Unified Faddeev treatment of high-energy electron capture

Steven Alston
Department of Physics, Pennsylvania State University, Wilkes-Barre Campus, Lehman, Pennsylvania 18627
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A second-order Faddeev scattering formalism is developed for treating high-energy electron capture in nonrelativistic ion-atom collisions. The approximation to the exact capture amplitude encompasses both forward-angle and large-angle scattering. Comparison with forward-angle experimental data for protons on hydrogen and helium at energies of a few MeV shows very good agreement. The contribution of the internuclear potential to the amplitude is analyzed, and an explicit explanation of its effects as described by the eikonal transformation is given in a multiple-scattering approach. The amplitude is shown to be well behaved for singly charged incident ions.

I. INTRODUCTION

Electron capture at high impact velocities has proven difficult to treat theoretically largely because multiple-scattering contributions play a more important role in this process than in direct excitation. Experimental measurements of the differential electron capture cross section at energies of a few MeV by Horsdal-Pedersen, Cocke, and Stockli for proton-helium[1] collisions and by Vogt *et al.* for proton-hydrogen[2] collisions have not only demonstrated the importance of these contributions but have also provided a more stringent test of models representing them.

Originally, Thomas proposed[3] a double-scattering mechanism as the only means, in a classical setting, of ridding the electron-projectile subsystem of its large internal momentum, thereby allowing capture to occur. The mechanism, shown schematically in Fig. 1(a), refers to an initial scattering of the electron off the projectile at roughly 60° to the incident direction followed by another collision, this time off the target nucleus, which redirects the electron to the forward direction. Since the projectile mass M_P is much greater than the electron mass m, the final electron-projectile bound system is detected at the very small angle $(m/M_P)\sin 60°$ (equal to 0.47 mrad for incident protons). The 60° results from conservation of transverse momentum in the first collision on assuming the electron's speed after the collision equals that of the projectile.

A second possible double-scattering mechanism[4] was later pointed out [Fig. 1(b)]. In this one the projectile suffers a collision with the target nucleus as well as the electron, and the final bound system is detected at roughly 60° to the forward direction for heavy targets. A third possibility [Fig. 1(c)] can also be envisioned in which the projectile scatters off the target nucleus (at 60° in the figure) and the recoiling target nucleus then collides with the previously passive electron, sending it in the direction of the projectile. However, this last mechanism is not classically allowed.

In a quantum-mechanical treatment of electron transfer, each of these mechanisms can contribute to the overall capture amplitude at *any* angle as a result of the momentum spreads of the initial and final bound states. On the other hand, as the electron must attain a final velocity of the order of the projectile's velocity **v**, minimum momentum transfers of the order of $\frac{1}{2}v$ must occur in each two-body collision. Consequently, the two-particle potentials are deeply probed. Additionally, the scatterings themselves are not truly elastic due to initial and final bindings of the electron to relatively moving nuclei.

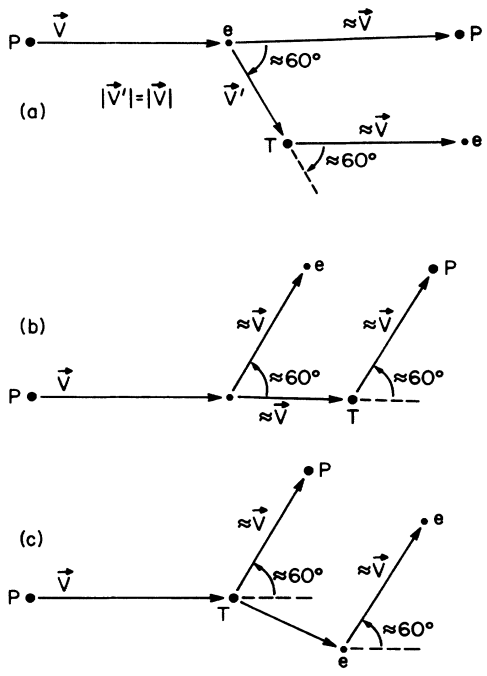

FIG. 1. Schematic representation of the double-scattering mechanism involving the projectile P, target-ion T, and electron e: (a) P-e collision followed by T-e collision, (b) P-e collision followed by P-T collision, and (c) P-T collision followed by T-e collision.

The second-Born (B2) approximation to the exact charge-transfer amplitude, including internuclear terms, provides the lowest-order quantum-mechanical representation of all of the double scattering mechanisms,[5,6] but because of the hard-collision and relative-binding aspects of the process this amplitude does not adequately reproduce the experimental results.[7] The purely electronic part of the amplitude (not including the internuclear terms) gives too large a cross section with the wrong shape. Furthermore, it has been shown[8] within a high-velocity peaking approximation that the partial amplitudes arising from the internuclear terms interfere and indeed cancel with the internuclear first-Born amplitude at near-forward scattering directions of the projectile. This result is in correspondence with the zero contribution of the internuclear terms to the total cross section which is known from the eikonal transformation,[9] but is at odds with the appearance of the nuclear scattering contribution at angles slightly away from the forward direction.

Within a multiple-scattering formalism, the question thus arises of how a better description of the experimental data can be obtained, how binding effects of the active electron affect the scattering, how the internuclear scattering contribution can be included, and yet how the conceptually simple picture of the scattering existing in the Born theory can be retained. Specifically, how is the differential cross section derived from the partial amplitude involving only electronic-nuclear potentials modified when a better description of the Coulomb scattering including binding effect is incorporated into the formalism, and when contributions from terms involving the internuclear potential are included?

An alternate and mathematically sounder theoretical decomposition of the entire collision process into two-body collisions is the scattering formalism of Faddeev.[10,11] Related treatments are those of Watson[12] and Lovelace.[13] This approach (FWL) to the collision process developed through second order is applied here to electron transfer. The resulting amplitude has several advantages over those of other high-order theories. A straightforward interpretation of the amplitude is afforded by its derivation through the simple replacement of the two-body potentials of the second-Born amplitude, except for the electronic part of the first-Born amplitude, with two-body transition operators, thereby automatically including infinite-order perturbation series in the treatment of each of the individual scatterings. Moreover, the replacement of potentials with transition operators affords the highest extension in second order of the Born approximation. An ability to deal with forward-angle and large-angle projectile scatterings within the same formalism also offers a unity of treatment. It is shown that in the second-order approximation used here, the internuclear contribution does not vanish in the differential cross section and in fact reproduces the effects of the eikonal transformation. Essentially, one obtains electronic capture superimposed on nuclear Rutherford scattering.[14] For collisions involving ions, modified Faddeev or other approaches[15] are needed to obtain a well-behaved Neumann expansion of the transition operator, although lower-order truncations of the expansion can be well defined.

An exact numerical calculation of the amplitude is extremely difficult and is not attempted here. However, an approximate evaluation is presented which relies on the smallness of the binding effects by employing near-the-energy-shell approximations[16] for the two-body transition matrices and on the further neglect of other factors all of which introduce errors on the order of the electron mass over heavy-particle masses and of the order of the square of the nuclear charges over the impact velocity squared.

Only forward-angle transfer is considered in the present article, but large-angle transfer could also be treated since the internuclear potential is included in the formalism. Calculated cross sections and the experimental data for proton-hydrogen[1] and proton-helium[2] collisions are compared with results obtained from other symmetric and asymmetric theoretical formalisms, including the second-Born, continuum distorted-wave (CDW),[17] and strong-potential Born[18,19] (SPB) approximations to the exact amplitude.

The contributions from terms involving the internuclear potential are treated separately. In particular, the amplitudes with and without internuclear terms are compared and the former shows good agreement with experiment at angles beyond the Thomas peak where the internuclear scattering is the main feature of the cross section. Furthermore, the contributions of the internuclear terms are seen to be in good agreement with the eikonal representation of the nuclear scattering.[9,17]

When nuclear scattering is neglected from the outset, the FWL amplitude reduces to a purely electronic part which can be derived within a distorted-wave Born formalism (hereafter DWB), as has been shown by Taulbjerg and Briggs.[20] Treatments of this amplitude have appeared elsewhere,[21,22] but without the present orientation where connections with the B2 approximation are stressed, internuclear contributions are considered, and off-the-energy-shell effects are explicitly treated.[22]

The plan of the paper is the following. An outline of the FWL formalism is given in Sec. II. In Sec. III, the application to electron capture is presented within a second-order approximation. The reduction of the amplitude to a form involving two-body T matrices is given in Sec. IV. Near-the-energy-shell approximations are introduced and the amplitude evaluated in Sec. V. Section VI presents calculated results and compares them with experiment and other theories. Concluding remarks are made in Sec. VII. Finally, three Appendixes present some of the details of the discussion. A very limited set of the present results has appeared elsewhere.[23] In the following discussion, atomic units are used but the electron mass m is retained in places for clarity. A plane wave of index $\mathbf{k}$ represented in coordinate space $\mathbf{r}$ is normalized as $\langle \mathbf{r}|\mathbf{k}\rangle = e^{i\mathbf{k}\cdot\mathbf{r}}$.

II. FADDEEV-WATSON-LOVELACE SCATTERING FORMALISM

A three-body collision is considered in which a projectile ion P is incident on a target consisting of an active

electron e and a target ion T. Both the target and projectile ions may contain nonactive electrons. It follows then that the two-body interactions between each pair of the three particles may assume the more general modified Coulomb[16] form, which still includes the pure Coulomb case.

The collision of the projectile and target system can result in three possible exit channels:

$$P+(T+e)\rightarrow \begin{cases} P+(T+e)^* , & \text{(1a)} \\ (P+e)^*+T , & \text{(1b)} \\ P+T+e , & \text{(1c)} \end{cases}$$

for excitation, rearrangement, and breakup, respectively, where the asterisk allows for excited states of the $(T+e)$ or $(P+e)$ aggregates. For the third channel, in general, a bound-state spectrum does not exist. A transition operator corresponds to each of the channels in the collision process: $\mathcal{T}_E$ for excitation, $\mathcal{T}_R$ for rearrangement, and $\mathcal{T}_B$ for breakup. We are interested in process (1b); processes (1a) and (1c) are not treated here.

The goal of the Faddeev-Watson-Lovelace scattering formalism, as in any Faddeev approach,[11] is to construct a set of operators and equations which they satisfy so that free propagation of one of the particles accompanied by any order of multiple scatterings of the other two is not allowed, although each of the individual scatterings may be represented at a higher level, e.g., through the use of two-body transition matrices. Such a procedure avoids the ensuing singular nature of the amplitude representing these types of subcollision. The actual transition operators for the individual scattering processes are then expressed in terms of the FWL operators. For potentials which are Coulomb-like at large distances, the Faddeev procedure should be modified[15] to account for the long-range distortions of the potentials, so that a Neumann expansion [Eq. (2) below] of the transition operator is well founded. However, if a certain order of the expansion in the original Faddeev equations can be shown to be well behaved and because the relation of the Faddeev expansion to the Born expansion is straightforward (as is seen below), it is still worthwhile to investigate the application of these equations to cases containing Coulomb-like potentials. It could be the case also that in an approximate form, the results are in accord with those obtained from the more rigorous theory, particularly so if good agreement with experiment is found. This then is the rationale behind the present study.

In order to keep the discussion self-contained, a brief presentation of the original Faddeev approach is outlined. Corresponding to the specific final-state interactions V_{Pe}, V_{Te}, and V_{PT}, the FWL "transition" operators $\mathcal{T}_{Pe}$, $\mathcal{T}_{Te}$, and $\mathcal{T}_{PT}$, or collectively $\mathcal{T}_a$ ($a=Te$, Pe, and PT), are introduced. The defining equations are

$$\mathcal{T}_{Te}=V_{Te}[G^+(E)(V_{Pe}+V_{PT})] ,$$
$$\mathcal{T}_{Pe}=V_{Pe}[1+G^+(E)(V_{Pe}+V_{PT})] ,$$
$$\mathcal{T}_{PT}=V_{PT}[1+G^+(E)(V_{Pe}+V_{PT})] ,$$

where

$$G^+(E)=(E-H_0-V_{Pe}-V_{Te}-V_{PT}-i\eta)^{-1}$$

is the full Green's operators of energy E satisfying an outgoing-wave boundary condition and η is an infinitesimal. The free-particle Hamiltonian of the system in the total center-of-mass frame is denoted by H_0.

Individual two-body transition operators with free propagation of the third particle are defined as solutions of the Lippmann-Schwinger equations

$$\tilde{\mathcal{T}}_{Te}=[1+\tilde{\mathcal{T}}_{Te}G_0^+(E)]V_{Te}=[1+V_{Te}G_{Te}^+(E)]V_{Te} ,$$
$$\tilde{\mathcal{T}}_{Pe}=[1+\tilde{\mathcal{T}}_{Pe}G_0^+(E)]V_{Pe}=[1+V_{Pe}G_{Pe}^+(E)]V_{Pe} ,$$
$$\tilde{\mathcal{T}}_{PT}=[1+\tilde{\mathcal{T}}_{PT}G_0^+(E)]V_{PT}=[1+V_{PT}G_{PT}^+(E)]V_{PT} ,$$

with $G_0^+(E)$ denoting the free Green's operator $(E-H_0+i\eta)^{-1}$ and $G_a^+(E)$, the Green's operator $(E-H_0-V_a+i\eta)^{-1}$ for the interaction V_a of two particles and free propagation of the third.

The equations for the $\mathcal{T}_a$ are derived using the relation

$$V_{Te}G^+(E)=\mathcal{T}_{Te}G_0^+(E)[1+(V_{Pe}+V_{PT})G^+(E)]$$

and ones analogous to it for the P-e and P-T interactions which are obtained by permutation of the potentials, and the definitions of the two-body transition operators. A unique set of equations[11] is found, in matrix form, as

$$\begin{bmatrix} \mathcal{T}_{Te} \\ \mathcal{T}_{Pe} \\ \mathcal{T}_{PT} \end{bmatrix} = \begin{bmatrix} 0 \\ \tilde{\mathcal{T}}_{Pe} \\ \tilde{\mathcal{T}}_{PT} \end{bmatrix} + \begin{bmatrix} 0 & \tilde{\mathcal{T}}_{Te} & \tilde{\mathcal{T}}_{Te} \\ \tilde{\mathcal{T}}_{Pe} & 0 & \tilde{\mathcal{T}}_{Pe} \\ \tilde{\mathcal{T}}_{PT} & \tilde{\mathcal{T}}_{PT} & 0 \end{bmatrix} G_0^+ \begin{bmatrix} \mathcal{T}_{Te} \\ \mathcal{T}_{Pe} \\ \mathcal{T}_{PT} \end{bmatrix} \quad (2)$$

after some manipulations. Zeros along the diagonal of the square matrix ensure the absence of terms representing multiple scatterings of the same two particles with free propagation of the third one.

Equation (2) can be solved approximately by iteration as a Neumann expansion. The first-order solution is $\mathcal{T}_a^{(1)}=\tilde{\mathcal{T}}_a$ for $a=Pe,PT$ and $\mathcal{T}_{Te}^{(1)}=0$; the second-order solution $\mathcal{T}_a^{(2)}$ is obtained by substituting $\mathcal{T}_a^{(1)}$ into the right-hand side of Eq. (2); the third-order solution $\mathcal{T}_a^{(3)}$ is obtained by substituting $\mathcal{T}_a^{(2)}$ into the right-hand side; the procedure is followed until the desired order of the solution is found. Considerations of the convergence of this procedure or of the compactness of the kernel matrix,[10,11] while being extremely important in the general setting, are beyond the scope of the present work.

