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Inner-shell charge transfer in a distorted-wave eikonal approximation using the asymptotic interaction*

Alvin M. Halpern
Department of Physics, Brooklyn College of the City University of New York, Brooklyn, New York 11210
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K-shell charge-transfer cross sections are calculated for swift fully stripped ions impinging on target atoms in a post-interaction distorted-wave formalism. The projectile interaction with the residual target atom is part of the unperturbed Hamiltonian, and is approximated by its asymptotic form while the consequent projectile distortion is approximated by an eikonal wave function. The results are compared to experiment and to other theoretical calculations and are used to shed light on some aspects of the three-body Coulombic rearrangement process and in particular on the significance of asymptotic properties of interactions and wave functions on the results of simple approximation schemes.

I. INTRODUCTION

The realization that charge transfer can play a competitive role to ionization in *K*-vacancy formation in target atoms due to collisions with swift fully stripped ions,[1] and the recent availability of experimental data on such charge-transfer processes[2,3,4] allow theoretical charge-transfer approximation schemes to be tested as a function of target and projectile charge, as well as energy. It has been shown for example, that the Jackson-Schiff (JS) full first Born plane-wave approximation for charge transfer, which is so successful for protons on hydrogen,[5] gives nonphysical results for *K*-shell charge transfer in most other systems.[6] This is in contrast to the Brinkman-Kramers (BK)[7] approximation which, while it overestimates these total cross sections by even larger factors than in the case of proton-hydrogen charge transfer, gives the correct energy and projectile charge dependence for other systems. Recent work[8] has shown that if one replaces the internuclear potential in the JS interaction Hamiltonian by its asymptotic form, i.e., by the interaction of the projectile with a single positive charge at the target nucleus, one gets remarkably good results for *K*-shell charge transfer for protons on He and argon. This is all the more surprising because in heavy targets such as argon one might expect that the projectile would be most effective in picking up the *K* electron in the vicinity of the *K* shell, and hence would see a much larger nuclear charge (see Ref. 6).

In this paper we have performed *K*-shell charge-transfer calculations for protons impinging on argon as well as for bare high-*Z* projectiles impinging on argon and chlorine, using a distorted-wave eikonal approximation. We use the asymptotic interaction of the projectile with the residual target (target atom minus active *K* electron), but that interaction now appears in the eikonal exponent rather than in the interaction potential. The results give good agreement with experiment, and further evidence the significance of the asymptotic approximation to the interaction of the projectile with the residual target atom.

Distorted-wave formalisms have been applied by a number of authors to charge transfer in proton-hydrogen collisions in the tens of kilovolts, and above range.[9,10,11] These were done in part to help clarify the still not fully resolved question of why the JS total cross sections for charge transfer in *p*-H scattering yield so much better results than those of BK, despite sound reasons for expecting the proton-proton interaction to become unimportant at high energies.[12] Numerous other relatively simple approximation schemes have been applied to proton-hydrogen charge transfer,[13] including an eikonal calculation within an impact-parameter formalism,[14] because of the well-known difficulties of getting a soundly based simple low-order approximation to yield good results for that system. More sophisticated calculations yielding good agreement with experiment have, of course, also been performed for that system.[15]

In our present calculation in examining distorted waves as applied to more complex charge-transfer systems, but systems where the essential three-body nature of the process can still be identified, we hope to contribute towards clarification of some of the ambiguities in the three-body Coulombic charge-transfer process. In addition, we present quantitative calculations of *K*-shell charge-transfer cross sections for bare high-*Z* projectiles impinging on heavy targets, as well as cross sections and angular distributions for protons on argon, and compare these with experimental and other theoretical results.

In Sec. II we develop our distorted-wave eikonal scheme and attempt to justify theoretically use of

the asymptotic interaction. In Sec. III we bring the formalism into a form suitable for calculation. In Sec. IV we present our results and conclusions.

II. FORMALISM

We assume that a bare projectile of charge Ze impinges on a neutral target atom of nuclear charge $Z_N e$ and picks up a K-shell electron into one of its own bound states. The other (inactive) electrons are treated as a static charge distribution seen by the projectile and active electron. Hence the problem reduces in this approximation to a three-body problem. The coordinates for the three bodies of interest are shown in Fig. 1.

We choose a "post" or "final-state" distorted-wave formalism in which the unperturbed Hamiltonian H_f includes (a) the interaction of the captured electron with the projectile, $-Ze^2/r_f$, (b) the projectile interaction with the residual target, U_f, (c) the kinetic energy of the electron-projectile system about its center of mass (CM), and (d) the relative kinetic energy of the two final-state bound fragments: the electron-projectile bound system and the residual target atom. Thus,

$$H_f = -\frac{\hbar^2}{2m_f}\nabla^2_{r_f} - \frac{Ze^2}{r_f} - \frac{\hbar^2}{2\mu_f}\nabla^2_{R_f} + U_f, \tag{1}$$

where

$$m_f = \frac{mM_p}{m+M_p}, \quad \mu_f = \frac{(M_p+m)M_N}{M_p+M_N+m}, \tag{2}$$

and m, M_p, and M_N are the electron, projectile, and residual-target-atom masses, respectively. If we ignore terms in U_f of order m/M_p, U_f can be considered a function of R_f rather than R in general, and H_f is separable. We shall assume this to be done in what follows. The "post" interaction Hamiltonian for the collisions, V_f, is then the Coulomb interaction of the captured electron with the target nucleus and the residual electron cloud.

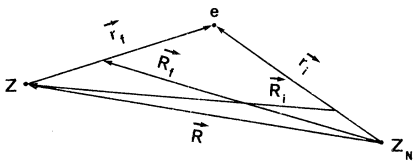

FIG. 1. Coordinate scheme for three active bodies. e, Z, Z_N locate the active electron, projectile, and target nucleus, respectively. $\vec{R}_i$ starts at the CM of the active-electron–residual-atom system. $\vec{R}_f$ ends at the CM of the active-electron–projectile system. These are the standard coordinates used for three-body rearrangement collisions and facilitate separating out the energy of relative motion of the colliding bound fragments in both initial and final states.

Then H, the total Hamiltonian for the system, is given by

$$H = H_f + V_f. \tag{3}$$

The essential distinction between the present formalism and a plane-wave formalism is that we include U_f in the unperturbed Hamiltonian H_f, instead of in the interaction potential V_f. There are in fact many possible choices for breaking up the Hamiltonian into an unperturbed part and an interaction part. The choice one makes becomes important in the context of a perturbative scattering series.[16(a)] The lowest-order term in such a Born series will depend on the particular breakup of the Hamiltonian chosen. The choice itself can depend on various considerations that one imposes from outside the formalism that one hopes gives it physical significance. In our case we choose to view the capture as a consequence of the active electron being disturbed, the disturbance of the projectile being accounted for in a distortion of the projectile wave function outside the framework of the perturbative scattering series. The motivation for this choice relates back to the historic controversy, still not fully resolved, of whether the BK or JS approach is the more physically and formally meaningful one for the plane-wave Born approximation applied to proton capture in hydrogen. Our approach is, in fact, the correct one for developing a first-order Born approximation in which only the active electron's potential appears in the interaction, and we will compare our results with recent plane-wave results based on the JS prototype.[8]

In our case the T matrix for the capture is then

$$T_{fi} = \langle \chi_f^- | V_f | \Psi_i^+ \rangle, \tag{4}$$

where Ψ_i^+ is the full outgoing scattered wave with initial-state boundary conditions and χ_f^- satisfies the unperturbed equation,

$$H_f \chi_f^- = E \chi_f^-, \tag{5}$$

where E is the energy of the colliding system, and obeys final-state boundary conditions with incoming scattered waves.

