Perturbation theory for strongly interacting atomic systems

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(Received 24 July 1989)

The strong-potential Born approximation has been formulated to include effects of elastic scattering in initial and final states. We use the standard distorted-wave theory and the eikonal approximation to derive closed-form expressions for scattering wave functions. Our results show that lowest-order theories must account for off-energy-shell electron propagation in the strong potential as well as for elastic scattering in initial and final states. Capture from inner shells and radiative electron capture are computed to illustrate the theory.

I. INTRODUCTION

To describe collisions of highly charged ions with atoms or ions of relatively low nuclear charge, Briggs[1] introduced an expansion in powers of the ratio λ of the small nuclear charge to the large nuclear charge. This idea, which has long been used in the theory of bound states of many-electron atoms, provides a comprehensive framework for understanding collisions between highly asymmetric systems. Further development has clarified the analytic properties of the expansion in the small parameter λ for one-electron systems.[2–5] The general theory based upon Briggs's expansion parameter is now referred to as the strong-potential Born (SPB) theory.[6,7]

Accurate representation, to lowest order in λ, of both asymptotic and intermediate states is necessary for a consistant theory of electron capture.[8] Previous work, which emphasizes only one of these aspects, is incomplete. In this paper we show how to incorporate both features without undue numerical complications and examine the effect of channel potentials which are needed to represent asymptotic states to lowest order in λ. In the formulation given by Macek,[5] several alternative forms of the transition amplitude are considered. In an exact theory all forms are naturally equivalent, but in approximate computations where the power series in λ is necessarily terminated at low order the different forms are not equivalent. Besides retention of all terms in a given power of λ inherent in a perturbation approach, it is desirable that the matrix element not draw contributions from regions of coordinate space where the approximate wave functions are inaccurate. This is particularly important in scattering theory since some expressions for transition matrix elements may draw contributions from large distances where only exact functions are adequate. For that reason expressions that draw the main contribution from regions concentrated near the "condensation point,"[9,10] where all particles are close together, are favored. Then values of matrix elements are sensitive to the asymptotic region mainly through normalization constants.

Distorted waves that incorporate channel potentials exactly serve both to describe elastic scattering in first approximation and to yield expressions for transition matrix elements which emphasize the condensation region. The main disadvantage of channel-distorted wave functions is the difficulty of computing terms in the perturbation expansion. For that reason the use of channel potentials has been restricted to first-order calculations[11] and to formal developments.[5] As noted earlier,[12] one effect of the application of the channel-distorted wave-function formulation is to exactly remove terms in the expansion of the T matrix associated with the divergences noted by Mapleton[13] and reemphasized in connection with the SPB expansion for electron capture by Dewangan and Eichler.[14] These terms were left out in previous evaluations of the SPB approximation. The original form of the SPB approximation for electron capture may accordingly be viewed as a derivation of the channel-distorted wave-function formulation in which the distorted waves are approximated by undistorted waves *after* the cancellation of these terms has been completed. The problem with divergences is accordingly completely solved and of no further concern in this paper. It is the influence of the channel distortion beyond this cancellation that is the main object in this work. Notice in particular that electron states pertaining to the smaller of the nuclear charges are perturbed by the *stronger* field. The elastic distortion of the corresponding channels can accordingly not be ignored in a consistent expansion to first order in λ. We show in this paper that it is possible, within the context of standard peaking approximations, to evaluate these terms without undue complications. The theory that emerges is more broadly applicable than the original SPB theory. Most importantly, it applies to radiative electron capture (REC) without the *ad hoc* modifications needed to bring cross sections into agreement with experiment and with more intuitive models.[15,16]

The notation and general formulation is given in Sec. II. Various perturbation expansions are discussed in Sec. III. Section IV introduces channel modified SPB wave functions. The wave functions are evaluated using peaking approximations that are consistent with expansions of transition amplitudes in powers of λ. We find that the channel modified SPB wave function interpolates between the impulse approximation (IA) and the unmodified SPB

wave function depending upon the characteristics of the channel potential. Capture from inner shells is considered in Sec. V. In Sec. VI we apply the theory to radiative electron capture and show that it is essentially identical to the impulse approximation in this case. Our conclusions are summarized in Sec. VII. Atomic units are used throughout, although we shall occasionally indicate the mass of the electron m explicitly for clarity.