In terms of the previously defined FWL operators, the individual channel transition operators assume the forms[11]

$$\mathcal{T}_E=\mathcal{T}_{Pe}+\mathcal{T}_{PT} , \quad \text{(3a)}$$

$$\mathcal{T}_R=V_{Pe}+\mathcal{T}_{Te}+\mathcal{T}_{PT} , \quad \text{(3b)}$$

$$\mathcal{T}_B=V_{PT}+\mathcal{T}_{Te}+\mathcal{T}_{Pe} . \quad \text{(3c)}$$

An approximate treatment of $\mathcal{T}_R$ in Eq. (3b), for example, is obtained by employing the corresponding order of the $\mathcal{T}_a$ found using Eq. (2).

III. APPLICATION TO ELECTRON TRANSFER

The present discussion of the FWL formalism centers on the transition operator $\mathcal{T}_R$ representing electron transfer. A second-order approximation to the $\mathcal{T}_a$ is used for calculating $\mathcal{T}_R$. Following Eqs. (2) and (3b), one finds

$$\begin{aligned}\mathcal{T}_R \approx \mathcal{T}_R^{(2)} &= V_{Pe} + \mathcal{T}_{Te}^{(2)} + \mathcal{T}_{PT}^{(2)} \\ &= [V_{Pe} + \tilde{\mathcal{T}}_{Te} G_0^+(E) \tilde{\mathcal{T}}_{Pe}] \\ &\quad + [\tilde{\mathcal{T}}_{PT} + \tilde{\mathcal{T}}_{PT} G_0^+(E) \tilde{\mathcal{T}}_{Pe} + \tilde{\mathcal{T}}_{Te} G_0^+(E) \tilde{\mathcal{T}}_{PT}] \\ &\equiv \mathcal{T}_e + \mathcal{T}_n \ . \end{aligned} \tag{4}$$

The various contributions to $\mathcal{T}_R^{(2)}$ have been collected into two sets of terms defined as $\mathcal{T}_e$ and $\mathcal{T}_n$. These two parts arise, respectively, from terms containing only electronic-nuclear operators and terms containing internuclear operators. The operators $\mathcal{T}_e$ and $\mathcal{T}_n$ describe different aspects of the capture problem, namely, the direct transfer of the electron and the role of the internuclear scattering. They also facilitate comparison with experiment and discussion of the eikonal transformation of the amplitude and of distorted-wave and second-Born treatments of the process.

The positions of the constituents of the system are represented by three sets of Jacobi coordinate vectors, each pair of which consists of a relative coordinate vector of one particle taken with respect to the center of mass of the other two and an internal coordinate vector for these two particles. The various sets of coordinate vectors are shown in Fig. 2; they are related by the following transformations:

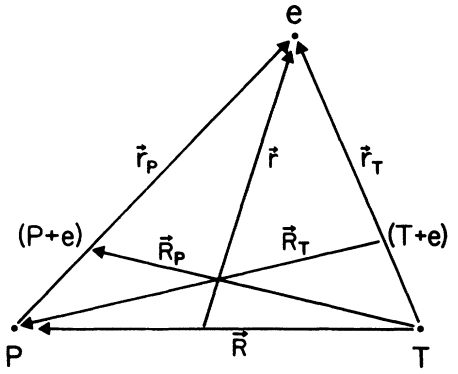

FIG. 2. Jacobi coordinate sets $\mathbf{r}_T, \mathbf{R}_T$; $\mathbf{r}_P, \mathbf{R}_P$; and $\mathbf{r}, \mathbf{R}$, corresponding to the three unique two-particle center of masses.

$$\begin{aligned}\mathbf{r}_T &= \beta \mathbf{r}_P + \mathbf{R}_P = \mathbf{r} + \gamma' \mathbf{R} \ , \\ \mathbf{R}_T &= -(1-\alpha\beta)\mathbf{r}_P + \alpha \mathbf{R}_P = -\alpha' \mathbf{r} + (1-\gamma'\alpha')\mathbf{R} \ , \\ \mathbf{r}_P &= \alpha \mathbf{r}_T - \mathbf{R}_T = \mathbf{r} - \gamma \mathbf{R} \ , \\ \mathbf{R}_P &= (1-\alpha\beta)\mathbf{r}_T + \beta \mathbf{R}_T = \beta' \mathbf{r} + (1-\gamma\beta')\mathbf{R} \ . \end{aligned} \tag{5}$$

Mass ratios in Eqs. (5) are defined as

$$\alpha = M_T/(m+M_T), \quad \beta = M_P/(m+M_P), \quad \gamma = M_T/(M_P+M_T) \ ,$$
$$\alpha' = m/(m+M_T), \quad \beta' = m/(m+M_P), \quad \gamma' = M_P/(M_P+M_T) \ ,$$

where m is the electron mass and M_P and M_T are the projectile- and target-ion masses, respectively; they satisfy the relations $\alpha+\alpha'=1$, $\beta+\beta'=1$, and $\gamma+\gamma'=1$.

Internal and relative reduced masses associated with the three two-body combinations are defined, respectively, as

$$\begin{aligned}\mu_i &= mM_T/(m+M_T) \ , \\ \nu_i &= M_P(m+M_T)/(m+M_P+M_T) \ , \\ \mu_f &= mM_P/(m+M_P) \ , \\ \nu_f &= M_T(m+M_P)/(m+M_P+M_T) \ , \\ \mu_n &= M_P M_T/(M_P+M_T) \ , \\ \nu_n &= m(M_P+M_T)/(m+M_P+M_T) \ . \end{aligned}$$

In terms of the reduced masses and Jacobi coordinates, the free-particle Hamiltonian assumes the possible forms

$$\begin{aligned}H_0 &= -\frac{1}{2\nu_i}\nabla^2_{\mathbf{R}_T} - \frac{1}{2\mu_i}\nabla^2_{\mathbf{r}_T} \\ &= -\frac{1}{2\nu_f}\nabla^2_{\mathbf{R}_P} - \frac{1}{2\mu_f}\nabla^2_{\mathbf{r}_P} \\ &= -\frac{1}{2\nu_n}\nabla^2_{\mathbf{r}} - \frac{1}{2\mu_n}\nabla^2_{\mathbf{R}} \ . \end{aligned} \tag{6}$$

The total energy of the system is given by

$$E = \frac{1}{2\nu_i}K_i^2 + \varepsilon_i = \frac{1}{2\nu_f}K_f^2 + \varepsilon_f \ , \tag{7}$$

where $\mathbf{K}_i$ and $\mathbf{K}_f$ are the initial and final heavy-particle wave vectors and ε_i and ε_f are the initial and final bound-state energies. The norm of a vector $\mathbf{K}$ is denoted by K.

Individual two-body potentials, owing to the possibly non-point-charge nature of the target and projectile ions, may have complicated dependences on their respective radial coordinates; however, they reduce asymptotically to the forms

$$\begin{aligned}V_{Te}(r_T) &\sim -Z_T^a/r_T \quad \text{as } r_T \to \infty \ , \\ V_{Pe}(r_P) &\sim -Z_P^a/r_P \quad \text{as } r_P \to \infty \ , \\ V_{PT}(R) &\sim Z_T^a Z_P^a/R \quad \text{as } R \to \infty \ . \end{aligned} \tag{8}$$

The projectile and target nuclear charges in Eqs. (8) are Z_P and Z_T and the corresponding asymptotic charges are Z_P^a and Z_T^a. The shielding of the projectile and target nuclei by the nonactive electrons leads to the values Z_P^a and Z_T^a; for neutral targets Z_T^a is unity.

Forming the matrix element of $\mathcal{T}_R^{(2)}$ between initial and

final asymptotic scattering states, the second-order FWL approximation to the exact capture amplitude at energy E takes the form

$$A_{\mathrm{FWL}}(E)=\langle\Phi_f|\mathcal{T}_R^{(2)}|\Phi_i\rangle=\langle\Phi_f|\mathcal{T}_e|\Phi_i\rangle+\langle\Phi_f|\mathcal{T}_n|\Phi_i\rangle \equiv A_e+A_n \ , \tag{9}$$

where the asymptotic states are given by

$$\langle\mathbf{R}_T,\mathbf{r}_T|\Phi_i\rangle=e^{i\mathbf{K}_f\cdot\mathbf{R}_T}\phi_i(\mathbf{r}_T) \ , \qquad \langle\mathbf{R}_P,\mathbf{r}_P|\Phi_f\rangle=e^{i\mathbf{K}_f\cdot\mathbf{R}_P}\phi_f(\mathbf{r}_P) \ . \tag{10}$$

The initial (final) bound-state wave function is ϕ_i (ϕ_f).

A simple picture of the second-order transition operator given in Eq. (4), and thus of the amplitude in Eq. (9), may be obtained by replacing the T matrices $\tilde{\mathcal{T}}_a$ in the second-order terms by their lowest-order approximations V_a and by replacing the first-order $\tilde{\mathcal{T}}_{PT}$ term by its second-order version $V_{PT}+V_{PT}G_0^+(E)V_{PT}$. One finds the operator

$$\mathcal{T}_{\mathrm{Born}}^{(2)}=[V_{Pe}+V_{Te}G_0^+(E)V_{Pe}] +[V_{PT}+V_{PT}G_0^+(E)V_{PT}+V_{PT}G_0^+(E)V_{Pe} +V_{Te}G_0^+(E)V_{PT}] \ , \tag{11}$$

which is the second-Born approximation[5-8] to $\mathcal{T}_R$. This can also be derived from the definition of the transition operator for capture by replacing the full Green's operator $G^+(E)$ with the free Green's operator $G_0^+(E)$.

Returning to Fig. 1, the three double-scattering mechanisms shown correspond to the second-order terms (containing G_0^+) in $\mathcal{T}_R^{(2)}$ and $\mathcal{T}_{\mathrm{Born}}^{(2)}$. In the second-Born approximation, each of the two collisions are treated using a simple (first) Born approximation to the scattering. The second-order FWL approximation goes very much further by treating each collision with a full two-body T matrix, implying an infinite summing of higher-order Born terms for *each* collision. It should be noted, however, that an effect such as the distortion of the scattering of one particle off the other by the interactions of these particles with the third one is not contained in the second-order FWL amplitude.

If the interion (internuclear for bare nuclei) contribution to $\mathcal{T}_R^{(2)}$ in Eq. (4) is small as is the case generally, for example, for forward-angle transfer, then $\mathcal{T}_n$ can be neglected. The transition operator reduces to the electronic-nuclear part

$$\mathcal{T}_R^{(2)}\approx\mathcal{T}_e=V_{Pe}+\tilde{\mathcal{T}}_{Te}G_0^+(E)\tilde{\mathcal{T}}_{Pe} \ .$$

This version of the transition operator, in different form, has been obtained elsewhere[20] using a distorted-wave Born formalism. The connection with the second-Born approximation is analogous to that discussed above.

IV. REDUCTION TO TWO-BODY T-MATRIX FORM

For each of the two-body collisions in the amplitude, it is useful to integrate the third free-particle motion so that two-body transition matrices can be obtained. In Sec. V, these T matrices will be approximated by their near-the-energy-shell forms. Toward this end, the bound-state wave functions are Fourier analyzed:

$$\phi_i(\mathbf{r}_T)=(2\pi)^{-3/2}\int d\mathbf{k}_i\tilde{\phi}_i(\mathbf{k}_i)e^{i\mathbf{k}_i\cdot\mathbf{r}_T} \ , \qquad \phi_f(\mathbf{r}_P)=(2\pi)^{-3/2}\int d\mathbf{k}_f\tilde{\phi}_f(\mathbf{k}_f)e^{i\mathbf{k}_f\cdot\mathbf{r}_P} \ . \tag{12}$$

Equations (5) are used to expand the plane-wave phases as

$$\begin{aligned}\mathbf{k}_i\cdot\mathbf{r}_T+\mathbf{K}_i+\mathbf{R}_T&=[\beta\mathbf{k}_i-(1-\alpha\beta)\mathbf{K}_i]\cdot\mathbf{r}_P+(\mathbf{k}_i+\alpha\mathbf{K}_i)\cdot\mathbf{R}_P\equiv\mathbf{t}_i\cdot\mathbf{r}_P+(\mathbf{k}_i+\alpha\mathbf{K}_i)\cdot\mathbf{R}_P\\ &=(\mathbf{k}_i-\alpha'\mathbf{K}_i)\cdot\mathbf{r}+[\gamma'\mathbf{k}_i+(1-\gamma'\alpha')\mathbf{K}_i]\cdot\mathbf{R}\equiv(\mathbf{k}_i-\alpha'\mathbf{K}_i)\cdot\mathbf{r}+\mathbf{U}_i\cdot\mathbf{R} \ ,\\ \mathbf{k}_f\cdot\mathbf{r}_P+\mathbf{K}_f+\mathbf{R}_P&=[\alpha\mathbf{k}_f+(1-\alpha\beta)\mathbf{K}_f]\cdot\mathbf{r}_T+(-\mathbf{k}_f+\beta\mathbf{K}_f)\cdot\mathbf{R}_T\equiv\mathbf{t}_f\cdot\mathbf{r}_T+(-\mathbf{k}_f+\beta\mathbf{K}_f)\cdot\mathbf{R}_T\\ &=(\mathbf{k}_f+\beta'\mathbf{K}_f)\cdot\mathbf{r}+[-\gamma'\mathbf{k}_f+(1-\gamma\beta')\mathbf{K}_f]\cdot\mathbf{R}\equiv(\mathbf{k}_f+\beta'\mathbf{K}_f)\cdot\mathbf{r}+\mathbf{U}_f\cdot\mathbf{R} \ .\end{aligned} \tag{13}$$

The electronic scattering energies (total energy minus heavy-particle energies) are given by

$$E_i=E-\frac{1}{2\nu_f}(\mathbf{k}_i+\alpha\mathbf{K}_i)^2, \quad E_f=E-\frac{1}{2\nu_i}(\mathbf{k}_f-\beta\mathbf{K}_f)^2 \ . \tag{14}$$

These various relations [Eqs. (12)–(14)] and Eq. (7) are used in the development below, first for the electronic part and then for the internuclear part of the amplitude.

A. Electronic-nuclear terms

The first-Born and higher-order parts of the amplitude are separated, giving

$$A_e=\langle\Phi_f|V_{Pe}|\Phi_i\rangle+\langle\Phi_f|\tilde{\mathcal{T}}_{Te}G_0^+(E)\tilde{\mathcal{T}}_{Pe}|\Phi_i\rangle \equiv A_{\mathrm{BI}}+A_e^{(2)} \ , \tag{15}$$

where A_{BI} is the first-Born amplitude and $A_e^{(2)}$ is the partial amplitude representing the higher-order scattering terms.