χ_f^- is the product of a continuum wave ψ_c^- for the relative motion of the CM's of the two final-state bound systems, with Φ_f the final bound-state wave function of the captured electron and projectile.

For our cases, Φ_f will be taken to be the exact hydrogenic 1s state, since capture into higher states is down by an order of magnitude from capture into the ground state.

ψ_c^- differs from a plane wave as a consequence of U_f. Since U_f has a Coulombic tail, one must be cautious in formulating an approximation to ψ_c^-. One clearly defined first-order approximation to

ψ_c^- that obeys the asymptotic boundary conditions and is the lead term in a clearly convergent series is that obtained by replacing U_f by its asymptotic form in Eq. (5). This asymptotic interaction U_f^a is just the Coulomb interaction of the projectile with a single positive charge at the target nucleus, and to order m/M_p as discussed earlier, we have

$$U_f^a = Ze^2/R_f. \tag{6}$$

Higher-order corrections to ψ_c^- then involve the well-behaved potential $U_f - U_f^a$. For the heavy projectiles and high velocities under consideration here we can further approximate ψ_c^- by using a Coulomb eikonal wave instead of a full hydrogenic Coulomb wave, yielding finally[16(b)]

$$\psi_c^-(\vec{R}_f) \approx e^{i\vec{K}_f\cdot\vec{R}_f} \exp\left(iA\int_{-\infty}^{-z_f} \frac{dz}{R_f}\right), \tag{7}$$

where $A = Ze^2/\hbar v$, $\vec{K}_i$ and $\vec{K}_f$ are the initial- and final-state momenta, and v is the relative velocity of the colliding system in CM. The integral is performed along the z axis corresponding to the direction $\vec{K}_f$.[16(c)] Returning to our T matrix, Eq. (4), we now approximate Ψ_i^+ by a plane wave times ϕ_i, the initial K-shell bound-state wave function of the active electron (which is taken to by hydrogenic), since this is the correct asymptotic form for a projectile impinging on a neutral atom. Furthermore, we can neglect the contribution to V_f of the interaction of the active electron with the residual electron cloud, since ϕ_i is significant over such a small radius that the electron cloud contribution in the matrix element is quite small compared to that of the nucleus. In addition, the small contribution of the cloud to the interaction is that of a constant potential, and this as has been shown in a similar context[6] gives a very small contribution to the capture matrix element. The final form of our T matrix is then

$$T_{fi} = \int \psi_c^-(\vec{R}_f)\phi_f(\vec{r}_f)\left(\frac{Z_N e^2}{r_i}\right)\phi_i(\vec{r}_i)e^{i\vec{K}_i\cdot\vec{R}_i}\, d^3r_i\, d^3R_i. \tag{8}$$

Before going on to reduce this to a form suitable for calculation, three points should be noted. One is that despite the ability to approximate $\vec{R}$ by $\vec{R}_f$ in U_f^a without introducing significant error, one cannot do the same in the wave functions, particularly in the phases. This is because $\vec{R}_f$ and $\vec{R}_i$ in the phases contain the information about the momentum transferred to the electron as a consequence of its changing from the nucleus to the projectile. This momentum transfer is the same order of magnitude as the momentum transfer to the heavy projectile, and hence plays a central role in the capture process. Second, although we have ignored the electron cloud contribution to V_f in the matrix element, we must use the correct energy of the initial state Φ_i in working out the kinematics of the problem. Indeed, the whole capture process is very sensitive to the bound-state energies of the initial and final systems. Third, one could develop the whole formalism from an initial-state rather than final-state perspective. This turns out to give considerably poorer results, and this is to be expected. In the initial-state formalism the T matrix is given by

$$T_{fi} = \langle \Psi_f^- | V_i | \chi_i^+ \rangle, \tag{9}$$

where Ψ_f^- is the full incoming scattering wave with final-state boundary conditions, V_i is the interaction of the active electron with the projectile, and χ_i^+ is the solution of the unperturbed Schrödinger equation obeying initial-state boundary conditions with outgoing scattered waves. The unperturbed Hamiltonian now includes the target atom Hamiltonian, the relative kinetic energy of the colliding systems, and the interaction of the projectile with the target nucleus and the residual electron cloud. If we attempt to approximate the continuum part of Ψ_f^- by a plane wave as was done with Ψ_i^+ before, we no longer get a valid description of the asymptotic final state, because asymptotically neither bound fragment is neutral. Similarly, the continuum part of χ_i^+ can formally be approximated by a Coulomb eikonal for a single positive charge at the nucleus, but physically the incoming state has no such Coulomb behavior because the projectile sees a neutral atom. Indeed it would be more sensible to approximate Ψ_f^- with an eikonal Coulomb wave and χ_i^+ with a plane wave, but this would violate the self-consistency of the distorted-wave formalism. As is well known, χ_i^+ must show the evidence of distortion due to that part of the interaction left out of the T matrix element. In the final-state formalism, on the other hand, the approximations made are consistent with both the requirements of the formalism and the physical boundary conditions.

III. CALCULATION

We now reduce Eq. (8), with Eq. (7) for ψ_c^-, to a form suitable for calculation. Letting

$$\begin{aligned} \Phi_i(\vec{r}_i) &= (\beta_i^3/\pi)^{1/2} e^{-\beta_i r_i}, \\ \Phi_f(\vec{r}_f) &= (\beta_f^3/\pi)^{1/2} e^{-\beta_f r_f}, \end{aligned} \tag{10}$$

where β_i and β_f are the reciprocals of the initial and final hydrogen-like Bohr radii for the active electron (corresponding to nuclear charges Z_N and Z, respectively), we get

$$T_{fi}=\frac{Z_N e^2(\beta_i^3\beta_f^3)^{1/2}}{\pi}\times\int\exp\left(-iA\int_{-\infty}^{-z_f}\frac{dz}{R_f}\right)e^{-i\vec{K}_f\cdot\vec{R}_f}\times e^{-\beta_f r_f}e^{-\beta_i r_i}e^{i\vec{K}_i\cdot\vec{R}_i}d^3r_i\,d^3R_i/r_i\,. \quad (11)$$

We note that

$$e^{-\beta_f r_f}=\frac{\beta_f}{\pi^2}\int\frac{d^3k'\,e^{-i\vec{k}'\cdot\vec{r}_f}}{(k'^2+\beta_f^2)^2}\,,\qquad \frac{e^{-\beta_i r_i}}{r_i}=\frac{1}{2\pi^2}\int\frac{d^3k\,e^{-i\vec{k}\cdot\vec{r}_i}}{(k^2+\beta_i^2)}\,, \quad (12)$$

and further that

$$\vec{r}_i=\gamma_f\vec{r}_f+\vec{R}_f\,,\quad \vec{R}_i=(\gamma_i\gamma_f-1)\vec{r}_f+\gamma_i\vec{R}_f\,, \quad (13a)$$

where

$$\gamma_i=M_N/(M_N+m)\,,\quad \gamma_f=M_p/(M_p+m)\,. \quad (13b)$$

Changing integration variables to $d^3r_f\,d^3R_f$ and substituting (12) into (11), we obtain with the aid of (13)

$$T_{fi}=\frac{Z_N e^2\beta_f(\beta_i^3\beta_f^3)^{1/2}}{2\pi^5}\times\int\exp\left(-iA\int_{-\infty}^{-z_f}\frac{dz}{R_f}\right)e^{-i\vec{q}\cdot\vec{R}_f}e^{i\vec{F}\cdot\vec{r}_f}\times(k^2+\beta_i^2)^{-1}(k'^2+\beta_f^2)^{-2}d^3r_f\,d^3R_f\,d^3k\,d^3k'\,, \quad (14)$$

where

$$\vec{q}=-\gamma_i\vec{K}_i+\vec{K}_f+\vec{k}\,,\quad \vec{F}=-\gamma_f\vec{k}-\vec{k}'+(\gamma_i\gamma_f-1)\vec{K}_i\,. \quad (15)$$