II. NOTATION AND GENERAL FORMULATION

In this work we are concerned with the following prototype reaction:

$$Z_P+(Z_T,e)_i\rightarrow(Z_P,e)_f+Z_T+\mathrm{ph}\ , \tag{2.1}$$

where Z_P and Z_T are the nuclear charge numbers of the projectile and the target, ph represents a photon to indicate the possibility of radiative electron capture. Throughout the paper the three-particle system is treated as a quantum-mechanical scattering problem. An entirely equivalent description based on the time-dependent impact-parameter method has been indicated in a separate publication.[17]

The initial and final states of reaction (2.1) are described in terms of different sets of Jacobi coordinates. We use a notation where $\mathbf{r}_T$ and $\mathbf{R}_T$ represent the position vector of the electron with respect to the target nucleus and the position of the projectile with respect to the center of mass of the target atom, respectively. In these coordinates the initial state of reaction (2.1) is

$$\langle\mathbf{r}_T,\mathbf{R}_T|\Phi_i\rangle=\varphi_i(\mathbf{r}_T)\phi_{\mathbf{K}_i}(\mathbf{R}_T)\ . \tag{2.2}$$

Here φ_i is the initial-state wave function of the target atom and $\phi_{\mathbf{K}_i}$ is a plane wave with wave vector $\mathbf{K}_i$,

$$\phi_{\mathbf{K}_i}(\mathbf{R}_T)=(2\pi)^{-3/2}\exp(i\mathbf{K}_i\cdot\mathbf{R}_T)\ . \tag{2.3}$$

A similar set of Jacobi coordinates are used to represent the final state of the reaction in Eq. (1)

$$\langle\mathbf{r}_P,\mathbf{R}_P|\Phi_f\rangle=\varphi_f(\mathbf{r}_P)\phi_{\mathbf{K}_f}(\mathbf{R}_P)\ . \tag{2.4}$$

We use a sign convention such that $\mathbf{R}_T$ and $\mathbf{R}_P$ are almost equal. It is, nevertheless, important to retain the small difference between the two vectors to account properly for the electronic and nuclear momentum exchange during the rearrangement collision. The two sets of coordinates are related according to

$$\begin{bmatrix}\mathbf{r}_P\\ \mathbf{R}_P\end{bmatrix}=\begin{bmatrix}\alpha & -1\\ 1-\alpha\beta & \beta\end{bmatrix}\begin{bmatrix}\mathbf{r}_T\\ \mathbf{R}_T\end{bmatrix}\ , \tag{2.5}$$

where α and β are defined by

$$\alpha=\frac{M_T}{m+M_T},\quad \beta=\frac{M_P}{m+M_P}\ , \tag{2.6}$$

and where M_T, M_P, and m represent the mass of the nuclei and the electron, respectively. The corresponding transformation in momentum space is

$$\begin{bmatrix}\mathbf{k}_P\\ \mathbf{K}_P\end{bmatrix}=\begin{bmatrix}\beta & \alpha\beta-1\\ 1 & \alpha\end{bmatrix}\begin{bmatrix}\mathbf{k}_T\\ \mathbf{K}_T\end{bmatrix}\ . \tag{2.7}$$

Following the notation of Ref. 18, we define for later convenience the average momentum transfer vectors

$$\mathbf{K}=\beta\mathbf{K}_f-\mathbf{K}_i,\quad \mathbf{J}=\alpha\mathbf{K}_i-\mathbf{K}_f\ . \tag{2.8}$$