Substituting Eqs. (12) and (13) into Eq (15), the partial amplitude $A_e^{(2)}$ becomes

$$A_e^{(2)}=(2\pi)^{-3}\int d\mathbf{k}_f d\mathbf{k}_i \tilde{\phi}_f^*(\mathbf{k}_f)\tilde{\phi}_i(\mathbf{k}_i)\langle -\mathbf{k}_f+\beta\mathbf{K}_f,\mathbf{t}_f|\tilde{T}_{Te}G_0^+(E)\tilde{T}_{Pe}|\mathbf{k}_i+\alpha\mathbf{K}_i,\mathbf{t}_i\rangle \ .$$

Letting G_0^+ and $\tilde{T}_{Pe}$ act on the $\mathbf{R}_P$ plane wave to the right and $\tilde{T}_{Te}$ act on the $\mathbf{R}_T$ plane wave to the left, inserting a complete set of plane-wave states in $\mathbf{r}_P$ and $\mathbf{R}_P$ between the $\tilde{T}_{Te}$ and G_0^+ factors, and applying Eq. (5), one obtains the expression

$$\begin{aligned}A_e^{(2)}=(2\pi)^{-3}\int d\mathbf{k}_f d\mathbf{k}_i \tilde{\phi}_f^*(\mathbf{k}_f)\tilde{\phi}_i(\mathbf{k}_i)\\ \times T_{Te}(\mathbf{t}_f,\mathbf{k}_i+\alpha(\mathbf{k}_f-\mathbf{K});E_f)\\ \times\tilde{G}_0^+(E_i)T_{Pe}(\mathbf{k}_f+\beta(\mathbf{k}_i+\mathbf{J}),\mathbf{t}_i;E_i)\end{aligned}$$

when the δ functions arising from the heavy-particle integrations are used to evaluate the momentum integrals of the complete set.

Initial and final heavy-particles velocities are defined in terms of the initial and final wave vectors as $\mathbf{v}_i=\mathbf{K}_i/v_i$ and $\mathbf{v}_f=\mathbf{K}_f/v_f$. The notation m/M is introduced to stand for either m/M_P or m/M_T. One can show that $v_f/v_i=1+O(m/M)$, and, for forward-angle capture, that $\mathbf{v}_f\cdot\mathbf{v}_i=1+O(m/M)$; therefore, the projectile velocity is written simply as $\mathbf{v}$. When terms of the order m/M are neglected, the expressions

$$\begin{aligned}&\mathbf{t}_i\approx\mathbf{k}_i-\mathbf{v},\quad E_i\approx\tfrac{1}{2}v^2-\mathbf{v}\cdot\mathbf{k}_i+\varepsilon_i\ ,\\ &\mathbf{t}_f\approx\mathbf{k}_f+\mathbf{v},\quad E_f\approx\tfrac{1}{2}v^2+\mathbf{v}\cdot\mathbf{k}_f+\varepsilon_f\end{aligned}\tag{16}$$

are obtained.

The target-ion and projectile momentum transfers experienced during the collision have been defined as

$$\mathbf{J}=\alpha\mathbf{K}_i-\mathbf{K}_f,\quad \mathbf{K}=\beta\mathbf{K}_f-\mathbf{K}_i\ .\tag{17}$$

They can be written as the vector sum of a component along $\mathbf{v}$ and a component perpendicular to it. The components parallel to $\mathbf{v}$ are $K_z=-v/2+(\varepsilon_i-\varepsilon_f)/v$ and $J_z=-v/2+(\varepsilon_f-\varepsilon_i)/v$, and the components perpendicular to it are $K_\perp$ for $\mathbf{K}$ and $-K_\perp$ for $\mathbf{J}$. Momentum conservation in the process takes the form[24]

$$\mathbf{K}+\mathbf{J}+\mathbf{v}=0\ .$$

The two-body transition matrices T_{Te} and T_{Pe} are defined as

$$T_{Te}(\mathbf{k}',\mathbf{k};\varepsilon)=\left\langle\mathbf{k}'\left|V_{Te}\left[1+\left[\varepsilon+\frac{1}{2\mu_i}\nabla_r^2-V_{Te}+i\eta\right]^{-1}V_{Te}\right]\right|\mathbf{k}\right\rangle\ ,$$

$$T_{Pe}(\mathbf{k}',\mathbf{k};\varepsilon)=\left\langle\mathbf{k}'\left|V_{Pe}\left[1+\left[\varepsilon+\frac{1}{2\mu_f}\nabla_r^2-V_{Pe}+i\eta\right]^{-1}V_{Pe}\right]\right|\mathbf{k}\right\rangle\ ;$$

they are completely off the energy shell, that is, $k^2\neq 2\mu\varepsilon$ and $k'^2\neq 2\mu\varepsilon$, with μ denoting μ_i for T_{Te} or μ_f for T_{Pe}. The scattering energy is given by ε. The free-particle Green's function in momentum space assumes the form

$$\tilde{G}_0^+(E_i)=\{E_i-[\mathbf{k}_f+\beta(\mathbf{k}_i+\mathbf{J})]/2\mu_i+i\eta\}^{-1}\ .$$

With these reductions, the partial amplitude is written

$$\begin{aligned}A_e^{(2)}=(2\pi)^{-3}\int d\mathbf{k}_f d\mathbf{k}_i \tilde{\phi}_f^*(\mathbf{k}_f)\tilde{\phi}_i(\mathbf{k}_i)\\ \times T_{Te}(\mathbf{k}_f+\mathbf{v},\mathbf{k}_i+\mathbf{k}_f-\mathbf{K};E_f)\\ \times\tilde{G}_0^+(E_i)T_{Pe}(\mathbf{k}_f+\mathbf{k}_i+\mathbf{J},\mathbf{k}_i-\mathbf{v};E_i)\ .\end{aligned}\tag{18}$$

Beginning with the far right-hand side of this equation, the interpretation of the amplitude is of the scattering of an electronic "wave packet" with momentum distribution $\mathbf{k}_i$ determined by $\tilde{\phi}_i$ centered about $-\mathbf{v}$ in the projectile frame. The energy of each component $\mathbf{k}_i$ of the packet is E_i. The wave packet collides with the projectile suffering a transfer of momentum $\mathbf{k}_f-\mathbf{K}$ such that after the collision the momentum becomes $\mathbf{k}_i+\mathbf{k}_f+\mathbf{J}$. The off-the-energy-shell scattering is described by the transition matrix T_{Pe}. Subsequently, the packet propagates freely to the next collision as represented by $\tilde{G}_0^+$.

Switching to the target frame, one must boost the momentum components of the packet by $\mathbf{v}$ so that $\mathbf{k}_i+\mathbf{k}_f+\mathbf{J}$ becomes $\mathbf{k}_i+\mathbf{k}_f-\mathbf{K}$. The corresponding shift in energy is

$$\begin{aligned}\Delta E&=\tfrac{1}{2}[(\mathbf{k}_i+\mathbf{k}_f-\mathbf{K})^2-(\mathbf{k}_i+\mathbf{k}_f+\mathbf{J})^2]\\ &=(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{v}+\tfrac{1}{2}(K^2-J^2)\\ &=(\mathbf{k}_i+\mathbf{k}_f)\cdot\mathbf{v}+(\varepsilon_f-\varepsilon_i)\ .\end{aligned}$$

Thus, in the target frame the wave-packet components have the energies

$$E_i+\Delta E=E_f\ .$$

Finally, in the collision with the target ion a momentum transfer $-\mathbf{k}_i-\mathbf{J}$ occurs, giving a final momentum of $\mathbf{k}_f+\mathbf{v}$; i.e., the packet then has a distribution of momentum $\mathbf{k}_f$ about $\mathbf{v}$ given by $\tilde{\phi}_f$. The second collision is described by the transition matrix T_{Te}.

From this discussion and using Eq. (6), it follows that the free Green's function assumes the two equivalent forms

$$\begin{aligned}\tilde{G}_0^+(E_i)&=[E_i-(\mathbf{k}_i+\mathbf{k}_f+\mathbf{J})^2/2+i\eta]^{-1}\\ &=[E_f-(\mathbf{k}_i+\mathbf{k}_f-\mathbf{K})^2/2+i\eta]^{-1}\\ &=\tilde{G}_0^+(E_f)\end{aligned}\tag{19}$$

which will be useful later.

Before considering the internuclear terms, we note that

the first-Born amplitude[25] is readily evaluated using Eqs. (6), (13), and (17) to give

$$A_{\mathrm{B1}} = -4\pi^3(K^2 - 2\varepsilon_f)\tilde{\phi}^*_f(\mathbf{K})\tilde{\phi}_i(\mathbf{J}) \ . \tag{20}$$

The well-known dependence of this partial amplitude on high-momentum components is evident since $K \sim v$ and $J \sim v$.

B. Internuclear terms

The partial amplitude A_n containing the internuclear terms is reduced in this section. The notation

$$\begin{aligned} A_n &= \langle \Phi_f | \tilde{T}_{PT} | \Phi_i \rangle + \langle \Phi_f | \tilde{T}_{Te} G_0^+(E) \tilde{T}_{PT} | \Phi_i \rangle \\ &\quad + \langle \Phi_f | \tilde{T}_{PT} G_0^+(E) \tilde{T}_{Pe} | \Phi_i \rangle \\ &\equiv A_n^{(1)} + A_n^{(2a)} + A_n^{(2b)} \ . \end{aligned} \tag{21}$$

is introduced.

1. First-order internuclear term

The first-order part of A_n is simplified using Eqs. (12) and (13):

$$A_n^{(1)} = \int d\mathbf{k}_f d\mathbf{k}_i \tilde{\phi}^*_f(\mathbf{k}_f)\tilde{\phi}_i(\mathbf{k}_i) \times \langle \mathbf{k}_f + \beta'\mathbf{K}_f, \mathbf{U}_f | \tilde{T}_{PT}(E) | \mathbf{k}_i - \alpha'\mathbf{K}_i, \mathbf{U}_i \rangle \ .$$

After the Green's function in $\tilde{T}_{PT}$ operates on the plane wave in $\mathbf{r}$, the δ function ensuing from the $\mathbf{r}$ integration forces the equality

$$\mathbf{k}_f = \mathbf{k}_i - \alpha'\mathbf{K}_i - \beta'\mathbf{K}_f = \mathbf{k}_i + \mathbf{J} + \mathbf{K} \approx \mathbf{k}_i - \mathbf{v} \ ,$$

which is valid, as before, to order m/M.

When the $\mathbf{k}_f$ integration is performed using the δ function, one obtains

$$A_n^{(1)} = \int d\mathbf{k}_i \tilde{\phi}^*_f(\mathbf{k}_i - \mathbf{v})\tilde{\phi}_i(\mathbf{k}_i) T_{PT}(\mathbf{U}_i - \mathbf{k}_i - \mathbf{J}, \mathbf{U}_i; E_n) \ , \tag{22}$$

where

$$E_n = E - (\mathbf{k}_i - \alpha'\mathbf{K}_i)^2/2\nu_n \ . \tag{23}$$

If $\mathbf{k}_i = \mathbf{0}$, the momentum transfer is $-\mathbf{J}$, and when $\mathbf{k}_i = \mathbf{v}$, it is $\mathbf{K}$. The two-body internuclear transition matrix is defined as

$$T_{PT}(\mathbf{k}', \mathbf{k}; \varepsilon) = \left\langle \mathbf{k}' \left| V_{PT} \left[1 + \left[\varepsilon + \frac{1}{2\mu_n}\nabla^2_{\mathbf{R}} - V_{PT} + i\eta \right]^{-1} V_{PT} \right] \right| \mathbf{k} \right\rangle \ .$$

In approximate form, neglecting m/M terms, one has

$$A_n^{(1)} = \int d\mathbf{k}_i \tilde{\phi}^*_f(\mathbf{k}_i - \mathbf{v})\tilde{\phi}_i(\mathbf{k}_i) T_{PT}(\mu_n\mathbf{v} - \mathbf{k}_i - \mathbf{J}, \mu_n\mathbf{v}; E_n) \tag{24}$$

with $E_n = \frac{1}{2}\mu_n v^2$. While Eq. (24) is conceptually useful, it cannot be used to approximate the two-body transition matrix, as is apparent from Appendix A; Eq. (22) must be used instead.

2. Second-order internuclear terms

(a) *Term including* $\tilde{T}_{Te}$. Using Eqs. (12) and (13) gives for the first term

$$A_n^{(2a)} = (2\pi)^{-3} \int d\mathbf{k}_f d\mathbf{k}_i \tilde{\phi}^*_f(\mathbf{k}_f)\tilde{\phi}_i(\mathbf{k}_i) \langle -\mathbf{k}_f + \beta\mathbf{K}_f, \mathbf{t}_f | \tilde{T}_{Te} G_0^+(E) \tilde{T}_{PT} | \mathbf{k}_i - \alpha'\mathbf{K}_i, \mathbf{U}_i \rangle \ .$$

Letting the operators $\tilde{T}_{Te}$ and G_0^+ act on the $\mathbf{R}_T$ plane wave to the left and the operator $\tilde{T}_{PT}$ act on the $\mathbf{r}$ plane wave to the right, inserting a complete set of plane-wave states in $\mathbf{r}$ and $\mathbf{R}$ between the G_0^+ and $\tilde{T}_{PT}$ factors, and using Eq. (5), one derives the expression

$$A_n^{(2a)} = (2\pi)^{-3} \int d\mathbf{k}_f d\mathbf{k}_i \tilde{\phi}^*_f(\mathbf{k}_f)\tilde{\phi}_i(\mathbf{k}_i) T_{Te}(\mathbf{t}_f, \mathbf{k}_i - \alpha'(\mathbf{k}_f - \mathbf{K}); E_f) \tilde{G}_0^+(E_f) T_{PT}(\mathbf{U}_i - \mathbf{k}_f + \mathbf{K}, \mathbf{U}_i; E_n) \tag{25}$$

when the δ functions arising from the $\mathbf{r}$ and $\mathbf{R}$ integrations are applied to evaluate the momentum integrals of the complete set. The momentum-space Green's function in this expression is given by

$$\tilde{G}_0^+(E_f) = \{ E_f - [\mathbf{k}_i + \alpha'(\mathbf{K} - \mathbf{k}_f)]^2/2\mu_i + i\eta \}^{-1} \ .$$

(b) *Term including* $\tilde{T}_{Pe}$. Equations (12) and (13) give for the second term

$$A_n^{(2b)} = (2\pi)^{-3} \int d\mathbf{k}_f d\mathbf{k}_i \tilde{\phi}^*_f(\mathbf{k}_f)\tilde{\phi}_i(\mathbf{k}_i) \langle \mathbf{k}_f + \beta'\mathbf{K}_f, \mathbf{U}_f | \tilde{T}_{PT} G_0^+(E) \tilde{T}_{Pe} | \mathbf{k}_i + \alpha\mathbf{K}_i, \mathbf{t}_i \rangle \ .$$

Letting the operators G_0^+ and $\tilde{T}_{Pe}$ act on the $\mathbf{R}_P$ plane wave to the right and the operator $\tilde{T}_{PT}$ act on the $\mathbf{r}$ plane wave to the left, inserting between the $\tilde{T}_{PT}$ and G_0^+ factors a complete set of plane-wave states in $\mathbf{R}$ and $\mathbf{r}$, and using Eq. (5), one obtains the expression

$$A_n^{(2b)} = (2\pi)^{-3} \int d\mathbf{k}_f d\mathbf{k}_i \tilde{\phi}^*_f(\mathbf{k}_f)\tilde{\phi}_i(\mathbf{k}_i) T_{PT}(\mathbf{U}_f, \mathbf{U}_f + \mathbf{k}_i + \mathbf{J}; E_n) \tilde{G}_0^+(E_i) T_{Pe}(-\mathbf{k}_f + \beta'(\mathbf{k}_i + \mathbf{J}), \mathbf{t}_i; E_i) \tag{26}$$

when the δ functions arising from the $\mathbf{r}$ and $\mathbf{R}$ integrations are applied to perform the momentum integrations of the

complete set. The momentum-space Green's function is given by

$$\tilde{G}_0^+(E_i)=\{E_i-[-\mathbf{k}_f+\beta'(\mathbf{k}_i+\mathbf{J})]^2/2\mu_f+i\eta\}^{-1} .$$

V. APPROXIMATE EVALUATION OF THE AMPLITUDE

Although the amplitude given in Eq. (9) permits a conceptually straightforward interpretation, its evaluation is conceptually daunting since it involves two-body transition matrices as opposed to the two-body potentials appearing in the B2 approximation. A further complication arises in the application to proton-helium collisions where the simple analytic form of the pure Coulomb potential is no longer valid. Since an exact evaluation of the amplitude is so difficult, an approximate treatment is used here based on the recently derived near-shell form of the two-body T matrix for a modified-Coulomb potential. This is a first look at results of the FWL formalism. The near-shell form is applicable provided the off-shell energy defect can be shown to be small. This is the case if one of our basic assumptions, viz., that $(Z_P/v)^2$ and $(Z_T/v)^2$ be small, is invoked.