Integrating d^3r_f yields a factor $(2\pi)^3\delta^3(\vec{F})$, and integrating over d^3k' yields

$$T_{fi}=D\int\frac{d^3k}{(k^2+\beta_i^2)(C^2+\beta_f^2)^2}\times\int e^{-i\vec{q}\cdot\vec{R}_f}\exp\left(-iA\int_{-\infty}^{-z_f}\frac{dz}{R_f}\right)d^3R_f\,, \quad (16)$$

where

$$D=4Z_N e^2\beta_f(\beta_i^3\beta_f^3)^{1/2}/\pi^2\,,\qquad C=\left|(\gamma_i\gamma_f-1)\vec{K}_i-\gamma_f\vec{k}\right|\,. \quad (17)$$

Changing integration variables from $\vec{k}$ to $\vec{q}$, we finally get

$$T_{fi}=\int d^3q\,f(\vec{q})\int d^3R\,e^{-i\vec{q}\cdot\vec{R}}\exp\left(-iA\int_{-\infty}^{-z}\frac{dz}{R}\right), \quad (18)$$

with

$$f(\vec{q})=D[\beta_i^2+(\gamma_i\vec{K}_i-\vec{K}_f+\vec{q})^2]^{-1}\times[\beta_f^2+(\gamma_f\vec{K}_f-\vec{K}_i-\gamma_f\vec{q})^2]^{-2}\,. \quad (19)$$

We have shown (see Appendix) that if $\vec{q}$ is expressed in cylindrical coordinates (q_b,q_z,ϕ) with the z axis along R_z, we can transform (18) into (to within an overall indeterminate phase)

$$T_{fi}=L_1\int_0^{2\pi}\int_0^{\infty}q_b^{-iA}\frac{\partial f(q_b,0,\phi)}{\partial q_b}\,dq_b d\phi+L_2\int_0^{2\pi}\int_0^{\infty}\int_{-\infty}^{\infty}e^{\pm\pi A/2}\frac{2F_1(iA+1,iA/2+1;iA/2+2;-q_b^2/q_z^2)}{|q_z|^{iA+2}}\frac{\partial f(q_b,q_z,\phi)}{\partial q_z}\times q_b\,dq_z dq_b d\phi\quad(\pm\text{ when }q_z\gtrless 0)\,, \quad (20)$$

where

$$L_1=(2\pi)^2 2^{iA+1}\Gamma(iA/2+1)/iA\,\Gamma(-iA/2)\,,\qquad L_2=4\pi A\,2^{iA}\Gamma(iA+1)/(iA+2)\,. \quad (21)$$

The expression for $f(\vec{q})$ can be simplified as follows. Let the x axis of our coordinate system be in the plane of $\vec{K}_i$ and $\vec{K}_f$, and let θ be the angle between $\vec{K}_i$ and $\vec{K}_f$. If $\hat{x}$, $\hat{y}$, $\hat{z}$ are the unit vectors for our coordinate system, then

$$\vec{K}_f=K_f\hat{z}\quad\text{and}\quad\vec{K}_i=K_i\cos\theta\,\hat{z}+K_i\sin\theta\,\hat{x}\,. \quad (22)$$

From conservation of energy,

$$\frac{\hbar^2K_f^2}{2\mu_f}-\frac{Z^2e^2}{2a_0}=\frac{\hbar^2K_i^2}{2\mu_i}-\frac{\overline{Z}_N^2e^2}{2a_0}\,, \quad (23)$$

where a_0 is the Bohr radius, $\mu_i=M_p(M_N+m)/(M_p+M_N+m)$ is the initial-state counterpart of μ_f defined in Eq. (2) above, and we ignore the difference in the electron reduced masses for the initial and final bound states. $\overline{Z}_N$ is the effective charge of the target so that $\overline{Z}_N^2e^2/2a_0$ is the correct binding energy of the active electron in the target.

In Eq. (19) we can see that β_i and β_f are essentially the momenta of the bound electron in the initial and final states. Since the velocities of the projectile in our calculations are comparable to the K-shell election velocity in the target, K_i and K_f are thousands of times greater than β_i or β_f. Furthermore, K_i-K_f is of the order of β_i or β_f, as can be seen from Eq. (23). Thus only small-angle scattering (θ or order m/M_p or m/M_N) is important, and we can use Eqs. (22) and (23) to

generate the lowest-order contributions to $f(\vec{q})$ in powers of m/M_p and m/M_N. In this approximation, after some lengthy algebra,

$$f(\vec{q}) = D(a_2 + q^2 - b_2 q_z + c q_b \cos\phi)^{-1} \times (a_1 + q^2 - b_1 q_z + c q_b \cos\phi)^{-2}, \tag{24}$$

where ϕ is the azimuthal angle of $\vec{q}$ in our coordinate system, so that $\vec{q}\cdot\hat{x} = q_b \cos\phi$ and

$$a_1 = \beta_f^2 + \epsilon_1^2 K_i^2 + \theta^2 K_i^2, \quad a_2 = \beta_i^2 + \epsilon_2^2 K_i^2 + \theta^2 K_i^2, \tag{25a}$$

$$b_1 = 2\epsilon_1 K_i, \quad b_2 = 2\epsilon_2 K_i, \quad c = 2\theta K_i, \tag{25b}$$

$$\epsilon_1 = \tfrac{1}{2}(\delta/k_i^2 - m/\overline{M}), \quad \epsilon_2 = \tfrac{1}{2}(\delta/k_i^2 + m/\overline{M}), \tag{25c}$$

with

$$\overline{M} = M_p M_N/(M_p + M_N), \quad \delta = (Z^2 - \overline{Z}_N^2) e^2 \mu_f/\hbar^2 a_0. \tag{25d}$$

Now $f(\vec{q})$ can be reexpressed as

$$f(\vec{q}) = -D\frac{\partial}{\partial a_1}\{[a_1 + q^2 - b_1 q_z + c q_b \cos\phi][a_2 + q^2 - b_2 q_z + c q_b \cos\phi]\}^{-1} \tag{26}$$

or

$$f(\vec{q}) = -D\frac{\partial}{\partial a_1}\frac{[a_2 + q^2 - b_2 q_z + c q_b \cos\phi]^{-1} - [a_1 + q^2 - b_1 q_z + c q_b \cos\phi]^{-1}}{(a_1 - a_2) - (b_1 - b_2) q_z}. \tag{27}$$

The integral over ϕ can be performed, yielding

$$\int_0^{2\pi} f(\vec{q})\, d\phi = -2\pi D\frac{\partial}{\partial a_1}\frac{[(a_2 + q^2 - b_2 q_z)^2 - c^2 q_b^2]^{-1/2} - [(a_1 + q^2 - b_1 q_z)^2 - c^2 q_b^2]^{-1/2}}{(a_1 - a_2) - (b_1 - b_2) q_z}. \tag{28}$$

