (-\epsilon_1^{(1)})^{5/4}}{\beta_{23}^2 \beta_{31}^2} I_{1s}(\kappa_i, \kappa_f, \hat{\kappa}_i \cdot \hat{\kappa}_f), \end{aligned} \quad (\text{A1})$$

where  $I_{1s}(\kappa_i, \kappa_f, \hat{\kappa}_i \cdot \hat{\kappa}_f)$  takes the form, for the  $m_1 = m_3$  case (with  $m_2$  being arbitrary),

$$\begin{aligned} I_{1s}(\kappa_i, \kappa_f, \hat{\kappa}_i \cdot \hat{\kappa}_f) \\ = \frac{2A^2 B^2 + 4B(1+A^2)\epsilon_1^{(1)} + 4(-\epsilon_1^{(1)})^2(1+A^2)^2}{16A^2 B^2(1+A^2)^2(-\epsilon_1^{(1)})^{5/2}} \\ + \tan^{-1}(A) \frac{B - 4\epsilon_1^{(1)}A^2 + \epsilon_1^{(1)}}{16A^2 B^2(-\epsilon_1^{(1)})^{3/2}}, \end{aligned} \quad (\text{A2})$$

with

$$\begin{aligned} A \equiv [(\vec{\kappa}_5 \cdot \vec{\kappa}_6 - \kappa_5^2)/2\epsilon_1^{(1)}]^{1/2}, \quad B \equiv \kappa_5^2 - \epsilon_1^{(1)}, \quad (\text{A3}) \\ \vec{\kappa}_5 \equiv (\vec{\kappa}_i + \alpha_{31}\vec{\kappa}_f)/\beta_{31}, \quad \vec{\kappa}_6 \equiv (\beta_{12}/\beta_{23})(\alpha_{31}\vec{\kappa}_i + \vec{\kappa}_f)/\beta_{31}. \end{aligned} \quad (\text{A4})$$

For the  $m_1 \neq m_3$  case with  $m_2$  being arbitrary,  $I_{1s}(\kappa_i, \kappa_f, \hat{\kappa}_i \cdot \hat{\kappa}_f)$  takes the form

$$I_{1s}(\kappa_i, \kappa_f, \hat{\kappa}_i \cdot \hat{\kappa}_f) = (\beta_{23}/\beta_{12})^7 (2A_1 + A_2 + \frac{3}{4}A_3)/C_1^3, \quad (\text{A5})$$

with

$$A_i = -B_i^{(2-i)} + (C_1 + 2C_2)B_i^{(3-i)} - C_2(C_1 + C_2)B_i^{(4-i)},$$

$$B_n^{(m)} \equiv \int_{C_2}^{C_1+C_2} \frac{\alpha y}{y^m(C_4 y^2 + C_5 y + C_6)^{n/2}},$$

$$C_1 = (\beta_{23}/\beta_{12})^2 (\kappa_6^2 - \kappa_5^2) - C_3,$$

$$C_2 = (\beta_{23}/\beta_{12})^2 (\kappa_5^2 - \epsilon_1^{(3)}),$$

$$C_3 = \epsilon_1^{(1)} - \epsilon_1^{(3)} (\beta_{23}/\beta_{12})^2,$$

$$C_4 = C_7/C_1^2,$$

$$C_5 = [-(C_7 + C_3)C_1 - 2C_2 C_7]/C_1^2,$$

$$C_6 = [C_7 C_2^2 + (C_7 + C_3)C_2 C_1 - \epsilon_1^{(3)} C_1^2 (\beta_{23}/\beta_{12})^2]/C_1^2,$$

$$C_7 = -(\vec{\kappa}_6 - \vec{\kappa}_5)^2 (\beta_{23}/\beta_{12})^2,$$

where the  $B_n^{(m)}$  integrals can be evaluated analytically.

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