An approximate evaluation has the advantages of isolating the important mechanisms of the capture process at the impact energies considered and allowing connections to be drawn with the more well-known methods for treating the high-energy capture problem such as the B2 approximation. Therefore the partial amplitudes of A_{FWL} given in Eqs. (18), (22), (25), and (26) are approximated to order $(Z_P/v)^2$ and $(Z_T/v)^2$ in this section.

For modified Coulomb potentials, the two-body transition matrix[16] reduces to a generalized elastic scattering amplitude multiplied by so-called off-energy-shell factors when the energy shell is approached. The limiting form mimics the known behavior for the pure Coulomb potential with the differences that the charge of the long-range pure Coulomb part of the modified Coulomb potential appears in the off-shell factors and that the Coulomb scattering amplitude is replaced by the sum of the amplitude for the Coulomb potential and the amplitude for the short-range part of the potential.

When the modified Coulomb potential is well represented by a scaled pure Coulomb potential in the inner region, the sum of the Coulomb and short-range amplitudes is approximated by the Coulomb amplitude for the screened potential. Such a simplification works when the impact energies are large, so that the individual collisions of the doubling scatterings are hard ones and the momentum transfers are large.

Appendix A gives a derivation of the near-shell form of the pure Coulomb two-body transition matrix. It lists also the analogous result for the modified Coulomb potential and the result when the inner form of the modified potential is Coulomb-like. Appendix B gives a discussion of order of magnitude estimates of certain parameters on which the Coulomb T matrices in the present work depend. In Appendix C, it is shown that for singly charged ions incident on neutral atoms the total amplitude A_{FWL} is well behaved: nonintegrable singularities are not present. If this were not the case, the approximations introduced below would not be quantitatively based, but only qualitative. In general, the conclusion is that the near-shell forms can be used to the order of the square of the projectile or target nuclear charges over impact velocity. The reader is referred to the Appendixes for details.

A. Electronic-nuclear terms

Because of the presence of the bound-state wave functions, the integral in the second-order electronic term [Eq. (18)] is dominated by momentum values in the regions $k_i \lesssim Z_T$ and $k_f \lesssim Z_P$. Consequently, the near-shell approximations to the T matrices in $A_e^{(2)}$ are

$$T_{Pe}(\mathbf{k}_f+\mathbf{k}_i+\mathbf{J},\mathbf{k}_i-\mathbf{v};E_i)\approx -4\pi Z_P e^{\pi\nu_P^a}[\Gamma(1+i\nu_P^a)^2\Gamma(1-i\nu_P)/\Gamma(1+i\nu_P)] \times(8E_i)^{i(2\nu_P^a-\nu_P)}[(k_i^2-2\varepsilon_i)/\tilde{G}_0^+]^{-i\nu_P^a}|\mathbf{k}_i+\mathbf{J}|^{-2+2i\nu_P}$$

and

$$T_{Te}(\mathbf{k}_f+\mathbf{v},\mathbf{k}_i+\mathbf{k}_f-\mathbf{K};E_i)\approx -4\pi Z_T e^{\pi\nu_T^a}[\Gamma(1+i\nu_T^a)^2\Gamma(1-i\nu_T)/\Gamma(1+i\nu_T)] \times(8E_f)^{i(2\nu_T^a-\nu_T)}[(k_f^2-2\varepsilon_f)/\tilde{G}_0^+]^{-i\nu_T^a}|\mathbf{k}_f-\mathbf{K}|^{-2+2i\nu_T} ,$$

with the Sommerfeld parameters given by $\nu_P^a=Z_P^a/(2E_i)^{1/2}$, $\nu_P=Z_P/(2E_i)^{1/2}$, $\nu_T^a=Z_T^a/(2E_f)^{1/2}$, and $\nu_T=Z_T/(2E_f)^{1/2}$. Using these expressions and the $1s$ hydrogenic wave function in momentum space

$$\tilde{\phi}_{1s}(\mathbf{k})=2^{3/2}Z^{5/2}/\pi(k^2+Z^2)^2 , \tag{27}$$

the amplitude is written

$$A_e^{(2)}=2(2/\pi)^2(Z_TZ_P)^{7/2}e^{\pi\nu_P^a}\frac{\Gamma(1+i\nu_P^a)^2\Gamma(1-i\nu_P)}{\Gamma(1+i\nu_P)}e^{\pi\nu_T^a}\frac{\Gamma(1+i\nu_T^a)^2\Gamma(1-i\nu_T)}{\Gamma(1+i\nu_T)}$$
$$\times(4v^2)^{i(2\nu_P^a-\nu_P)}J^{-2+2i\nu_P}(4v^2)^{i(2\nu_T^a-\nu_T)}K^{-2+2i\nu_T}$$
$$\times\int d\mathbf{k}_f d\mathbf{k}_i(k_i^2-2\varepsilon_i)^{-2-i\nu_P^a}(k_f^2-2\varepsilon_f)^{-2-i\nu_T^a}[\tilde{G}_Q^{+}(E_i)]^{1+i\nu_T^a+i\nu_P^a}\ , \tag{28}$$

where $\tilde{G}_Q^{+}(E_i)$ is a quadratic approximation to the Green's function [Eq. (19)] in which the $\mathbf{k}_i\cdot\mathbf{k}_f$ term is neglected:

$$\tilde{G}_0^{+}(E_i)\approx\tilde{G}_Q^{+}(E_i)=[\tfrac{1}{2}(v^2-K^2+\varepsilon_i)-\mathbf{k}_f\cdot\mathbf{J}+\mathbf{k}_i\cdot\mathbf{K}$$
$$-\tfrac{1}{2}(k_i^2+k_f^2)+i\eta]^{-1}\ , \tag{29}$$

and where now

$$\nu_P^a=Z_P^a/v,\quad \nu_P=Z_P/v\ ,$$
$$\nu_T^a=Z_T^a/v,\quad \nu_T=Z_T/v\ . \tag{30}$$

The evaluation of the six-dimensional integral in Eq. (28) proceeds by reducing it to two radial integrals through straightforward angular integrations along with radial integrations by part. The radial variables are then written as $k_i=k\cos\theta$ and $k_f=k\sin\theta$. By means of Cauchy's integral theorem, the integration path for k along the positive real axis is converted into two straight lines, one from $0+i0$ to k_x+ik_y and the other from k_x+ik_y to $\infty+i0$, with k_x and k_y denoting constants. The deformed path is parametrized on the real-line segment (0,1). In this manner, the singularity in the Green's function is avoided during the integration. The θ and parameterized k integrations are performed numerically using an adaptive quadrature routine.[26] Tolerances were given as 10^{-8} and 10^{-6}, respectively. The output of cross sections was explicitly checked. Better than four-digit accuracy is maintained, even in the difficult Thomas peak region.

If the remaining quadratic terms k_i^2 and k_f^2 in Eq. (29) are neglected, an approximation to the free Green's function is obtained which is linear in $\mathbf{k}_i$ and $\mathbf{k}_f$. When this linearized Green's function is substituted into Eq. (28) the integrals can be evaluated to give a closed-form expression for the electronic part of the FWL amplitude in terms of F_4 generalized hypergeometric functions. A discussion of this version of the amplitude is presented elsewhere.[27] Such a treatment is valuable for its isolation of the velocity dependence of a high-order multiple-scattering amplitude.

B. Internuclear terms

1. *First-order internuclear term*

The T-matrix approximation in the first-order internuclear term in Eq. (22) is

$$T_{PT}(\mathbf{U}_i-\mathbf{k}_i-\mathbf{J},\mathbf{U}_i;E_n)\approx 4\pi Z_PZ_Te^{-\pi\nu_{PT}^a}[\Gamma(1-i\nu_{PT}^a)^2\Gamma(1+i\nu_{PT})/\Gamma(1-i\nu_{PT})]$$
$$\times(8E_n)^{-i(2\nu_{PT}^a-\nu_{PT})}\{[(\mathbf{k}_i-\mathbf{v})^2-2\varepsilon_f](k_i^2-2\varepsilon_i)\}^{i\nu_{PT}^a}|\mathbf{k}_i+\mathbf{J}|^{-2-2i\nu_{PT}}\ ,$$

with the Sommerfeld parameters given by $\nu_{PT}^a=\mu_nZ_P^aZ_T^a/(2\mu_nE_n)^{1/2}$ and $\nu_{PT}=\mu_nZ_PZ_T/(2\mu_nE_n)^{1/2}$. Using the same approximations as in Sec. V A, one finds the partial amplitude

$$A_n^{(1)}=\frac{2^5}{\pi}(Z_PZ_T)^{7/2}e^{-\pi\nu_{PT}^a}\frac{\Gamma(1-i\nu_{PT}^a)^2\Gamma(1+i\nu_{PT})}{\Gamma(1-i\nu_{PT})}(4\mu_nv^2)^{-i(2\nu_{PT}^a-\nu_{PT})}$$
$$\times\int d\mathbf{k}_i\{[(\mathbf{k}_i-\mathbf{v})^2-2\varepsilon_f](k_i^2-2\varepsilon_i)\}^{-2+i\nu_{PT}^a}|\mathbf{k}_i+\mathbf{J}|^{-2-2i\nu_{PT}}\ ,$$

where now

$$\nu_{PT}^a=Z_P^aZ_T^a/v,\quad \nu_{PT}=Z_PZ_T/v\ . \tag{31}$$

The μ_n factor appearing in this intermediate version of $A_n^{(1)}$ arises because the inner and outer charges of the modified Coulomb potential are not equal.

The remaining integral is evaluated by treating the two dominant peaks in the integrand at $\mathbf{k}_i=0$ and $\mathbf{v}$ as if they were separate peaks and by neglecting the $\mathbf{k}_i$ variation about the peaks of the other factors. This is justified if the two peaks are well separated in momentum space, as is true for $v\gg Z_P$ and $v\gg Z_T$. Noting that

$$\int d\mathbf{k}(k^2+Z^2)^{-2+i\nu}=\pi^{3/2}Z^{-1+2i\nu}\Gamma(\tfrac{1}{2}-i\nu)/\Gamma(2-i\nu)\ , \tag{32}$$

the result

$$A_n^{(1)}=2^5\pi^{1/2}(Z_PZ_T)^{5/2}e^{-\pi\nu_{PT}^a}\frac{\Gamma(1-i\nu_{PT}^a)\Gamma(\frac{1}{2}-i\nu_{PT}^a)\Gamma(1+i\nu_{PT})}{(1-i\nu_{PT}^a)\Gamma(1-i\nu_{PT})}(4\mu_n v^2)^{-i(2\nu_{PT}^a-\nu_{PT})}$$
$$\times[Z_TZ_P^{2i\nu_{PT}^a}(v^2+Z_T^2)^{-2+i\nu_{PT}^a}K^{-2-2i\nu_{PT}}+Z_PZ_T^{2i\nu_{PT}^a}(v^2+Z_P^2)^{-2+i\nu_{PT}^a}J^{-2-2i\nu_{PT}}] \tag{33}$$

is obtained, assuming $\varepsilon_i=\varepsilon_{1s}=-\frac{1}{2}Z_T^2$ and $\varepsilon_f=\varepsilon_{1s}=-\frac{1}{2}Z_P^2$. The relation $\mathbf{K}=-\mathbf{v}-\mathbf{J}$ has also been used.

2. *Second-order internuclear terms*

(a) *Term including* T_{Te}. The T matrix approximations to the term in Eq. (25) are

$$T_{PT}(\mathbf{U}_i-\mathbf{k}_f+\mathbf{K},\mathbf{U}_i;E_n)\approx 4\pi Z_PZ_Te^{-\pi\nu_{PT}^a}[\Gamma(1-i\nu_{PT}^a)^2\Gamma(1+i\nu_{PT})/\Gamma(1-i\nu_{PT})]$$
$$\times(8E_n)^{-i(2\nu_{PT}^a-\nu_{PT})}[(k_i^2-2\varepsilon_i)/\tilde{G}_0^+]^{i\nu_{PT}^a}|\mathbf{k}_f-\mathbf{K}|^{-2-2i\nu_{PT}}$$

and

$$T_{Te}(\mathbf{t}_f,\mathbf{k}_i-\alpha'(\mathbf{k}_f-\mathbf{K});E_f)\approx -4\pi Z_Te^{\pi\nu_T^a}[\Gamma(1+i\nu_T^a)^2\Gamma(1-i\nu_T)/\Gamma(1+i\nu_T)]$$
$$\times(8E_f)^{i(2\nu_T^a-\nu_T)}[(k_f^2-2\varepsilon_f)/\tilde{G}_0^+]^{-i\nu_T^a}|\mathbf{k}_i-\mathbf{k}_f-\mathbf{v}|^{-2+2i\nu_T},$$

where the Sommerfeld parameters are $\nu_{PT}^a=\mu_nZ_P^aZ_T^a/(2\mu_nE_n)^{1/2}$, $\nu_{PT}=\mu_nZ_PZ_T/(2\mu_nE_n)^{1/2}$, $\nu_T^a=Z_T^a/(2E_f)^{1/2}$, and $\nu_T=Z_T/(2E_f)^{1/2}$. Retaining only those terms in the integrand in which the momentum variation is rapid in the sense used in Sec. V B 1, one obtains the intermediate expression

$$A_n^{(2a)}=-2(2/\pi)^3Z_T(Z_PZ_T)^{7/2}e^{\pi\nu_T^a}\frac{\Gamma(1+i\nu_T^a)^2\Gamma(1-i\nu_T)}{\Gamma(1+i\nu_T)}e^{-\pi\nu_{PT}^a}\frac{\Gamma(1-i\nu_{PT}^a)^2\Gamma(1+i\nu_{PT})}{\Gamma(1-i\nu_{PT})}$$
$$\times(2v)^{i2(2\nu_T^a-\nu_T)}v^{-2+2i\nu_T}(\tfrac{1}{2}v^2+\varepsilon_f)^{-1-i\nu_T^a+i\nu_{PT}^a}(4\mu_nv^2)^{-i(2\nu_{PT}^a-\nu_{PT})}K^{-2-2i\nu_{PT}}$$
$$\times\int d\mathbf{k}_fd\mathbf{k}_i(k_i^2-2\varepsilon_i)^{-2+i\nu_{PT}^a}(k_f^2-2\varepsilon_f)^{-2-i\nu_T^a}.$$

Using Eq. (32) gives the result

$$A_n^{(2a)}=-2^4(Z_PZ_T)^{5/2}Z_T^{1+2i\nu_{PT}^a}Z_P^{-2i\nu_T^a}e^{\pi\nu_T^a}e^{-\pi\nu_{PT}^a}$$
$$\times\frac{\Gamma(1+i\nu_T^a)\Gamma(\frac{1}{2}+i\nu_T^a)\Gamma(1-i\nu_T)\Gamma(1-i\nu_{PT}^a)\Gamma(\frac{1}{2}-i\nu_{PT}^a)\Gamma(1+i\nu_{PT})}{(1+i\nu_T^a)\Gamma(1+i\nu_T)(1-i\nu_{PT}^a)\Gamma(1-i\nu_{PT})}$$
$$\times(2v)^{i2(2\nu_T^a-\nu_T)}v^{-2+2i\nu_T}[\tfrac{1}{2}(v^2-Z_P^2)]^{-1-i\nu_T^a+i\nu_{PT}^a}(4\mu_nv^2)^{-i(2\nu_{PT}^a-\nu_{PT})}K^{-2-2i\nu_{PT}}, \tag{34}$$

where ν_{PT}^a, ν_{PT}, ν_T^a, and ν_T are defined in Eqs. (30) and (31).