This leads to

$$\int_0^{2\pi} \frac{\partial f}{\partial q_b}\bigg|_{q_z = 0} d\phi = -2\pi D\frac{\partial}{\partial a_1} g_1(a_1, a_2, c; q_b) \tag{29}$$

and

$$\int_0^{2\pi} \frac{\partial f}{\partial q_z} d\phi = -2\pi D\frac{\partial}{\partial a_1} g_2(a_1, a_2, b_1, b_2, c; q_b, q_z), \tag{30}$$

where

$$g_1 = \frac{q_b}{a_1 - a_2}\left(\frac{c^2 - 2(a_2 + q_b^2)}{[(a_2 + q_b^2)^2 - c^2 q_b^2]^{3/2}} - \frac{c^2 - 2(a_1 + q_b^2)}{[(a_1 + q_b^2)^2 - c^2 q_b^2]^{3/2}}\right), \tag{31}$$

$$g_2 = \frac{b_1 - b_2}{[(a_1 - a_2) - (b_1 - b_2) q_z]^2}\left(\frac{1}{[(a_2 + q^2 - b_2 q_z)^2 - c^2 q_b^2]^{1/2}} - \frac{1}{[(a_1 + q^2 - b_1 q_z)^2 - c^2 q_b^2]^{1/2}}\right) + \frac{1}{(a_1 - a_2) - (b_1 - b_2) q_z}\left(\frac{(b_2 - 2q_z)(a_2 + q^2 - b_2 q_z)}{[(a_2 + q^2 - b_2 q_z)^2 - c^2 q_b^2]^{3/2}} - \frac{(b_1 - 2q_z)(a_1 + q^2 - b_1 q_z)}{[(a_1 + q^2 - b_1 q_z)^2 - c^2 q_b^2]^{3/2}}\right). \tag{32}$$

Substituting Eqs. (32), (31), (30), and (29) into Eq. (20) yields

$$T_{fi} = -2\pi D[L_1 G_1(a_1, a_2, c) + L_2 G_2(a_1, a_2, b_1, b_2, c)], \tag{33}$$

where

$$G_1 = \frac{\partial}{\partial a_1}\int_0^\infty g_1(a_1, a_2, c; q_b) q_b^{-iA}\, dq_b, \tag{34}$$

$$G_2 = \int_0^\infty \int_{-\infty}^\infty e^{\pm\pi A/2}\, {}_2F_1(iA + 1, \tfrac{1}{2}iA + 1; \tfrac{1}{2}iA + 2; -q_b^2/q_z^2)/|q_z|^{iA+2} \times\left(\frac{\partial}{\partial a_1} g_2\right) q_b\, dq_z\, dq_b. \tag{35}$$

G_2 can be simplified by changing integration variables. Letting $q_z = q\cos\psi$ and $q_b = q\sin\psi$, and noting $q_b\, dq_b\, dq_z \to q^2\, dq\, d(\cos\psi)$, we get (letting $x = \cos\psi$)

$$G_2 = \int_0^\infty \int_0^1 {}_2F_1(iA + 1, \tfrac{1}{2}iA + 1; \tfrac{1}{2}iA + 2; (x^2 - 1)/x^2) \times\frac{\partial}{\partial a_1}\{e^{+\pi A/2} g_+(a_1, a_2, b_1, b_2, c; q, x) + e^{-\pi A/2} g_+(a_1, a_2, b_1, b_2, c; q, -x)\}\frac{dx\, dq}{q^{iA}}, \tag{36}$$

where

$$g_+(a_1,a_2,b_1,b_2,c;q,x)=g_2(a_1,a_2,b_1,b_2,c;q_b,q_z). \tag{37}$$

Eq. (36) has the advantage of leaving only one variable of integration in the hypergeometric function. Transforming Eqs. (20) and (33) into dimensionless units with all lengths in units of a_0 and all momenta/$\hbar$ in units of $\beta_0 \equiv a_0^{-1}$, and letting $m=1$ and noting $\mu_i \approx \mu_f \approx \overline{M}$, we get

$$K_i=\overline{M}(v/v_0),\quad \beta_i=z,\quad \beta_f=Z_N,\quad \delta=(Z^2-\overline{Z}_N^2)\overline{M}, \tag{38}$$

where v_0 is the electron velocity in the ground state of hydrogen and v, defined earlier, is the incoming projectile laboratory velocity. Eq. (25) now gives

$$\begin{aligned} a_1&=Z^2+b_1^2/4+(v/v_0)^2(\overline{M}\theta)^2,\\ a_2&=Z_N^2+b_2^2/4+(v/v_0)^2(\overline{M}\theta)^2,\\ b_1&=(Z^2-\overline{Z}_N^2)(v_0/v)-(v/v_0),\\ b_2&=(Z^2-\overline{Z}_N^2)(v_0/v)+(v/v_0),\\ c&=2(v/v_0)\overline{M}\theta,\quad A=Z(v_0/v). \end{aligned} \tag{39}$$

Noting that a $1/\beta_0^{6+iA}$ factors out of Eq. (20) or (33) and that $\mu_f e^2 Z_N/\hbar^2 \approx \beta_i \overline{M}$, we get for the differential scattering amplitude [recalling the expression for D Eq. (17)]:

$$f(\theta)=-\frac{\mu_f}{2\pi\hbar^2}T_{fi}=\frac{4\overline{M}(ZZ_N)^{5/2}}{\pi^2\beta_0^{1+iA}}\{L_2G_2+L_1G_1\}. \tag{40}$$

The differential cross section is then (assuming two electrons in the target K shell)

$$d\sigma/d\Omega=2|f(\theta)|^2, \tag{41}$$

and the total cross section is [recalling that $f(\theta)$ is negligible for $\theta \gg m/M_N$ or m/M_p]

$$\sigma=4\pi\int_0^\infty |f(\theta)|^2\theta\,d\theta. \tag{42}$$

Since $f(\theta)$ is a function of $y=\overline{M}\theta$ only,

$$\sigma=\frac{64(ZZ_N)^5a_0^2}{\pi^3}\int_0^\infty [L_2G_2(y)+L_1G_1(y)]^2 y\,dy. \tag{43}$$

After differentiation with respect to a_1, the G_1 and G_2 integrations were performed numerically using Gaussian quadratures on the CUNY IBM 370/168 Computer.

IV. RESULTS AND CONCLUSIONS

We now present the results of our calculations and discuss their significance.[16(d)]

In Table I we compare our results, σ_A, with σ_{BK}[17] and the experimental results σ_E for bare nuclei $Z=+6$, 7, 8, 9 impinging on neutral argon targets at three velocities. The experimental numbers are obtained from the K-vacancy formation cross sections of Ref. 2 by subtracting Z^2-scaled ionization cross sections based on proton-on-argon data from the same reference. Because of the experimental uncertainties and the limitations of Z^2 scaling, not all the experimental numbers are meaningful at the lowest velocity. Nonetheless, the agreement is quite remarkable, and indeed if increased binding effects[18] account for the violation of Z^2 scaling at the lowest velocity, the agreement there would improve.

TABLE I. K-shell to K-shell charge-transfer calculations. Fully stripped ions on argon; all cross sections in units of 10^{-20} cm^2.