In previous developments it has been customary to ignore the internuclear potential $V_P=Z_PZ_T/R$ from the outset with the implicit understanding that an eikonal transformation must be implemented if angular differential cross sections are required. It should be noticed that the validity of the eikonal approximation relies on the fact that M_P and M_T are much larger than m for ion-atom collisions. If positrons are used as projectiles ($M_P=m$) or if positronium targets are considered ($M_T=m$), full inclusion of V_{PT} is essential for a proper description of the reaction processes.[19,20] The present work is restricted to ion-atom collisions only. We may therefore ignore the internuclear potential from the outset. For completeness a general discussion is given in Appendix A to show that any distortion potential common to initial and final channels can be eliminated in the eikonal approximation.

The coupling to the radiation field will be ignored throughout, except for radiative processes in which case a first-order perturbation treatment of the coupling to the radiation field suffices. The full Hamiltonian of the system may therefore be written

$$H=H_0+V_P+V_T=H_T+V_P=H_P+V_T\ , \tag{2.9}$$

where $V_T=-Z_T/r_T$ and $V_P=-Z_P/r_P$. The free Hamiltonian H_0 is given by

$$H_0=-\frac{1}{2\mu_i}\nabla^2_{\mathbf{R}_T}-\frac{1}{2}\nabla^2_{\mathbf{r}_T}=-\frac{1}{2\mu_f}\nabla^2_{\mathbf{R}_P}-\frac{1}{2}\nabla^2_{\mathbf{r}_P}\ , \tag{2.10}$$

where μ_i (μ_f) is the reduced mass in the initial (final) ion-atom configuration.

The initial state given in Eq. (2.2) is, by definition, an eigenstate of the initial Hamiltonian

$$H_i|\Phi_i\rangle=H_T|\Phi_i\rangle=E_i|\Phi_i\rangle\ . \tag{2.11}$$

The corresponding channel perturbation is accordingly given by

$$V_i=V_P\ . \tag{2.12}$$

Similarly, we write

$$H_f|\Phi_f\rangle=H_P|\Phi_f\rangle=E_f|\Phi_f\rangle \tag{2.13}$$

and

$$V_f=V_T \tag{2.14}$$

in the final channel. Using ε_i and ε_f to denote the internal energy of the initial and final electron states φ_i and φ_f, the total energy of the states may be expressed as

$$E_i=\varepsilon_i+\frac{1}{2\mu_i}K_i^2\ , \tag{2.15}$$

$$E_f=\varepsilon_f+\frac{1}{2\mu_f}K_f^2 \ . \tag{2.16}$$

Since the potentials in Eqs. (2.12) and (2.14) contain long-range Coulomb terms, the standard T matrix is not well defined on the energy shell. Rather a satisfactory theory may be based on the distorted-wave theory of scattering amplitudes. This relies on a separation of the channel potential V_c ($c=i$ or f), into two components

$$V_c=U_c+W_c \ , \tag{2.17}$$

where the residual interaction W_c is effectively of short range and the distortion potential U_c is simple enough that corresponding distorted waves $|\Phi_c^{\pm}\rangle$ can be determined. That $W_i(\mathbf{r}_T,\mathbf{R}_T)$ is of short range means that $R_T W_i$ goes to zero as R_T becomes large, while r_T is kept fixed. Reaction cross sections may then be obtained in the usual way from the absolute square of distorted-wave transition elements

$$T_{fi}=\langle\Phi_f^-|W_f|\Psi_i^+\rangle \ . \tag{2.18}$$

Here, the exact scattering state is given by

$$|\Psi_i^+\rangle=(1+G^+W_i)|\Phi_i^+\rangle \ , \tag{2.19}$$

where G^+ is the full Green's operator

$$G^+=(E-H\pm i\eta)^{-1} \ . \tag{2.20}$$

More explicitly, we may write the distorted-wave T-matrix element as

$$T_{fi}=\langle\Phi_f^-|(V_f-U_f)+(V_f-U_f)G^+(V_i-U_i)|\Phi_i^+\rangle \ , \tag{2.21}$$

which is well defined on the energy shell $E_i=E_f=E$ provided the residual potentials V_c-U_c vanish faster than $1/R$ at large internuclear separations R.