(b) *Term including* T_{Pe}. The T-matrix approximations to the other second-order internuclear term Eq. (26) are

$$T_{PT}(\mathbf{U}_f,\mathbf{U}_f+\mathbf{k}_i+\mathbf{J};E_n)\approx 4\pi Z_PZ_Te^{-\pi\nu_{PT}^a}[\Gamma(1-i\nu_{PT}^a)^2\Gamma(1+i\nu_{PT})/\Gamma(1-i\nu_{PT})]$$
$$\times(8E_n)^{-i(2\nu_{PT}^a-\nu_{PT})}[(k_f^2-2\varepsilon_i)/\tilde{G}_0^+]^{i\nu_{PT}^a}|\mathbf{k}_i+\mathbf{J}|^{-2-2i\nu_{PT}}$$

and

$$T_{Pe}(-\mathbf{k}_f+\beta'(\mathbf{k}_i+\mathbf{J}),\mathbf{t}_i;E_i)\approx -4\pi Z_Pe^{\pi\nu_P^a}[\Gamma(1+i\nu_P^a)^2\Gamma(1-i\nu_P)/\Gamma(1+i\nu_P)]$$
$$\times(8E_i)^{i(2\nu_P^a-\nu_P)}[(k_i^2-2\varepsilon_i)/\tilde{G}_0^+]^{-i\nu_P^a}|\mathbf{k}_f-\mathbf{k}_i+\mathbf{v}|^{-2+2i\nu_P},$$

with $\nu_{PT}^a=\mu_nZ_P^aZ_T^a/(2\mu_nE_n)^{1/2}$, $\nu_{PT}=\mu_nZ_PZ_T/(2\mu_nE_n)^{1/2}$, $\nu_P^a=Z_P^a/(2E_i)^{1/2}$, and $\nu_P=Z_P/(2E_i)^{1/2}$. Retaining only those terms in the integrand in which the momentum variation is rapid as was done above, one finds the expression

$$A_n^{(2b)}=-2(2/\pi)^3Z_P(Z_PZ_T)^{7/2}e^{-\pi\nu_{PT}^a}\frac{\Gamma(1-i\nu_{PT}^a)^2\Gamma(1+i\nu_{PT})}{\Gamma(1-i\nu_{PT})}e^{\pi\nu_P^a}\frac{\Gamma(1+i\nu_P^a)^2\Gamma(1-i\nu_P)}{\Gamma(1+i\nu_P)}$$
$$\times(4\mu_nv^2)^{-i(2\nu_{PT}^a-\nu_{PT})}J^{-2-2i\nu_{PT}}(\tfrac{1}{2}v^2+\varepsilon_i)^{-1+i\nu_{PT}^a-i\nu_P^a}(2v)^{i2(2\nu_P^a-\nu_P)}v^{-2+2i\nu_P}$$
$$\times\int d\mathbf{k}_fd\mathbf{k}_i(k_i^2-2\varepsilon_i)^{-2-i\nu_P^a}(k_f^2-2\varepsilon_f)^{-2+i\nu_{PT}^a},$$

which becomes

$$A_n^{(2b)} = -2^4(Z_P Z_T)^{5/2} Z_T^{-2i\nu_P^a} Z_P^{1+2i\nu_{PT}^a} e^{-\pi\nu_{PT}^a} e^{\pi\nu_P^a} \times \frac{\Gamma(1-i\nu_{PT}^a)\Gamma(\frac{1}{2}-i\nu_{PT}^a)\Gamma(1+i\nu_{PT})\Gamma(1+i\nu_P^a)\Gamma(\frac{1}{2}+i\nu_P^a)\Gamma(1-i\nu_P)}{(1-i\nu_{PT}^a)\Gamma(1-i\nu_{PT})(1+i\nu_P^a)\Gamma(1+i\nu_P)} \times (4\mu_n v^2)^{-i(2\nu_{PT}^a-\nu_{PT})} J^{-2-2i\nu_{PT}} [\tfrac{1}{2}(v^2-Z_T^2)]^{-1+i\nu_{PT}^a-i\nu_P^a} (2v)^{i2(2\nu_P^a-\nu_P)} v^{-2+2i\nu_P} , \quad (35)$$

where ν_{PT}^a, ν_{PT}, ν_P^a, and ν_P are given by Eqs. (30) and (31).

3. *Total internuclear term*

Combining the terms in Eqs. (33)–(35) and regrouping some of the factors, one finds

$$A_n = 2^4(Z_P Z_T)^{5/2} e^{-\pi\nu_{PT}^a} \frac{\Gamma(1-i\nu_{PT}^a)\Gamma(\frac{1}{2}-i\nu_{PT}^a)\Gamma(1+i\nu_{PT})}{(1-i\nu_{PT}^a)\Gamma(1-i\nu_{PT})} (4\mu_n v^2)^{-i(2\nu_{PT}^a-\nu_{PT})} \times \Big[Z_T K^{-2-2i\nu_{PT}} \Big\{ 2\pi^{1/2} Z_P^{2i\nu_{PT}^a} (v^2+Z_T^2)^{-2+i\nu_{PT}^a} - Z_T^{2i\nu_{PT}^a} Z_P^{-2i\nu_T^a} e^{\pi\nu_T^a} \frac{\Gamma(1+i\nu_T^a)\Gamma(\frac{1}{2}+i\nu_T^a)\Gamma(1-i\nu_T)}{(1+i\nu_T^a)\Gamma(1+i\nu_T)} \times (4v^2)^{i(2\nu_T^a-\nu_T)} v^{-2+2i\nu_T} [\tfrac{1}{2}(v^2-Z_P^2)]^{-1-i\nu_T^a+i\nu_{PT}^a} \Big\} + Z_P J^{-2-2i\nu_{PT}} \Big\{ 2\pi^{1/2} Z_T^{2i\nu_{PT}^a} (v^2+Z_P^2)^{-2+i\nu_{PT}^a} - Z_T^{-2i\nu_P^a} Z_P^{2i\nu_{PT}^a} e^{\pi\nu_P^a} \frac{\Gamma(1+i\nu_P^a)\Gamma(\frac{1}{2}+i\nu_P^a)\Gamma(1-i\nu_P)}{(1+i\nu_P^a)\Gamma(1+i\nu_P)} \times [\tfrac{1}{2}(v^2-Z_T^2)]^{-1+i\nu_{PT}^a-i\nu_P^a} (4v^2)^{i(2\nu_P^a-\nu_P)} v^{-2+2i\nu_P} \Big\} \Big] , \quad (36)$$

which is symmetric in the two charges, momentum transfers, etc. The dependence of Eq. (36) on K^{-2} and J^{-2} reflects the nuclear Coulomb scattering. Also noteworthy is the appearance of two terms of opposite sign in each set of large parentheses. Ignoring the different multiplying factors and neglecting factors of order $(Z_P/v)^2$ and $(Z_T/v)^2$, a cancellation of contributions would be expected in Eq. (36).

VI. RESULTS AND DISCUSSION

Sections VI A and VI B present results calculated using the FWL formalism and compares them with other theoretical results and with experimental results. The internuclear contribution is discussed in Sec. VI C. Although only a small angular region from 0 to 1 mrad is of interest, one should still keep in mind that there are four separate subregions involving different scattering effects: first, an extreme forward direction where the first-Born term dominates; second, an interference region where large cancellations of the various terms occur; third, the Thomas peak region where double-scattering dominates; and finally, the region beyond the secondary peak where internuclear scattering takes over. Extensive analysis of the many different contributions is made.

A. Proton-helium collisions

Results for proton-helium collisions are presented in Figs. 3–5. Figure 3 compares full FWL calculated cross

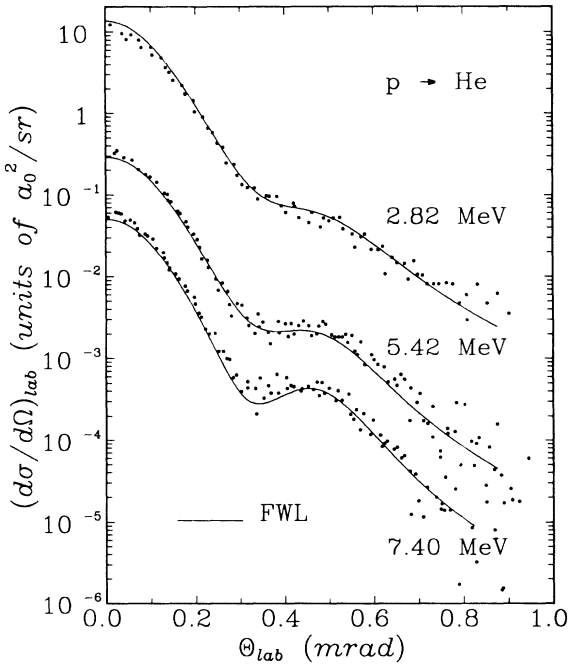

FIG. 3. Differential cross sections for $1s \rightarrow 1s$ capture in 2.82-, 5.42-, and 7.40-MeV proton-helium collisions. Results of Faddeev-Watson-Lovelace (FWL) calculations including the internuclear terms in the amplitude are compared with the experimental data of Horsdal-Pedersen, Cocke, and Stockli (Ref. 1). The theoretical results have been convoluted with the beam profiles (Ref. 28).

sections [i.e., ones derived from the sum of A_e in Eq. (28) and A_n in Eq. (36)] with the experimental data of Horsdal-Pedersen, Cocke, and Stockli[1] for the incident proton energies 2.82, 5.42, and 7.40 MeV. These energies correspond respectively to the velocities 10.6, 14.7, and 17.1 a.u. The data, which include capture to all excited states, have good statistics (significantly better than for hydrogen targets); individual points are estimated to be accurate to within 30%. The theoretical cross sections have been convoluted with the experimental beam profiles[28] and are for $1s \rightarrow 1s$ capture only. In the numerical calculations, the values assumed for the charges in the Sommerfeld parameters are $Z_P = 1.0$, $Z_P^a = 1.0$, $Z_T = 1.6875$, and $Z_T^a = 1.0$. This figure shows extremely good agreement, both in magnitude and shape, between theory and experiment at all three energies.

In Fig. 4, the FWL cross sections and experimental data at 2.82 and 5.42 MeV are compared with the continuum distorted-wave cross sections of Rivarola, Salin, and Stockli[17] and the transverse-peaking SPB cross sections of Alston,[19] both of which are also convoluted. It is seen that the FWL results agree significantly better with the data than do the CDW or SPB results. Up to about 0.2 mrad where the first-Born amplitude dominates, the variation is smallest but even in this region there are differences of 50%. Beyond the Thomas peak at ~0.5 mrad where the nuclear scattering produces the main effect, the FWL and CDW curves agree better. In this region, the SPB curve becomes too small due to the omission of the nuclear part. The largest differences are found between 0.2 and 0.4 mrad, reflecting significant cancellation of the different parts of the amplitudes there. This exposes the level of accuracy to which secondary contributions are treated as well as the inclusion of different higher-order effects in the separate theories. These differences are discussed further below. Finally, rather large differences are also found at the Thomas peak, even though one might have expected better agreement between the theories because of the applicability of the classical picture at this angle. It should be noted, however, that some of the large differences seen in Fig. 4 are exaggerated as a result of the convolution process, as comparison with Fig. 5 shows.

Figure 5 presents unconvoluted cross sections calculated using the FWL formalism *without* the internuclear terms, i.e., the DWB theory of Taulbjerg and Briggs,[20] and compares them with corresponding values of the CDW, SPB, and B2 theories. The small differences between the three unconvoluted curves in the forward-peak region again reflect the dominance of the first-Born amplitude whose contribution is identical in the DWB, SPB, and B2 theories and which is included in another manner in the CDW theory. Beyond the Thomas peak region at 0.47 mrad, the DWB and B2 curves agree very well and the SPB curve has the same slope and curvature but is shifted upward due to the overall momentum-transfer dependence having a different multiplicative coefficient. The CDW curve has the nuclear contribution included,

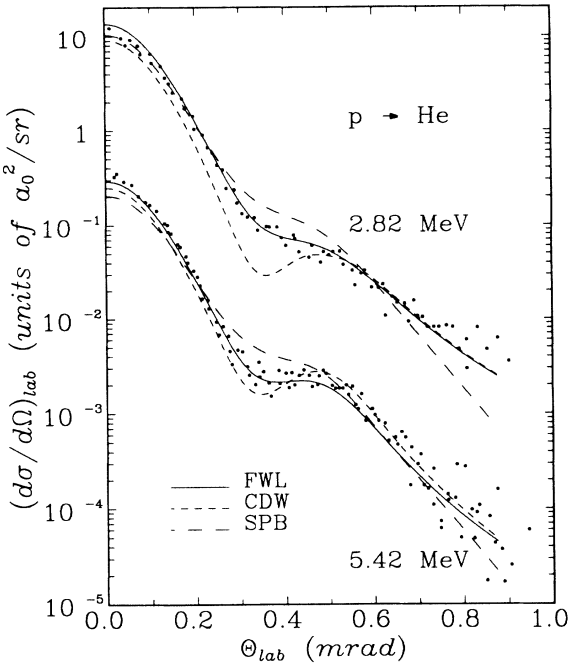

FIG. 4. Differential cross sections for $1s \rightarrow 1s$ capture in 2.82- and 5.42-MeV proton-helium collisions. Results of (FWL) (solid lines), SPB (long-dashed lines, Ref. 19), and CDW (short-dashed lines, Ref. 17) calculations are compared with the experimental data of Horsdal-Pedersen, Cocke, and Stockli (Ref. 1). The theoretical results have been convoluted with the beam profiles (Ref. 28).

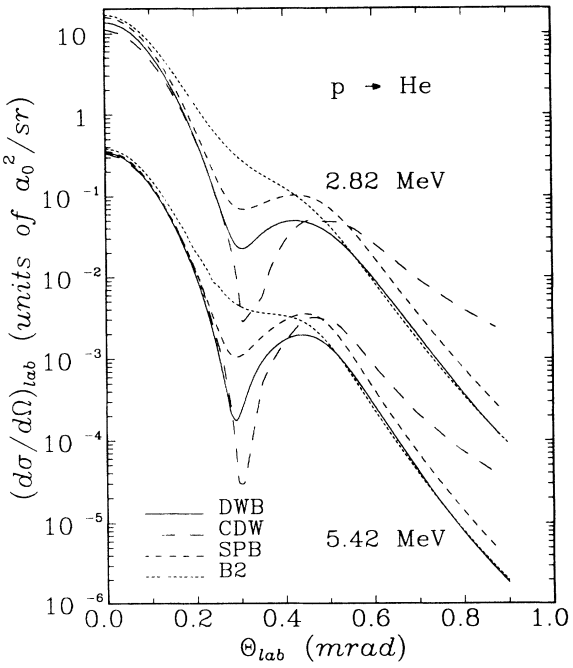

FIG. 5. Differential cross sections for $1s \rightarrow 1s$ capture in 2.82- and 5.42-MeV proton-helium collisions. Results of unconvoluted (DWB) (solid lines), SPB (short-dashed lines, Ref. 19), CDW (long-dashed lines, Ref. 17), and B2 (dotted lines) calculations are compared.

explaining the difference of this curve here.