Z	σ_{BK}[a]	σ_A	σ_E[b]
	(1) $v/v_0=6.504$ (1.05 MeV/amu)		
6	19.3	6.3	...
7	54.9	8.2	...
8	144.7	10.2	2
9	359.6	12.9	12
	(2) $v/v_0=7.777$ (1.50 MeV/amu)		
6	30.7	8.3	4.0
7	80.8	12.0	5.7
8	194.5	16.6	15.0
9	434.9	22.6	30.7
	(3) $v/v_0=8.713$ (1.88 MeV/amu)		
6	37.1	8.3	5.1
7	93.1	12.9	12.8
8	212.4	19.1	22.9
9	446.8	27.7	43.3

[a] See Ref. 17.

[b] Data from Ref. 2 (pickup to all states). Pickup extracted from K-vacancy rate by assuming Z^2 scaling for ionization.

In Table II we show similar results for Cl^{+17} on krypton. Here the experimental cross sections for charge transfer are obtained from Ref. 4 by

TABLE II. K-shell to K-shell charge-transfer calculations for Cl^{+17} on krypton. All cross sections in units of 10^{-21} cm^2.

v/v_0	E[a] (MeV)	σ_{BK}[b]	σ_A	σ_E[c]
10.615	100	146	4.3	8.5
11.628	120	205	8.5	14
12.560	140	261	13.5	27
13.427	160	314	19.5	48

[a] Lab energy.

[b] See Ref. 17.

[c] Data from Ref. 4 (pickup to all states). Pickup extracted from K vacancy by subtracting Z^2-scaled K vacancy for Cl^{+15}.

subtracting a Z^2-scaled target K-vacancy cross section for Cl^{+15} projectiles from the K-vacancy cross section for Cl^{+17} projectiles, since the Cl^{+15} vacancy formation is almost solely due to ionization.

In Table III we show the results for protons on argon. The experimental data in this case directly measures charge transfer and is that of Ref. 3. Also included is another theoretical cross section σ_C, which results from the modified full first plane-wave Born calculation[8] in which the projectile–residual-atom interaction is taken to be its asymptotic form; i.e., the residual atom presents a single positive charge to the projectile. σ'_A is σ_A scaled to include capture into higher states using σ_{BK} scaling. σ'_{BK} is capture to all states.[17]

Finally, Fig. 2 shows the differential scattering cross section for 6-MeV protons on argon. (K shell to 1s state only) for BK, the modified first Born approximation, and our own results. (We have also calculated the eikonal cross section for protons on hydrogen, and the results are consistent with other distorted-wave calculations[9,10,11] and will be reported elsewhere.)

The key features of the above results can be summarized as follows: (a) We obtain relativity good quantitative agreement with available experimental results for all the high-Z projectile cases, and give both the correct projectile-charge and projectile-velocity dependence. (b) In the case of protons on argon, both the present result and the modified first Born results yield improvement over σ_{BK} at the higher energies shown, but show a rapid rise at the lower energies where the experimental cross section decreases. (c) The differential scattering cross section for protons on argon agrees remarkably well with that of the modified first Born, and both give rise to the same interference dip that is characteristic of first Born for protons on hydrogen. The fact that a distorted-wave calculation exhibits this interference dip is of particular interest and lends weight to its possible physical significance for protons on argon. It should be noted, however, that a recent measurement of the proton-on-argon K-shell charge-transfer angular distribution at 6 MeV[19] does not indicate the existence of such a dip. It would be interesting to see angular distributions for protons on hydrogen in the comparable energy region, 20–100 KeV, since the possibility of the narrow dip being obscured due to residual target electron interaction with the projectile would not arise. Such experimental results exist at lower energies[20] and exhibit considerable structure in the very-small-angle region.

What is perhaps most interesting about the eikonal results is that the asymptotic form of the projectile–residual-atom interaction gives as good

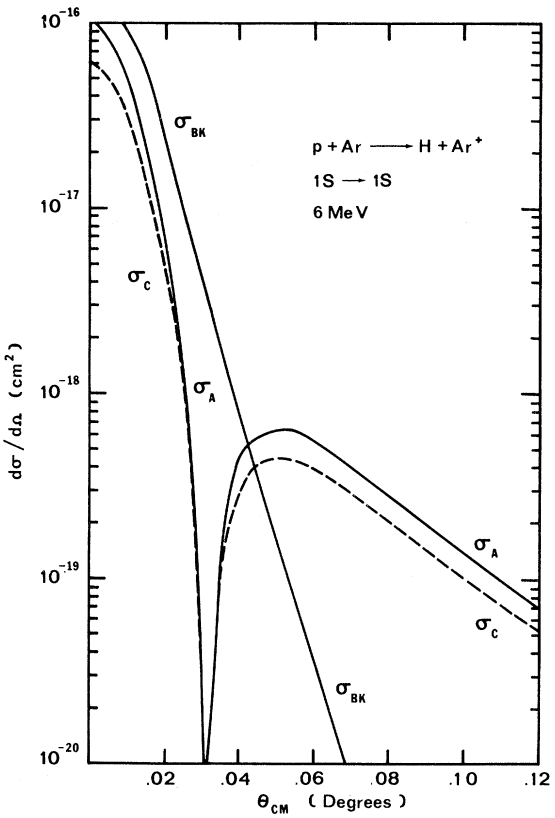

FIG. 2. Angular distribution for protons on argon. σ_A is our result, σ_c is modified first Born of Ref. 8, and σ_{BK} is Brinkman-Kramers result. For this case $\Theta_{lab} \approx \Theta_{CM}$.

TABLE III. Proton-on-argon K-shell to all-states charge-transfer calculations. All cross sections in units of 10^{-22} cm^2.

v/v_0	E[a] (MeV)	σ'_{BK}[b]	σ'_A[c]	σ_C[d]	σ_E[e]
10.00	2.5	0.467	0.533	0.36	0.192
10.96	3.0	0.513	0.389	0.272	0.272
12.65	4.0	0.521	0.289	0.192	0.262
14.15	5.0	0.470	0.262	0.15	0.196
15.49	6.0	0.402	0.245	0.147	0.168
17.32	7.5	0.303	0.206	0.12	0.110
17.89	8.0	0.273	0.194	0.114	0.099
18.98	9.0	0.223	0.166	0.096	0.072
20.00	10.0	0.180	0.142	0.083	0.056
20.98	11.0	0.147	0.118	0.068	0.050
21.91	12.0	0.120	0.099	0.059	0.034

[a]Lab energy $\sim 0.1(v/2v_0)^2$.
[b]Pickup to all states, see Ref. 17.
[c]Scaled to give pickup to all states.
[d]Results of Ref. 8, pickup to all states.
[e]Data of Ref. 3, pickup to all states.

results as it does. The results of a standard impact parametrization of our angular distribution indicates that for high Z on argon most of the capture takes place near the L shell of the target where projectile distortion is due to an effective charge at the nucleus much greater than 1. It is interesting to note, however, that when we performed our eikonal calculation using such an effective interaction of the projectile with the residual atom, we obtained cross sections which were four orders of magnitude to small. This is, perhaps, not surprising, in light of our arguments about the asymptotic boundary conditions.