Since the distortion potential U_c is of long range, the Lippmann-Schwinger equation cannot be used to define the distorted states $|\Phi_c^{\pm}\rangle$. Rather these states may be obtained directly by solving the Schrödinger equation with suitable asymptotic conditions. The distortion potential U_c is formally arbitrary except for an asymptotic condition that makes W_c of finite range, but the choice of U_c is important in practice when the T-matrix element in Eq. (2.21) is approximated by some perturbation expansion of the exact scattering state in Eq. (2.19). In this connection it should be realized that the phase variation of the initial and final states over the region of space where the T-matrix element receives its main contributions is as important for a correct determination of the magnitude of the transition amplitude as is the absolute normalization of the states. Phase variations are, however, difficult to represent accurately over an extended interaction zone. It is therefore essential to choose the distortion potentials in initial and final channels so as to minimize the effective range of the residual interactions.

To examine this problem further, consider the T matrix in a multichannel representation using asymptotic eigenstates as basis states. Then, it appears natural to exactly eliminate all diagonal—so called secular—terms from the coupling matrix by standard procedures. The corresponding distortion potentials are given by[12]

$$U_i(R_T)=\int d\mathbf{r}_T|\varphi_i(\mathbf{r}_T)|^2V_P(\mathbf{r}_P) \tag{2.22}$$

in the initial channel and

$$U_f(R_P)=\int d\mathbf{r}_P|\varphi_f(\mathbf{r}_P)|^2V_T(\mathbf{r}_T) \tag{2.23}$$

in the final channel. This choice of distortion represents the static potential between the aggregates in initial and final channels and thus accounts for elastic scattering to a reasonable accuracy at intermediate and high velocities. It is, in principle, possible to go beyond the level of a static channel potential to include polarization and virtual transitions in the distortion potentials, but in the present context it suffices to allow for such effects as higher-order terms in a perturbation expansion of the exact T matrix in Eq. (2.21). Equation (2.21) has been previously discussed where U_i and U_f were regarded as arbitrary. The present considerations serve to obtain more precisely defined channel distortion potentials U_i and U_f. We emphasize that the internuclear potential $V_{PT}=Z_PZ_T/R$ is correctly omitted in Eq. (2.21) within the eikonal approximation. The formulation is accordingly valid for ion-atom collisions, but not if light projectiles such as positrons are involved. In a more general formulation, the residual potentials would remain unchanged since the internuclear potential in V_c and U_c would cancel, but the complete distortion potential should be retained to define the distorted initial and final states. Further, V_{PT} would then be retained in the Green's operator in Eq. (2.21). Practical evaluation beyond the eikonal approximation is, however, a formidable computational task.

III. PERTURBATION EXPANSIONS

Apart from the eikonal approximation to remove the internuclear potential, the expression in Eq. (2.21) for the T-matrix element is exact, but too complicated to be evaluated without further approximations. To arrive at a manageable form the exact Green's operator G^+ may be suitably approximated, preferably by expanding in powers of a small parameter. In the case of highly asymmetric collisions $Z_P\gg Z_T$ such an expansion is provided by the strong-potential Born series

$$G^+=G_P^+ +G_P^+V_TG_P^+ +\cdots \ , \tag{3.1}$$

where the first-order term is given by the projectile Green's operator

$$G_P^+=(E-H_0-V_P+i\eta)^{-1} \ . \tag{3.2}$$

Considering specifically an initial target state, we may use the fact that $i\eta G_P^+|\Phi_i^+\rangle$ is identically zero since $|\Phi_i^+\rangle$ is asymptotically orthogonal to the complete spectrum of the projectile Hamiltonian $H_P=H_0+V_P$ to prove the following identity, derived by Faddeev:[21]