To study the FWL and B2 amplitudes further, it is useful to compare the second-order parts of these complex amplitudes. Figure 6(a) shows the imaginary parts of the amplitudes. At the Thomas peak (or hump), there are local maxima that represent scattering via on-energy-shell intermediate states. Within the B2 approximation, the peaking of the imaginary part of the amplitude and the association with on-shell scattering are expected features if the free Green's operator is written as a sum of principal-part and δ function terms: $G_0^+(E)=\mathcal{P}(E-E')-i\pi\delta(E-E')$, noting in addition that the potentials and wave functions are real.[29] In a classical and, consequently, on-shell treatment of the capture process a similar peak in the amplitude is found.[3] A comparison of the imaginary parts of the FWL and B2 amplitudes shows that the FWL treatment of this component of the scattering is not appreciably modified. Even though a consistent treatment of off-energy-shell effects has been incorporated in the FWL approximation, the off-shell effects vanish. For angles to the left of Thomas peak, the FWL curves becomes much smaller than the B2 curves, the more so for the higher energy. The very large differences are not reflected in the differential cross sections since in this region the imaginary parts are considerably smaller than the real parts. [See Fig. 6(b)].

Associated with the much less accentuated dips in the B2 cross sections relative to the FWL (or DWB) cross sections in Fig. 5 (for helium only a shoulder appears) are the smaller real parts of the second-order term of the B2 amplitude in Fig. 6(b). The absolute values of the real parts are actually plotted in Fig. 6(b) and the sharp dips

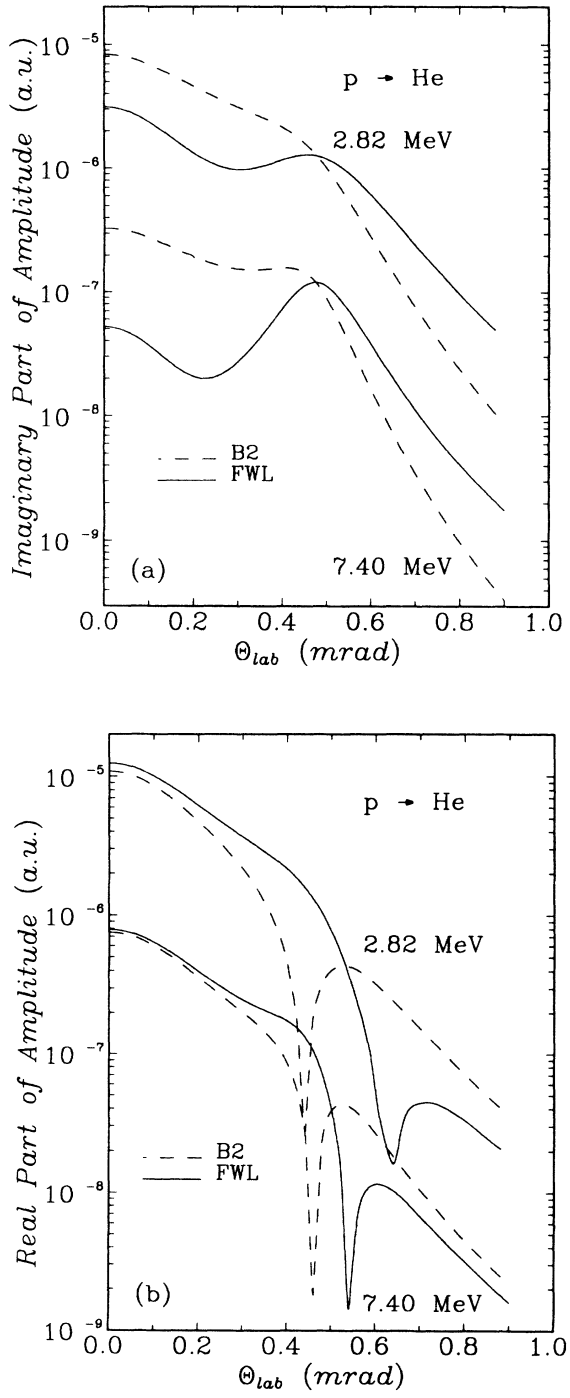

FIG. 6. (a) Real and (b) imaginary parts of the FWL (solid lines) and B2 (dashed lines) amplitudes are shown for $1s \rightarrow 1s$ capture in 2.82- and 7.40-MeV proton-helium collisions.

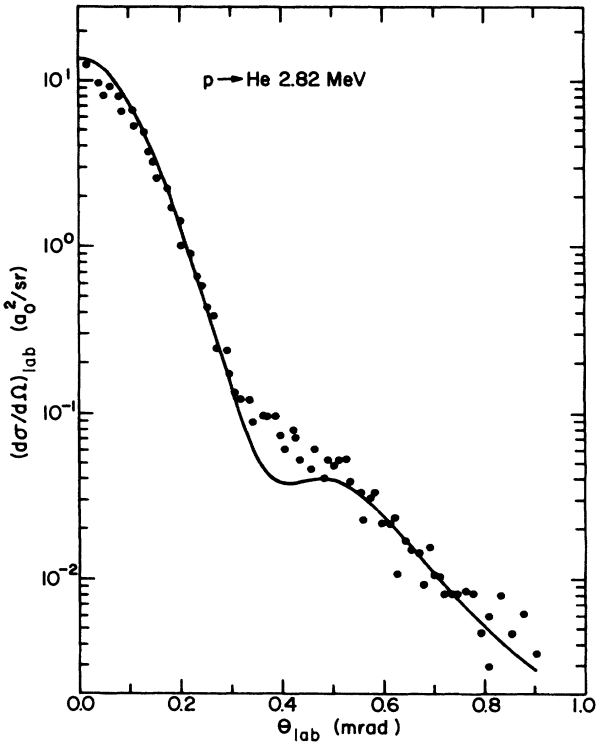

FIG. 7. Differential cross sections for $1s \rightarrow 1s$ capture in 2.82-MeV proton-helium collisions are shown. An FWL calculation performed using a scaled-charge pure Coulomb formalism is compared with the experimental data of Horsdal-Pedersen, Cocke, and Stockli (Ref. 1). The theoretical curve has been convoluted with the beam profile (Ref. 28).

in the curves reflect the real parts passing through zero. Since the Thomas peak or shoulder results from a partial cancellation in the amplitude of the real first-Born term (for $1s \rightarrow 1s$ capture) with the real part of the second-order term, much more cancellation takes place in the FWL amplitude. According to the above decomposition of the free Green's function, the real part of the second-order contributions to the B2 amplitude represents scattering via off-energy-shell intermediate states,[29] which have no classical analog. According to the experimental data, the FWL treatment of this part of the intermediate scattering is much better. The inclusion of the "off-shell" Q factors of Eq. (A4) in the calculation is the reason for the improvement.[16] The shifting of the sharp dips in the real parts of the FWL curves relative to the B2 curves is due to the intermediate terms. The DWB real parts go through zero in a manner similar to the B2 real parts.

In Fig. 7, a cross section derived using an FWL formalism[30] with pure Coulomb potentials is compared with the helium data. The calculation is performed using pure Coulomb T matrices approximated by their near-shell representations [see Eq. (A3)]. Equations (28) and (36) can be used by simply employing the charge $Z_T^a = 1.6875$ instead of 1. A comparison of the FWL curves in Figs. 3 and 7 reveals little change over much of the angular region. From roughly 0.3 to 0.6 mrad, however, considerable differences are apparent. The large change in the local-minimum region is not unexpected considering the cancellations of various terms there. The significant variation at the Thomas peak, though, points out differences in the treatment of the off-shell effects and the necessity of using the better, modified Coulomb potential approximation. Similar results (not shown) are also found for 5.42 and 7.40 MeV collisions.

B. Proton-hydrogen collisions

Results for proton-hydrogen collisions are presented in Figs. 8 and 9. The full FWL cross sections are compared in Fig. 8 with full-peaking SPB cross sections and the experimental data of Vogt *et al.*[2] for proton energies of 2.8 and 5.0 MeV. The velocities corresponding to these energies are 10.6 and 14.1 a.u., respectively. The data are estimated to be accurate to within 50% and include capture to all final states. The SPB results were calculated using Eq. (5.8) of Macek and Alston.[18] The theoretical $1s \rightarrow 1s$ cross sections have been convoluted with the experimental beam profiles.[31]

Starting at roughly 0.3 mrad, the SPB cross section is seen to become larger than the FWL cross sections, with a maximum difference at the Thomas peak. The curves converge again at larger angles. For the lower energy collisions, the SPB curve is too high relative to the experimental data. At the higher energy, the SPB curve fits the data better in magnitude, but the FWL curve fits the shape of the cross section around the Thomas peak better. Although hard to estimate, the contribution of excited-state capture is expected to contribute more relative to ground-state capture in the Thomas peak region. This would make the SPB results higher still than they presently are. A recent, improved-peaking calculation of the SPB amplitude by Macek and Dong[18] gives much closer agreement with the FWL results, more like the transverse-peaking results seen in the helium case above. Both of the SPB results could be modified by recent work which would lead to larger cross sections.[32]

A comparison of unconvoluted DWB, SPB, and B2 cross sections is given in Fig. 9. The relative positions of the cross sections in this figure follow quite closely those for the helium case in Fig. 5 except that the exaggerated peaking of the SPB curve results from the use of the full-peaking approximation instead of the more accurate transverse-peaking approximation there. A boundary-corrected second-Born approximation[33] has also been developed. For 5-MeV collisions, the unconvoluted $1s$-$1s$ cross section calculated using this theory follows the DWB cross section fairly closely, especially in the local-minimum and Thomas peak regions, though it is lower by perhaps a factor of 2 in the extreme forward direction. Since the boundary-corrected second-Born approximation gives a better account of the Coulomb scattering of the problem by means of asymptotically correct scattering states, the agreement is very encouraging, but a formal justification appears difficult to obtain.

C. Internuclear contribution

Consideration of the internuclear amplitude [Eq. (36)] shows that a contribution of the first-order T_{PT} term

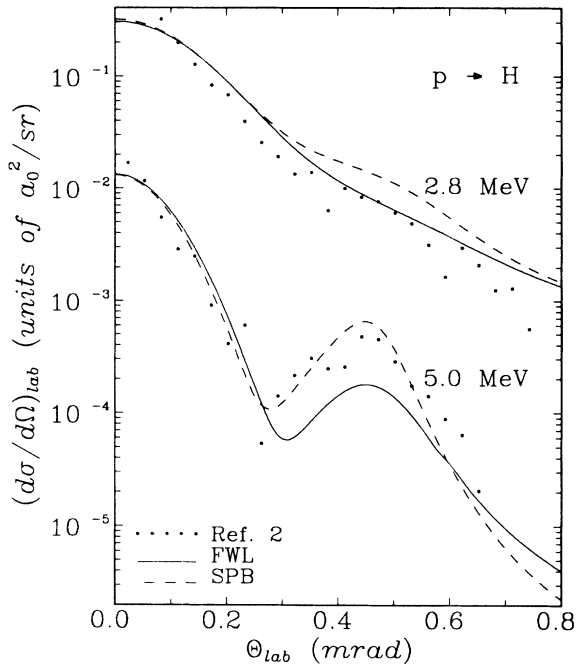

FIG. 8. Differential cross sections for $1s \rightarrow 1s$ capture in 2.8- and 5.0-MeV proton-hydrogen collisions. Results of FWL (solid lines) and SPB (dashed lines, Ref. 18) calculations are compared with the experimental data of Vogt (Ref. 2). The theoretical results have been convoluted with the beam profiles (Ref. 31).

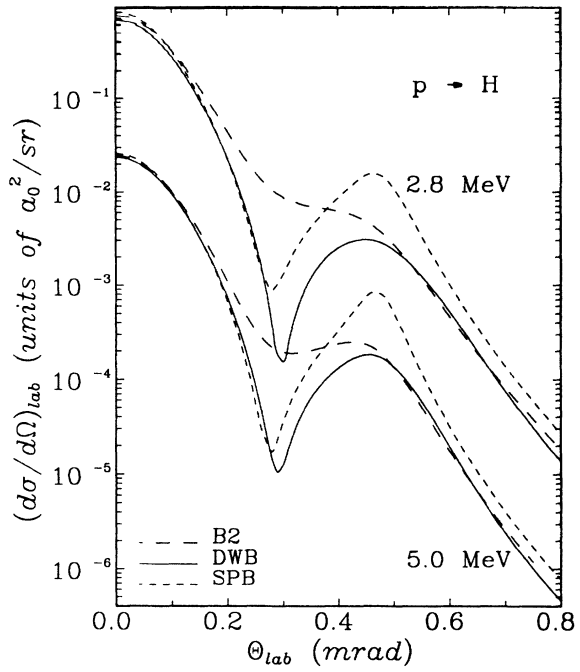

FIG. 9. Differential cross sections for $1s \rightarrow 1s$ capture in 2.8- and 5.0-MeV proton-hydrogen collisions. Results of unconvoluted DWB (solid lines), SPB (short-dashed lines, Ref. 18) and B2 (long-dashed lines) calculations are compared.

arises for each of the second-order terms, which appear with opposite signs. If the off-shell effects and the explicit nature of the Coulomb scattering are neglected by setting the Sommerfeld parameters equal to zero, one finds, to orders $(Z_P/v)^2$ and $(Z_T/v)^2$ (which are the orders of our approximations overall), that the internuclear term vanishes. The resulting amplitude is the second-Born approximation.

This behavior of the second-Born approximation to A_n was first noted some time ago.[8] In the FWL case, however, A_n is not zero to leading order because the factors multiplying the common velocity and momentum-transfer dependences are not the same in the different terms and thus do not cancel. In other words, the coherent addition of the double-scattering partial amplitudes and the single-scattering nuclear amplitude in A_n is not zero when a proper treatment (by use of T matrices) of each two-body collision is considered.

Considering Fig. 6(a) again, one notes that beyond 0.5 mrad the imaginary part of the B2 amplitude decreases rapidly as opposed to the imaginary part of the FWL amplitude. Noting also that the real parts of the B2 and FWL amplitudes in Fig. 6(b) converge, roughly, to each other, one concludes that the nuclear scattering contribution is contained largely in the imaginary part. The reason for this behavior is not known.