Despite the above reservations, we believe that the agreement with experiment for the wide range of cases tested, and the success of the asymptotic approximation in the quite different contexts of plane-wave Born and distorted-wave eikonal calculations, sheds new light on the question of how to treat the projectile–residual-atom interaction in a Coulombic rearrangement collision. Indeed, just as our present work can be deemed a distorted-wave calculation in which part of the interaction appears in the unperturbed Hamiltonian, so can the modified plane-wave Born calculation of Ref. 8. In our case all the interaction of the projectile with the residual atom is included in the unperturbed Hamiltonian, in the case of Ref. 8 the interaction of the projectile with a single positive charge at the target nucleus is included in the interaction, and the remainder of the projectile interaction with the residual atom is in the unperturbed Hamiltonian. In both cases the unperturbed wave function (χ_f^- in our case) is approximated by its asymptotic form. In the case of Ref. 8 this is of course a plane wave; in our case it is a Coulomb wave due to a single positive charge at the target nucleus which we approximate by an eikonal exponent. Thus both formalisms treat the unperturbed wave function in the same asymptotic approximation, but they break up the Hamiltonian differently.

When the asymptotic wave function for the given formalism also conforms to the physical asymptotic behavior, we should not be surprised if we get the best results. This explains the success of our calculations in the "post" formalism, and the lack of success of the same calculation in the "prior" formalism as discussed in Sec. II. This same fact perhaps explains why plane-wave Born (i.e., JS for protons on hydrogen and Ref. 8 for protons on argon) gives better results than either our present calculation or other typical distorted-wave calculations for those systems. Charge transfer to a proton is the only case we are considering where in both the initial and final states one of the fragments is neutral. Thus the physical boundary conditions call for a plane wave while the formal boundary conditions call for a Coulomb tail in our χ_f^- for protons on argon. A similar result is true for the proton-on-hydrogen calculation of Ref. 11. The plane-wave calculations for these systems, on the other hand, satisfy both the physical and formal boundary conditions. Interestingly, the proton-on-hydrogen distorted-wave calculation of Ref. 9 is weak for the reverse reason (although the issue there is not that of a Coulomb tail). The formalism requires the unperturbed wave to show distortion, but is none the less approximated by a plane wave which satisfies the physical boundary conditions. In our calculations for the case of high-Z projectiles both the formal and physical boundary conditions are (at least approximately) satisfied, and it is in these cases that our technique should be most useful. We are presently further examining these questions and hope our present results will stimulate additional theoretical work in this area.

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APPENDIX

We wish to evaluate the integral[21]

$$\int f(\vec{q})\,d^3q \int e^{-i\vec{q}\cdot\vec{R}} \exp\left(-iA\int_{-\infty}^{-z}\frac{d\bar{z}}{(b^2+\bar{z}^2)^{1/2}}\right) d^3R\,, \tag{44}$$

where

$$\vec{R}=\vec{z}+\vec{b}, \quad d^3R_b = dz\,b\,db\,d\phi_b, \tag{45}$$

in cylindrical coordinates. Letting $\vec{q}=\vec{q}_z+\vec{q}_b$, with $\vec{q}_z$ along $\vec{z}$, we choose ϕ_b to be the angle between $\vec{q}_b$ and $\vec{b}$.

Equation (44) can then be cast in the form (letting $z \to -z$)

$$\int f(\vec{q})\,d^3q \int e^{iq_z z} e^{-iq_b b\cos\phi_b} \times \exp\left(-iA\int_{-\infty}^{z}\frac{d\bar{z}}{(b^2+\bar{z}^2)^{1/2}}\right) dz\,b\,db\,d\phi_b. \tag{46}$$

Integrating over ϕ_b yields

$$\int f(\vec{q})\,d^3q \left[2\pi\int e^{iq_z z} J_0(q_b b) \times \exp\left(-iA\int_{-\alpha}^{z}\frac{d\bar{z}}{(b^2+\bar{z}^2)^{1/2}}\right) b\,db\,dz\right]. \tag{47}$$

The eikonal exponent $\int_{-\infty}^{z}(\bar{z}^2+b^2)^{-1/2}d\bar{z}$ can be evaluated as follows:

$$\int_{z_0}^{z}\frac{d\bar{z}}{(b^2+\bar{z}^2)^{1/2}}=\ln[z+(b^2+z^2)^{1/2}]-\ln[z_0+(b^2+z_0^2)^{1/2}]. \quad (48)$$

If we take the limit as $z_0\to-\infty$, we get for fixed b

$$\lim_{z_0\to-\infty}\ln[z_0+(b^2+z_0^2)^{1/2}]=\lim_{z_0\to-\infty}\ln[b^2/(2|z_0|)], \quad (49)$$

and

$$\exp\left(-iA\int_{-\alpha}^{z}\frac{d\bar{z}}{(b^2+\bar{z}^2)^{1/2}}\right)=[z+(b^2+z^2)^{1/2}]^{-iA}b^{2iA}\lim_{z_0\to-\infty}(2|z_0|)^{-iA}. \quad (50)$$

This last form has an indeterminant limit because of the oscillating phase term, but because that term appears as an overall multiplicative phase factor which cannot affect the cross sections, we factor it out. That this limiting procedure is the correct one to use is evidenced by the fact that the result does conform to the required asymptotic phase behavior of ψ_c^-.

Substituting Eq. (50) into Eq. (47) and factoring out the indeterminant phase, we get for our integral

$$\int f(\vec{q})\,d^3q\,\mathcal{F}(q_b,q_z), \quad (51)$$

where

$$\mathcal{F}(q_b,q_z)=2\pi\int e^{iq_zz}J_0(q_bb)\times[z+(b^2+z^2)^{1/2}]^{-iA}b^{2iA}b\,db\,dz. \quad (52)$$

We now turn to the z integration in Eq. (52). Let us add a convergence factor $e^{-\nu|z|}$, $\nu>0$, to the integrand. Then we have to calculate

$$\int_{-\infty}^{\infty}e^{iq_zz}e^{-\nu|z|}[z+(b^2+z^2)^{1/2}]^{-iA}dz, \quad (53)$$

and take the limit $\nu\to0$. This is a standard technique for exhibiting the δ-function singularity structure of such an integral. Splitting the integral into the two intervals $[-\infty,0]$ and $[0,\infty]$, performing an integration by parts for each segment, taking limit $\nu\to0$, and recombining, we get for expression (53)

$$2\pi\delta(q_z)b^{-iA}+\frac{A}{q_z}\int_{-\alpha}^{\infty}e^{iq_zz}(b^2+z^2)^{-1/2}\times[z+(b^2+z^2)^{1/2}]^{-iA}dz. \quad (54)$$

Noting that

$$\ln[z+(b^2+z^2)^{1/2}]=\sinh^{-1}(z/b)+\ln b, \quad (55)$$

and that[22]

$$\int_{-\infty}^{\infty}e^{iqz}(b^2+z^2)^{-1/2}\exp[-iA\sinh^{-1}(z/b)]\,dz=2e^{\pm\pi A/2}K_{iA}(|q_z|b)\quad(\pm\text{ for }q_z\gtrless0), \quad (56)$$

and substituting (56) into (54), and then into (52), we get

$$\mathcal{F}(q_b,q_z)=(2\pi)^2\delta(q_z)F(q_b)+G(q_b,q_z), \quad (57)$$

where

$$F(q_b)=\int_0^{\infty}J_0(q_bb)b^{iA+1}db, \quad (58)$$

$$G(q_b,q_z)=2\pi(2A/q_z)e^{\pm\pi A/2}\times\int_0^{\infty}J_0(q_bb)K_{iA}(|q_z|b)b^{iA+1}db\quad(\pm\text{ for }q_z\gtrless0). \quad (59)$$

It should be noted that expression (59) and indeed the right-hand side of (54) are valid only for $|q_z|\neq0$. We must check the behavior of $\mathcal{F}(q_b,q_z)$ at $q_z=0$ for further possible singularities. Let $G(q_b,q_z)$ include the correct singular behavior at the origin $q_z=0$, so that it is represented by Eq. (59) for $q_z>0$, and by whatever δ-function-type singularities are necessary at the origin. We will shortly return to the singular properties of G. First we carry out the integration in Eq. (59) which yields[23]

$$\int_0^{\infty}J_0(q_bb)K_{iA}(|q_z|b)b^{iA+1}db=\frac{\Gamma(iA+1)(2|q_z|)^{iA}}{(q_b^2+q_z^2)^{iA+1}}, \quad (60)$$

and hence

$$G(q_b,q_z)\big|_{q_z\neq0}=\frac{4\pi A2^{iA}\Gamma(iA+1)e^{\pm\pi A/2}|q_z|^{iA}}{q_z(q_b^2+q_z^2)^{iA+1}}. \quad (61)$$

To test the $q_z=0$ behavior of G, let us integrate $\mathcal{F}$ over q_z directly from the defining Eq. (52). Integrating q_z first yields a $\delta(z)$, and integrating over z then gives

$$\int_{-\infty}^{\infty}\mathcal{F}(q_b,q_z)\,dq_z=(2\pi)^2\int_0^{\infty}J_0(q_bb)b^{iA+1}db=(2\pi)^2F(q_b), \quad (62)$$

but this is the result one gets by integrating just the first term in Eq. (57) over q_z. Hence we conclude

$$\int_{-\infty}^{\infty}G(q_b,q_z)\,dq_z=0. \quad (63)$$

It should be noted that if we assume the form Eq. (61) for G for all q_z and integrate directly, we get an indeterminant answer due to the widely oscillatory behavior of the integral:

$$\int_{q_z}^{\infty}G\,dq_z'\to\lambda_1q_z^{iA}+\lambda_2\ \text{ as }\lim q_z\to0 \quad (64)$$

[λ_1 and λ_2 constants, see Eq. (72) below]. Thus the singular properties of G at $q_z=0$ must cancel this effect. The important point as we shall see is that the full G function has the well-defined integral property, Eq. (63). Returning to Eqs. (57) and (51), we need to obtain

$$\int f(\vec{q})\, d^3q\, G(q_b, q_z) = \int f(q_b, q_z, \phi) G(q_b, q_z)\, dq_z\, q_b\, dq_b\, d\phi, \quad (65)$$

where ϕ is the azimuthal angle for $\vec{q}$ in cylindrical coordinates. Performing the integral over q_z first, and integrating by parts yields

$$\int_{-\infty}^{\infty} fG\, dq_z = \left(\int_{-\infty}^{q_z} G\, dq_z'\right) f\Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty}\left(\int_{-\infty}^{q_z} G dq_z'\right)\frac{\partial f}{\partial q_z}\, dq_z. \quad (66)$$

The surface term vanishes at $-\infty$ and $+\infty$ because of the asymptotic behavior of $f(\vec{q})$ and the integral property of G [Eq. (63)]. To obtain the integral term one needs an analytic expression for

$$\int_{-\infty}^{q_z} G(q_b, q_z')dq_z'. \quad (67)$$

This can be done if we can use expression (61) for G, but that would give a correct answer for the integral (67) only for $q_z<0$. For $q_z>0$ we can still obtain an analytic result using expression (61) by again using the integral property [Eq. (63)], obtaining

$$\int_{-\infty}^{q_z} G(q_b, q_z')dq_z' = -\int_{q_z}^{\infty} G(q_b, q_z')dq_z', \quad (68)$$

and evaluating the right-hand side for $q_z>0$. Proceeding to do this, we have

$$\int_{|q_z|}^{\infty} G(q_b, q_z')dq_z' = 4\pi A 2^{iA}\Gamma(iA+1)e^{\pi A/2} \times \int_{|q_z|}^{\infty} |q_z'|^{iA-1}(q_b^2+q_z'^2)^{-iA-1}dq_z', \quad q_z>0. \quad (69)$$

$$\int_{-\infty}^{-|q_z|} G(q_b, q_z')dq_z' = -4\pi A 2^{iA}\Gamma(iA+1)e^{-\pi A/2} \times \int_{-\infty}^{-|q_z|} |q_z'|^{iA-1}(q_b^2+q_z'^2)^{-iA-1}dq_z', \quad q_z<0. \quad (70)$$

Letting $q_z' \to -q_z'$ in Eq. (70) we immediately see

$$\int_{-\infty}^{-|q_z|} G(q_b, q_z')\, dq_z' = -e^{-\pi A}\int_{|q_z|}^{\infty} G(q_b, q_z')\, dq_z'. \quad (71)$$

We can perform the integral on the right obtaining[24]

$$\int_{|q_z|}^{\infty} |q_z'|^{iA-1}(q_b^2+q_z'^2)^{-iA-1}dq_z' = \frac{{}_2F_1(iA+1, iA/2+1; iA/2+2; -q_b^2/q_z^2)}{(iA+2)|q_z|^{iA+2}}. \quad (72)$$

Putting (72) and (71) into the integral term on the right-hand side of (66), and recalling (68), we get

$$\int_{-\infty}^{\infty} f(q_b, q_z, \phi)G(q_b, q_z)\, dq_z = L_2\int_{-\infty}^{\infty} e^{\pm\pi A/2}\, {}_2F_1(iA+1, iA/2+1; iA/2+2; -q_b^2/q_z^2)\,(\partial f/\partial q_z)\,|q_z|^{-iA-2}\, dq_z \quad (\pm \text{ for } q_z \gtrless 0), \quad (73)$$

where

$$L_2 = 4\pi A 2^{iA}\Gamma(iA+1)/(iA+2). \quad (74)$$

Although the integrand in Eq. (73) still has a singular behavior at the origin, it is of the form $|q_z|^{iA}$ and the integral converges unambiguously at the origin.

We now return to the first term on the right-hand side of Eq. (57), and in particular to the form of $F(q_b)$. We could actually evaluate $F(q_b)$ by using convergence factors and proceed to obtain our final result, but rather than do that we can obtain our final result directly by noting

$$(2\pi)^2\int f(\vec{q})\delta(q_z)F(q_b)q_b\, dq_b\, dq_z = (2\pi)^2\int_0^{\infty} f(q_b, 0, \phi)F(q_b)q_b\, dq_b, \quad (75)$$

We now rewrite the expression for $F(q_b)$ [Eq. (58)] by introducing the integral representation[25]

$$b^{iA-1} = 2^{iA}\frac{\Gamma(1+iA/2)}{\Gamma(1-iA/2)}\int_0^{\infty} t^{-iA}J_1(bt)\, dt, \quad (76)$$

and noting

$$J_1(bt) = -\frac{1}{b}\frac{\partial J_0(bt)}{\partial t}, \quad (77)$$

we get, substituting (77) into (76), and (76) into (58) into (75),

$$(2\pi)^2\int_0^\infty f(q_b,0,\phi)F(q_b)q_b\,dq_b = L_1\int_0^\infty\int_0^\infty\int_0^\infty f(q_b,0,\phi)J_0(q_bb)t^{-iA} \times\frac{\partial J_0(bt)}{\partial t}bq_b\,db\,dq_b\,dt, \quad (78)$$

where

$$L_1 = 2^{iA+1}\frac{\Gamma(1+iA/2)}{iA\Gamma(-iA/2)} \quad (79)$$

[which follows from (76) and the minus sign in (77) after some manipulation of the Γ functions]. Integrating over b gives

$$L_1\int_0^\infty\int_0^\infty f(q_b,0,\phi)t^{-iA}\frac{\partial}{\partial t}\left(\frac{\delta(t-q_b)}{q_b}\right)q_b\,dq_b\,dt. \quad (80)$$