Figures 10(a) and 10(b) compare the full FWL cross sections (unconvoluted) with the DWB cross sections obtained when the internuclear terms are removed. Proton energies of 2.8 and 5.0 MeV for the hydrogen target and 2.82 and 7.40 MeV for the helium target are treated. In the angular region beyond the local maximum, the enhancement of the FWL cross sections relative to those obtained from the purely electronic term is apparent. The FWL curves exhibit a K^{-4} (or J^{-4}) momentum dependence in this region consistent with the Coulomb

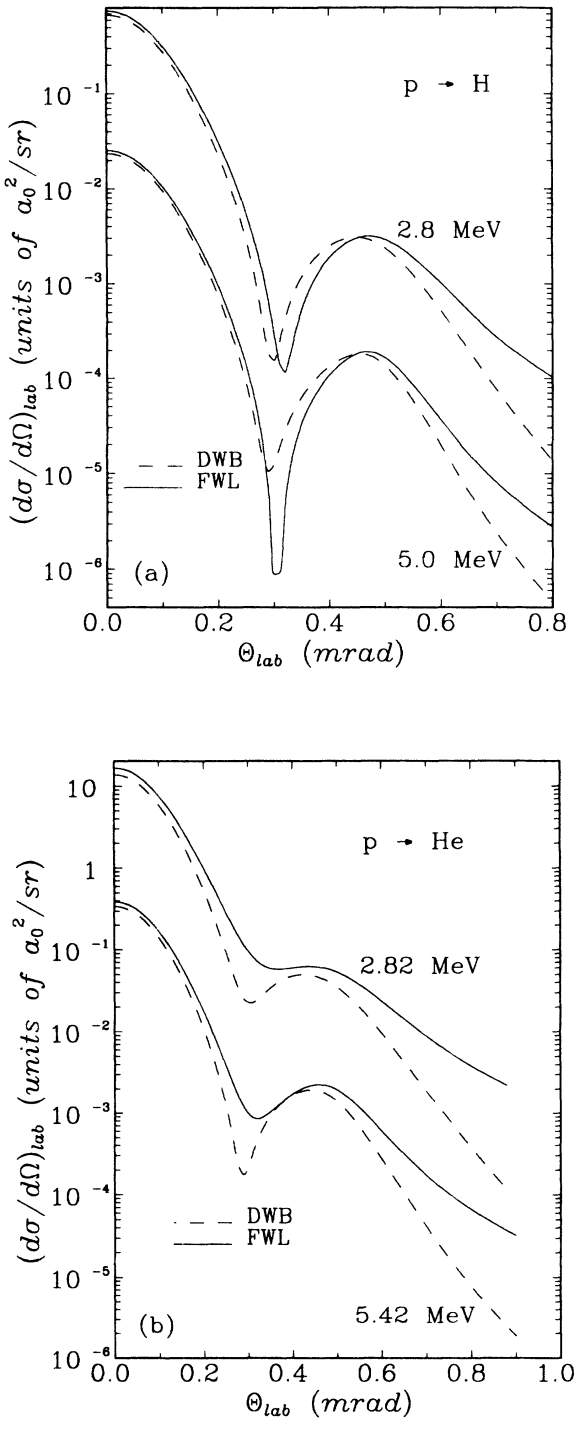

FIG. 10. Comparison of FWL differential cross sections for $1s \rightarrow 1s$ capture calculated with (solid lines) and without (dashed lines, DWB) the internuclear terms in the amplitude for (a) proton-hydrogen and (b) proton-helium collisions.

scattering of the projectile off the target nucleus. Since A_e exhibits a K^{-4} dependence at angles larger than the Thomas peak, so that its contribution can be neglected, it follows that the total cross section factors into the product of electronic and nuclear parts,[14] as Eq. (36) shows. Compare this with the discussion at the end of this section.

The helium data in Fig. 3 support the higher FWL curves extremely well while the hydrogen data in Fig. 8 do not really extend to large enough angles except, perhaps, in the 5.0-MeV case where the slope of the FWL curve agrees with the data. The agreement of the FWL cross sections with the data beyond the Thomas peak and the formal discussion of the amplitude in the preceding paragraphs show that A_n gives the first explicit representation in a multiple-scattering formalism of the mechanism by which the internuclear potential contributes to the capture of the electron. This is in contrast to the second-Born approximation where no such contribution at all is found.

At angles less than 0.2 mrad, the internuclear terms do not modify the electronic amplitude appreciably, and the height of the Thomas peak is not altered to within the accuracy of the present approximation. In the vicinity of the local minimum, however, the two sets of curves differ considerably. It is this angular region which is most sensitive to the approximations used because of the cancellation of the various terms in the full amplitude. The relatively large changes are thus not surprising. However, this region contributes only slightly to the total cross section.

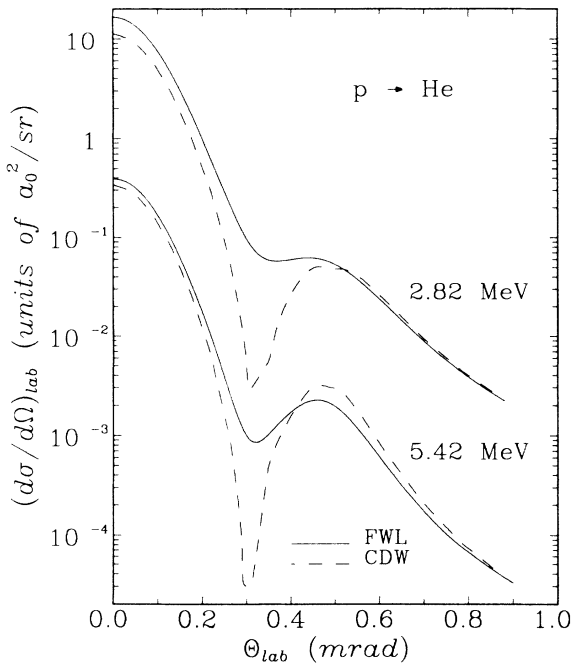

FIG. 11. Comparison of unconvoluted FWL (solid lines) and CDW (dashed lines, Ref. 17) differential cross sections for $1s \rightarrow 1s$ capture calculated for 2.82- and 5.42-MeV collisions of protons on helium.

In Fig. 11, a comparison of the uncovoluted FWL and CDW curves reveals agreement beyond the Thomas peak. The CDW theory includes the internuclear contribution via the eikonal transformation of the electronic amplitude.[9] The good agreement gives further evidence for the conclusions drawn above about the internuclear terms included in the FWL theory. The eikonal transformation of an electronic amplitude shows how the internuclear contribution can be represented though a multiplicative phase factor and it thus provides a method for including the effects of the internuclear potential; however, it does not elucidate a mechanism of the nuclear scattering in a multiple-scattering theory. The FWL theory does because it shows how incomplete cancellation (i.e., interference) of the various scattering terms occurs in A_n when these terms are accurately described through the use of T matrices.

The large differences between the FWL and DWB curves in the vicinity of the local minimum similarly result from cancellation of the second-order terms with the first-Born term and thus are expected to expose nonleading-order components of the second-order terms which, however, are not treated as accurately as the leading-order components. The convoluted DWB cross sections (not shown) give agreement comparable to the FWL ones in the forward-peak and Thomas-peak regions but not as good agreement with experiment in the minimum region.

When the Coulomb and off-shell natures of Eqs. (28) and (36) are neglected (by once again setting the Sommerfeld parameters equal to zero) the expression for the B2 amplitude in the same approximation is derived. As a consequence of this connection and the specific forms of the factors which become unity one equating the parameters to zero [see Eq. (36)], the pronounced structure (peaks or valleys) exhibited[4] by the B2 amplitude at specific and *not* necessarily small critical scattering angles exists also in the FWL amplitude, and at the *same* angles, although the shape and height of the structures will be altered. This conclusion follows even though infinitely many terms in each of the potentials have been summed in the FWL amplitude.

VII. CONCLUSION

In summary, it has been shown that a second-order Faddeev expansion of the transition operator for electron capture leads to differential cross sections in excellent agreement with experimental data for proton-helium collisions and good agreement for proton-hydrogen collisions. Significant improvement is obtained over results of other theories. An explanation has been given for how the contribution of the internuclear potential arises and fits within a time-independent scattering formalism. Finally, a direct and explicit relation of the FWL theory to the second-Born theory has been derived. A simple picture of capture involving double scatterings is maintained while a much more accurate treatment of each of the scatterings is employed. Comparison of the various theories with experiment reveals an acute need for more accurate data and better control of the incident beam width.

ACKNOWLEDGMENTS

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APPENDIX A: NEAR-SHELL COULOMB T MATRICES

The pure Coulomb two-body transition matrix is defined as

$$T_C(\mathbf{k}',\mathbf{k};\varepsilon)=\left\langle \mathbf{k}' \left| V_C \left[1+\left[\varepsilon-\frac{1}{2\mu}\nabla_r^2-V_C+i\eta \right]^{-1} V_C \right] \right| \mathbf{k} \right\rangle , \tag{A1}$$

with $V_C=-Z/r$ and $\langle \mathbf{r}|\mathbf{k}\rangle=e^{i\mathbf{k}\cdot\mathbf{r}}$. Shastry, Kumar, and Callaway[34] have reduced this T matrix to a form involving hypergeometric functions, namely,

$$T_C(\mathbf{k}',\mathbf{k};\varepsilon)=(2\pi)^{3/2}\tilde{V}_C(\mathbf{k}'-\mathbf{k})\left[1+\frac{4i\nu}{(1+i\nu)(t_+-t_-)}[x_+\,{}_2F_1(1,1;2+i\nu;x_+)-x_-\,{}_2F_1(1,1;2+i\nu;x_-)] \right] \tag{A2}$$

with

$$x_\pm=(1-t_\pm)^{-1} ,$$

$$t_\pm=1+(2/\delta)[1\pm(1+\delta)^{1/2}] ,$$

$$\delta=(2\mu\varepsilon-k'^2)(2\mu\varepsilon-k^2)/2\mu\varepsilon|\mathbf{k}'-\mathbf{k}|^2 ,$$

$$\nu=\mu Z/(2\mu\varepsilon+i\eta)^{1/2} ,$$

and $\eta\to 0+$. The dimensionless quantity δ isolates parameters relative to the (nonrelativistic) off-the-energy-shell scattering, including the off-shell energy defects, the on-shell energy, the momentum transfer of the scattering, and the reduced mass μ.

If either of the energy defects are small and the energy ε or magnitude of the momentum transfer $|\mathbf{k}'-\mathbf{k}|$ is large so that δ is small, an approximate expression for the T matrix can be derived. Expanding the radical in t_+ in powers of δ and neglecting quadratic and higher terms, one finds that

$$t_+\approx 4/\delta,\quad x_+\approx-\delta/4,\quad t_-\approx\delta/4,\quad x_-\approx 1+\delta/4 .$$

One also finds that $\delta(t_+-t_-)\approx 4$.

With these approximations, the factor $x_+\,{}_2F_1(1,1;2+i\nu;x_+)$ gives only a second-order contribution. Analytic continuation of the other hypergeometric function gives

$$[i\nu/(1+i\nu)]x_-\,{}_2F_1(1,1;2+i\nu;x_-)\approx 1-|\Gamma(1+i\nu)|^2(-\delta/4)^{-i\nu}$$

to the same order. The T matrix expression in Eq. (A2) is thus seen to assume the form

$$T_C(\mathbf{k}',\mathbf{k};\varepsilon)\approx(2\pi)^{3/2}\tilde{V}_C(\mathbf{k}'-\mathbf{k})|\Gamma(1+i\nu)|^2(-\delta/4)^{-i\nu}$$
$$=(2\pi)^{3/2}\tilde{V}_C(\mathbf{k}'-\mathbf{k})|\Gamma(1+i\nu)|^2[-(2\mu\varepsilon-k'^2)(2\mu\varepsilon-k^2)/8\mu\varepsilon|\mathbf{k}'-\mathbf{k}|^2]^{-i\nu} \tag{A3}$$

when δ is small, where $\tilde{V}_C(\mathbf{k})=-(2/\pi)^{1/2}Z/k^2$.

This equation can be recast as a relation between the off-shell T matrix and the on-shell scattering amplitude $f^C_{\mathbf{k}',\mathbf{k}}(\varepsilon)$, written in slightly generalized form.[16] The result is

$$T_C(\mathbf{k}',\mathbf{k};\varepsilon)\approx -2\pi Q(Z,k',\varepsilon)Q(Z,k,\varepsilon)f^C_{\mathbf{k}',\mathbf{k}}(\varepsilon) , \tag{A4}$$

where the so-called off-shell factor is given by

$$Q(Z,k,\varepsilon)=e^{\pi\nu/2}\Gamma(1+i\nu)[(2\mu\varepsilon-k^2)/8\mu\varepsilon]^{-i\nu} , \tag{A5}$$

and

$$f^C_{\mathbf{k}'\mathbf{k}}(\varepsilon)=(-2Z/|\mathbf{k}'-\mathbf{k}|)e^{2i\sigma_0}[|\mathbf{k}'-\mathbf{k}|/(k'+k)]^{2i\nu}$$

is the generalized elastic Coulomb scattering amplitude with $\sigma_0=\arg\Gamma(1-i\nu)$.

For the case of a modified Coulomb potential

$$V_{MC}(r)\sim -Z^a/r \quad \text{as } r\to\infty ,$$

where Z^a is the charge of the asymptotic pure Coulomb part, one can show that the T matrix $T_{MC}(\mathbf{k}',\mathbf{k};\varepsilon)$ reduces to the analogous pure Coulomb form

$$T_{MC}(\mathbf{k}',\mathbf{k};\varepsilon)\approx -2\pi Q(Z^a,k',\varepsilon)Q(Z^a,k,\varepsilon)\times[f^C_{\mathbf{k}',\mathbf{k}}(\varepsilon)+f^{SR}_{\mathbf{k}',\mathbf{k}}(\varepsilon)] , \tag{A6}$$

with $f^{SR}_{\mathbf{k}',\mathbf{k}}(\varepsilon)$ denoting the elastic scattering amplitude for the short-range part of the potential. The Coulomb part of the modified Coulomb amplitude is a function of the asymptotic charge Z^a.

At large impact velocities and deep penetration of the potential, the modified Coulomb potential is approximated in the inner region by a pure Coulomb potential with an effective charge Z^e,

$$V_{MC}(r)\approx V_{\text{eff}}(r)\equiv -Z^e/r+V_0 ,$$

where V_0 is chosen to make the ground-state energy of the potential agree with the experimental binding energy. Given an effective Coulomb potential, the modified Coulomb amplitude is approximated by a pure Coulomb amplitude, and thus one writes

$$\begin{aligned} T_{MC}(\mathbf{k}',\mathbf{k};\varepsilon)\approx &-2\pi Q(Z^a,k',\varepsilon)Q(Z^a,k,\varepsilon) \\ &\times(-2Z^e/|\mathbf{k}'-\mathbf{k}|)e^{2i\sigma_0} \\ &\times[|\mathbf{k}'-\mathbf{k}|/(k'+k)]^{2i\nu^e} , \end{aligned} \tag{A7}$$

with

$$\nu^e=\mu Z^e/(2\mu\varepsilon+i\eta)^{1/2} . \tag{A8}$$

This formula is used for the calculation of the various partial amplitudes in the present work.

APPENDIX B: ORDER OF MAGNITUDE ESTIMATES OF T-MATRIX PARAMETERS

Following the discussion of Appendix A, if approximate forms of the two-body T matrices are to be derived, one must show that the dimensionless δ parameters on which the T matrices in the FWL amplitude depend are small. This analysis, which is based on order of magnitude estimates using the pure Coulomb case, is performed here. Although a similar analysis for the modified Coulomb case is not a trivial generalization[16] of the pure Coulomb case, it is a necessary condition for the applicability of the near-shell approximation to the modified Coulomb T matrices.

Considering $A_e^{(2)}$ in Eq. (18), the δ parameters for T_{Pe} and T_{Te} have the forms

$$\begin{aligned} \delta_i &= [(\mathbf{k}_t+\mathbf{k}_f+\mathbf{J})^2-2\mu_f E_i] \\ &\quad\times[(\mathbf{k}_t-\mathbf{v})^2-2\mu_f E_i]/2\mu_f E_i|\mathbf{k}_f-\mathbf{K}|^2 , \\ \delta_f &= [(\mathbf{k}_i+\mathbf{k}_f-\mathbf{K})^2-2\mu_i E_f] \\ &\quad\times[(\mathbf{k}_f+\mathbf{v})^2-2\mu_i E_f]/2\mu_i E_f|\mathbf{k}_i+\mathbf{J}|^2 , \end{aligned}$$

respectively. As noted in Sec. V, the peaking of the initial and final bound-state momentum wave functions $\tilde{\phi}_i(\mathbf{k}_t)$ about $\mathbf{k}_i=0$ and $\tilde{\phi}_f(\mathbf{k}_f)$ about $\mathbf{k}_f=0$, implying that $k_i\lesssim Z_T$ and $k_f\lesssim Z_P$, means that

$$\begin{aligned} &(\mathbf{k}_i-\mathbf{v})^2-2\mu_f E_t=k_i^2-2\varepsilon_t=O(Z_T^2) , \\ &|\mathbf{k}_f-\mathbf{K}|^2=O(v^2) , \\ &E_i=O(v^2) , \\ &(\mathbf{k}_f+\mathbf{v})^2-2\mu_i E_f=k_f^2-2\varepsilon_f=O(Z_P^2) , \\ &|\mathbf{k}_i+\mathbf{J}|^2=O(v^2) , \\ &E_f=O(v^2) . \end{aligned}$$

Furthermore, one has the range of values

$$(\mathbf{k}_i+\mathbf{k}_f-\mathbf{K})^2-2\mu_i E_f=(\mathbf{k}_i+\mathbf{k}_f+\mathbf{J})^2-2\mu_f E_t = \begin{cases} O(v^2) & \text{for } K_\perp\approx 0 \\ O(Z^2) & \text{for } K_\perp\approx v \end{cases}$$

where Z stands for Z_P or Z_T. Combining these relations gives at least the estimates

$$\begin{aligned} &\delta_i=O((Z_T/v)^2)\ll 1 , \\ &\delta_f=O((Z_P/v)^2)\ll 1 . \end{aligned} \tag{B1}$$

For $A_n^{(1)}$, the δ parameter for T_{PT} in Eq. (22) is

$$\begin{aligned} \delta_n &= [2\mu_n E_n-(\mathbf{U}_t-\mathbf{k}_t-\mathbf{J})^2] \\ &\quad\times(2\mu_n E_n-U_t^2)/2\mu_n E_n|\mathbf{k}_i+\mathbf{J}|^2 , \end{aligned}$$

where $\mathbf{U}_t=\gamma'\mathbf{k}_t+(1-\gamma'\alpha')\mathbf{K}_i$ and $E_n=E-(\mathbf{k}_t-\alpha'\mathbf{K}_i)^2/2\nu_n$. Using the definitions of $\mathbf{J}$ and $\mathbf{K}_i$ and writing all factors to order m/M, one finds the relations

$$2E_n-U_t^2/\mu_n\approx \begin{cases} 2\varepsilon_t-k_i^2=O(Z_T^2) & \text{for } \mathbf{k}_i\approx 0 \\ 2\varepsilon_i-(\mathbf{k}_t-\mathbf{v})^2=O(v)^2 & \text{for } \mathbf{k}_i\approx\mathbf{v} \end{cases}$$

$$2E_n-(\mathbf{U}_i-\mathbf{k}_t-\mathbf{J})^2/\mu_n\approx \begin{cases} 2\varepsilon_f-(\mathbf{k}_i-\mathbf{v})^2=O(v^2) \\ \qquad\text{for } \mathbf{k}_t\approx 0 \\ 2\varepsilon_f-\mathbf{k}_t^2=O(Z_P^2) \\ \qquad\text{for } \mathbf{k}_t\approx\mathbf{v} \end{cases}$$

$$|\mathbf{k}_i+\mathbf{J}|^2= \begin{cases} O(v^2) & \text{for } \mathbf{k}_i\approx 0 \\ K^2=O(v^2) & \text{for } \mathbf{k}_i=\mathbf{v} \end{cases}$$

$$E_n/\mu_n=O(v^2) .$$

It follows from these expressions that the estimates

$$\delta_n= \begin{cases} O((Z_T/v)^2)\ll 1 & \text{for } \mathbf{k}_i\approx 0 \\ O((Z_P/v)^2)\ll 1 & \text{for } \mathbf{k}_t\approx\mathbf{v} \end{cases} \tag{B2}$$

hold.

In the partial amplitude $A_e^{(2a)}$ of Eq. (25), the δ parameters for T_{Te} and T_{PT} are

$$\begin{aligned} \delta_T &= \{2\mu_t E_f-[\mathbf{k}_t-\alpha'(\mathbf{k}_f-\mathbf{K})]^2\} \\ &\quad\times(2\mu_t E_f-t_f^2)/2\mu_t E_f|\mathbf{k}_f-\mathbf{k}_t+\mathbf{v}|^2 , \\ \delta_n &= [2\mu_n E_n-(\mathbf{U}_t-\mathbf{k}_f+\mathbf{K})^2] \\ &\quad\times(2\mu_n E_n-U_t^2)/2\mu_n E_n|\mathbf{k}_f-\mathbf{K}|^2 , \end{aligned}$$

respectively. Using $E_f=\mathbf{v}\cdot(\mathbf{k}_f-\mathbf{K})+\varepsilon_i$ (see Appendix C), neglecting terms of order m/M, and assuming again the peaking of the bound-state momentum wave functions, one obtains the estimates

$$\begin{aligned} &2E_f-k_t^2=O(v^2) , \\ &2E_f-(\mathbf{k}_f+\mathbf{v})^2=2\varepsilon_f-k_f^2=O(Z_P^2) , \\ &|\mathbf{k}_f-\mathbf{k}_t+\mathbf{v}|=O(v^2) , \\ &E_f=O(v^2) , \\ &2E_n-U_t^2/\mu_n\approx 2\varepsilon_t-k_t^2=O(Z_T^2) , \\ &2E_n-(\mathbf{U}_t-\mathbf{k}_f+\mathbf{K})^2/\mu_n=O(v^2) , \\ &|\mathbf{k}_f-\mathbf{K}|=O(v^2) , \\ &E_n/\mu_n=O(v^2) . \end{aligned}$$

Combining these estimates the δ parameters become

$$\delta_T = O((Z_P/v)^2) \ll 1 ,$$
$$\delta_n = O((Z_T/v)^2) \ll 1 . \tag{B3}$$

In the partial amplitude $A_e^{(2b)}$ of Eq. (26), the δ parameters for T_{PT} and T_{Pe} are, respectively,

$$\delta_n = [2\mu_n E_n - (\mathbf{U}_f + \mathbf{k}_i + \mathbf{J})^2] \times (2\mu_n E_n - U_f^2)/2\mu_n E_n |\mathbf{k}_i + \mathbf{J}|^2 ,$$
$$\delta_P = \{2\mu_f E_i - [-\mathbf{k}_f + \beta'(\mathbf{k}_i + \mathbf{J})]^2\} \times (2\mu_f E_i - t_i^2)/2\mu_f E_i |\mathbf{k}_i - \mathbf{k}_f - \mathbf{v}|^2 ,$$

where $\mathbf{U}_f = -\gamma \mathbf{k}_f + (1-\gamma\beta')\mathbf{K}_f$. Using $E_i = -\mathbf{v}\cdot(\mathbf{k}_i + \mathbf{J}) + \varepsilon_f$, neglecting terms of order m/M, and assuming the peaking, one finds the estimates

$$2E_n - U_f^2/\mu_n \approx 2\varepsilon_f - \mathbf{k}_f^2 = O(Z_T^2) ,$$
$$2E_n - (\mathbf{U}_f + \mathbf{k}_i + \mathbf{J})^2/\mu_n = O(v^2) ,$$
$$|\mathbf{k}_i + \mathbf{J}| = O(v^2) ,$$
$$E_n/\mu_n = O(v^2) ,$$
$$2E_i - k_f^2 = O(v^2) ,$$
$$2E_i - (\mathbf{k}_i - \mathbf{v})^2 = 2\varepsilon_i - k_i^2 = O(Z_T^2) ,$$
$$|\mathbf{k}_i - \mathbf{k}_f - \mathbf{v}| = O(v^2) ,$$
$$E_f = O(v^2) .$$

Combining these estimates, one obtains the δ-parameter sizes

$$\delta_P = O((Z_P/v)^2) \ll 1 ,$$
$$\delta_n = O((Z_T/v)^2) \ll 1 . \tag{B4}$$

In conclusion, the estimates listed in Eqs. (B1)–(B4) are seen to be small and thus near-shell approximations to the respective T matrices are valid.

APPENDIX C: INTEGRABLE SINGULARITIES OF THE AMPLITUDE

When considering near-shell approximations to the two-body T matrices appearing in the second-order FWL amplitude, the question arises as to the possible presence of nonintegrable singularities,[35] for if such singularities are present, the approximations are not quantitatively based, but are rather only conceptual in nature. It is shown here that no such singularities overall are present in the amplitude for the case when singly charged ions are incident on neutral targets. Only the simpler case of $1s \rightarrow 1s$ transfer is discussed, although the conclusions hold for excited states as well. First, an explicit demonstration of the singularities is given for pure Coulomb potentials.

Using the expression [Eq. (A2)] for the Coulomb T matrix in terms of ${}_2F_1$ functions, it is clear that singularities are contained in certain of the individual terms of the amplitude: one notes that if $\nu = Z/(2\varepsilon + i\eta)^{1/2} = +i$, then $1 + i\nu = 0$, and so the T matrix is singular. The energies where this occurs correspond to bound states. On the other hand, if $\mathbf{k}' \rightarrow \mathbf{k}$, so that $\delta \rightarrow \infty$, one has

$$t_+ \approx 1 \pm 2/\delta^{1/2}, \quad x_+ \approx \mp \tfrac{1}{2}\delta^{1/2}, \quad t_+ - t_- \approx 4/\delta^{1/2}$$

and

$${}_2F_1(1,1;2+i\nu;x_+) \approx \pm\tfrac{1}{2}(1+i\nu)\delta^{1/2}[C + \ln(\pm\tfrac{1}{2}\delta^{1/2})] ,$$

with C a constant. Therefore the T matrix assumes the form

$$T_C(\mathbf{k}',\mathbf{k};\varepsilon) \approx (2\pi)^{3/2}\tilde{V}_C(\mathbf{k}'-\mathbf{k}) \times \{1 + (2i\nu/\delta^{1/2})[\ln(\tfrac{1}{2}\delta^{1/2}) - \ln(\tfrac{1}{2}\delta^{1/2})]\}$$
$$= (2\pi)^{3/2}\tilde{V}_C(\mathbf{k}'-\mathbf{k})(1 \pm 4\pi\nu\delta^{-1/2}) , \tag{C1}$$

where the actual sign (unimportant for our purposes) depends on the phase of δ. That is, the leading-order term in the approximation to the full two-body T matrix at small momentum transfers is the potential itself, which is singular.

The partial amplitude $A_e^{(2)}$ consists of a double integral over $\mathbf{k}_i$, $\mathbf{k}_f$ involving, among other factors, the T matrices $T_{Te}(\mathbf{k}_f + \mathbf{v}, \mathbf{k}_i + \mathbf{k}_f - \mathbf{K}; E_f)$ and $T_{Pe}(\mathbf{k}_f + \mathbf{k}_i + \mathbf{J}, \mathbf{k}_i - \mathbf{v}; E_i)$. The first one depends on $Z_T/(2E_f + i\eta)^{1/2}$ and the second on $Z_P/(2E_i + i\eta)^{1/2}$. These quantities can equal $+i$, since, from the definitions of K_z and J_z, one has that $E_i = -\mathbf{v}\cdot(\mathbf{k}_i + \mathbf{J}) + \varepsilon_f$ and $E_f = \mathbf{v}\cdot(\mathbf{k}_f - \mathbf{K}) + \varepsilon_i$, with $\varepsilon_i = -\frac{1}{2}Z_T^2$ and $\varepsilon_f = -\frac{1}{2}Z_P^2$. Further, the relation $\mathbf{v} + \mathbf{J} + \mathbf{K} = 0$ shows that a momentum transfer $\mathbf{k}_i + \mathbf{J}$ occurs for the first T matrix and $\mathbf{k}_f - \mathbf{K}$ for the second T matrix.

Thus, for pure Coulomb T matrices, $A_e^{(2)}$ is seen to contain two singularities at $\mathbf{k}_i = -\mathbf{J}$ and $\mathbf{k}_f = \mathbf{K}$, each of which are the confluence of two separate singularities. The confluences of singularities are not integrable. In the more general case of a modified Coulomb potential, the singularities arising from zero momentum transfers are still present as they result from scattering at large distances where the potentials reduce to pure Coulomb form. The other singularities are present as well, as follows from an eigenfunction expansion of the Green's functions present in the T matrices, since they result from T matrix energies coinciding with specific bound-state energies: a term is present in the expansion (the ground-state term here) whose energy denominator vanishes at a certain momentum transfer.

It can be shown that the other terms $\tilde{T}_{Te}G_0^+(E)\tilde{T}_{PT}$ and $\tilde{T}_{PT}G_0^+(E)\tilde{T}_{Pe}$ of the FWL amplitude contain analogous singularities, but only one each since the P-T interaction does not support a bound-state spectrum. In combination with the above singularities, though, which are independent of each other, consideration of the sums $\tilde{T}_{Te}G_0^+(E)[\tilde{T}_{PT} + \tilde{T}_{Pe}]$ and $[\tilde{T}_{PT} + \tilde{T}_{Te}]G_0^+(E)\tilde{T}_{Pe}$ is necessary.

Taking the long-range forms [Eq. (C1)] of the square-bracketed terms since it is the zero-momentum transfer limits which concern us, and expanding them in common coordinate vectors, one finds

$$V_{Pe}(r_P)\sim -Z_P^a/r_P=-Z_P^a/|\alpha \mathbf{r}_T-\mathbf{R}_T| \quad \text{as } r_P\to\infty ,$$

$$V_{PT}(R)\sim -Z_P^aZ_T^a/R=Z_P^aZ_T^a/|\alpha' \mathbf{r}_T+\mathbf{R}_T|$$
$$=Z_P^aZ_T^a/|-\beta' \mathbf{r}_P+\mathbf{R}_P| \quad \text{as } R\to\infty ,$$

$$V_{Te}(r_T)\sim -Z_T^a/r_T=-Z_T^a/|\beta \mathbf{r}_P+\mathbf{R}_P| \quad \text{as } r_T\to\infty .$$

For capture to and from bound states and for large intersystem coordinate separations, one finds

$$\tilde{T}_{PT}+\tilde{T}_{Pe}\sim V_{PT}+V_{Pe}$$
$$\approx Z_P^a(Z_T^a-1)/R_T-Z_P^a(\alpha+\alpha' Z_T^a)\mathbf{r}_T\cdot\mathbf{R}_T/R_T^3 ,$$

$$\tilde{T}_{PT}+\tilde{T}_{Te}\sim V_{PT}+V_{Te}$$
$$\approx (Z_P^a-1)Z_T^a/R_P+(\beta+\beta' Z_P^a)Z_T^a\mathbf{r}_P\cdot\mathbf{R}_P/R_P^3 .$$

For singly charged ions, the long-range Coulomb force vanishes and the corresponding zero-momentum singularities cancel, leading to a finite amplitude in this case. This conclusion renders the analysis of Appendix A valid from a quantitative point of view.

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