Integrating over q_b then yields

$$L_1\int_0^\infty\left(\frac{\partial f(t,0,\phi)}{\partial t}\right)t^{-iA}dt = L_1\int_0^\infty q_b^{-iA}\frac{\partial f(q_b,0,\phi)}{\partial q_b}dq_b. \quad (81)$$

Combining Eqs. (73) and (81) in Eq. (51) yields the desired result [Eq. (20)]. Equation (20) was tested as a check by choosing $f(\vec{q})$, so that

$$\int f(q)e^{-i\vec{q}\cdot\vec{R}}d^3q = e^{-\alpha R} = e^{-\alpha(b^2+z^2)^{1/2}}. \quad (82)$$

T_{fi} was evaluated analytically in coordinate space using Eq. (18), and was then evaluated analytically using our result [Eq. (20)], yielding the same result.

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[1]A. M. Halpern and J. Law, Phys. Rev. Lett. 31, 4 (1973); 31, 620 (E) (1973); J. H. McGuire, Phys. Rev. A 8, 2760 (1973).

[2]J. R. Macdonald, L. M. Winters, M. D. Brown, L. D. Ellsworth, T. Chiao, and E. W. Pettus, Phys. Rev. Lett. 30, 251 (1973).

[3]J. R. Macdonald, C. L. Cocke, and W. W. Eidson, Phys. Rev. Lett. 32, 648 (1974).

[4]F. Hopkins, N. Cue, and V. Dutkiewicz, Phys. Rev. A 12, 1710 (1975).

[5]J. D. Jackson and H. Schiff, Phys. Rev. 89, 359 (1953).

[6]A. M. Halpern and J. Law, Phys. Rev. A 12, 1776 (1975); Similar conclusions for unshielded full first Born approximation have been obtained by K. Omidvar and J. McGuire (private communication).

[7]M. C. Brinkman and H. A. Kramers, Proc. Acad. Sci. Amsterdam 33, 973 (1930); V. S. Nikoleav, Zh. Eksp. Teor. Fiz. 51, 1263 (1966) [Sov. Phys.-JETP 24, 847 (1967)].

[8]K. Omidvar, J. E. Golden, J. H. McGuire, and L. Weaver, Phys. Rev. A 13, 500 (1976); and private communication.

[9]R. H. Bassel and E. Gerjuoy, Phys. Rev. 117, 749 (1960).

[10]J. Grant and J. Shapiro, Proc. Phys. Soc. 86, 1007 (1965).

[11]S. Geltman, J. Phys. B 4, 1288 (1971).

[12]See, e.g., discussion in "Note added in proof" of Ref. 5.

[13]Y. B. Band, Phys. Rev. A 8, 243 (1973); 8, 2857 (1973); 8, 2866 (1973); J. Choudhuri, A. S. Ghosh, and N. C. Sil, Phys. Rev. A 7, 1544 (1973); R. Shakeshaft and L. Spruch, Phys. Rev. A 8, 206 (1973); also many other papers on charge transfer for protons on other targets and into different excited states, e.g., R. A. Mapleton, J. Phys. B 1, 529 (1968); 1, 850 (1968).

[14]M. H. Mittleman and J. Guong, Phys. Rev. 167, 74 (1968).

[15]I. M. Cheshire, D. F. Gallaher, and A. J. Taylor, J. Phys. B 3, 813 (1970).

[16](a) We do not here address the problem of the formal convergence of such rearrangement Born series, which are in question. (b) The form shown for χ_f^- follows from the formal relation $\langle\vec{r}|\chi_f^-\rangle = \langle -\vec{r}|\chi_f^+\rangle^*$ and the well-known result for χ_f^+, as well as directly from the linearized Lippmann-Schwinger equation for χ_f^-. (c) The choice of z axis along $\vec{K}_f$ gives the same result as that along $\vec{K}_i$ in the small-scattering-angle approximation used here. Indeed the only difference in our equations is to change c to $-c$ in Eq. (24), (26), and (27). After integrating over the azimuthal angle, only c^2 appears, and hence the resultant amplitudes are the same. (d) All the calculations and the experimental data are in the interesting "resonant" region where the projectile velocity is comparable to the velocity of the active electron in the target atom. Total cross sections are referred to unless otherwise specified.

[17]σ_{Bk} is calculated using the basic approach of Nikoleav (see Ref. 7). σ_{Bk}' of Table III uses the scaling of Ref. 7, which yields a 20% increase over pickup into the ground state, for protons on argon. (For p + Ar this is essentially $1/n^3$ scaling.)

[18]G. Basbas, W. Brandt, R. Laubert, A. Ratkowski, and A. Schwarzschild, Phys. Rev. Lett. 27, 171 (1971).

[19]C. L. Cocke, J. R. Macdonald, B. Curnutte, S. L. Varghese, and R. Randall, Phys. Rev. Lett. 36, 782 (1976).

[20]See e.g., J. C. Houver, J. Fayeton, and M. Barat,

J. Phys. B 7, 1358 (1974); James E. Bayfield, Phys. Rev. Lett. 25, 1 (1970). (Although this latter paper has angular distributions for the relative probability of capture into the 2S state at energies up to 30 keV, the question of the Jackson-Schiff dip is still unresolved. J. E. Bayfield, private communication.)

[21]Strictly speaking, the $\vec{q}$ integration should be performed first. In interchanging integration we are left with a coordinate integration which has δ-function-type singularities which are dealt with in the standard ways. $f(\vec{q})$ is assumed here to be well behaved at $q=0$ and is assumed to vanish as $q \to \infty$. In our case, $f(\vec{q})$ falls off far more rapidly at ∞, and the actual existence of the integrals in Eqs. (18) and (20), in addition to their formal equality, is not in question.

[22]*Tables of Integral Transforms*, edited by A. Erdelyi (McGraw-Hill, New York, 1954), Vol. 1, p. 122, formula 32.

[23]Reference 22, Vol. 2, p. 63, Formula 3; also F. Oberhettinger, *Tables of Bessel Transforms* (Springer-Verlag, Heidelberg, Germany, 1972), p. 109, formula 12.9.

[24]I. S. Gradshtyn and I. M. Ryzhik, *Tables of Integral Series and Products* (Academic, New York, 1965) p. 298, No. 3.254.2 [Translated from: *Tablitsy Integralov Summ, Ryadov I Proievedeniy* (Gosudarstvennoe Izdatel'stvo Fiziko-Matematicheskoy Literatury, Moscow, 1963)]. (Please note misprint in formula: $\Gamma(\lambda - 2\nu)$ should replace $\Gamma(\lambda - \mu)$ in denominator on right side of the equation.)

[25]W. Magnus, F. Oberhettinger and R. P. Soni, *Formulas and Theorems for the Special Functions of Mathematical Physics*, 3rd ed. (Springer-Verlag, New York, 1966) p. 91, first formula on page. The result, Eq. (81), obtained using this formula, was also derived by independent techniques.