$$[1+G_P^+(V_P-U_i)]|\Phi_i^+\rangle=G_P^+V_T|\Phi_i^+\rangle \ . \tag{3.3}$$

Then Eq. (2.21), with G^+ approximated by G_P^+, appears

in the form

$$T_{fi}=\langle\Phi_f^-|(V_T-U_f)G_P^+V_T|\Phi_i^+\rangle\ . \tag{3.4}$$

This may be viewed as the channel-distorted strong-potential Born (DSPB) approximation for electron capture in asymmetric collisions. It retains, however, some higher-order contributions in the small parameter $\lambda=Z_T/Z_P$ via the *weak* channel distortion included in the distorted final state $|\Phi_f^-\rangle$. These contributions may be consistently omitted in lowest order by replacing $|\Phi_f^-\rangle$ by the undistorted final state $|\Phi_f\rangle$. Since U_f in Eq. (3.4) is chosen according to Eq. (2.23), it is easy to show, following Macek,[12] that the contribution from $U_fG_P^+V_T$ is exactly canceled by the elastic pole contribution from $V_TG_TV_T$ to obtain

$$T_{fi}^{\mathrm{DSPB}}=\langle\Phi_f|V_TG_P'^+V_T|\Phi_i^+\rangle\ , \tag{3.5}$$

where $G_P'^+$ is the projectile Green's operator excluding intermediate scattering in the final electron state

$$G_P'^+=\sum_{n\neq f}\frac{|\Phi_n\rangle\langle\Phi_n|}{E-E_n+i\eta}\ . \tag{3.6}$$

We note that if the distortion in the initial channel is ignored Eq. (3.5) is readily shown to be identical to the form evaluated, for example, by Macek and Alston and by Sil and McGuire.[22]

In formal derivations and in approximate evaluations using various peaking approximations, it has been useful to introduce the SPB approximation to the complete scattering state.[7,23,24] In the present distorted-channel generalization the SPB wave function is defined by

$$\begin{aligned}|\Psi_i^{+\mathrm{DSPB}}\rangle&=[1+G_P^+(V_P-U_i)]|\Phi_i^+\rangle\\&=G_P^+V_T|\Phi_i^+\rangle\ .\end{aligned} \tag{3.7}$$

where the last equality derives from Eq. (3.3). The original form of the SPB wave function is obtained if the distortion is ignored. In most applications, $|\Psi_i^{+\mathrm{DSPB}}\rangle$ is further approximated. Usually, the final-state pole contribution to G_P is then automatically omitted. This is the case in the often employed near-shell approximation. Under this proviso we have

$$T_{fi}^{\mathrm{DSPB}}=\langle\Phi_f|V_T|\Psi_i^{+\mathrm{DSPB}}\rangle\ . \tag{3.8}$$

The compact form of the electron-capture amplitude given by Eq. (3.5) and of the scattering state given by Eq. (3.7) is peculiar to the SPB expansion. The expression for the capture amplitude is particularly interesting because it emphasizes the double-collision nature of the capture process and that the leading term in an ordered expansion in powers of $\lambda=Z_T/Z_P$ is proportional to λ^2. In this connection it is of interest to compare with a similar development for target excitation by a highly charged projectile. As in case of electron capture, we may use the relation given by Eq. (3.3) to show that Eq. (2.21) in this case may be expressed as

$$T_{fi}^{\mathrm{exc,DSPB}}=\langle\Phi_f^-|(V_P-U_f)G_P^+V_T|\Phi_i^-\rangle\ . \tag{3.9}$$

Here, G_P^+ is the complete projectile Green's operator and the distortion must be retained in the residual interaction in the final channel since the final state pertains to the target atom and accordingly is distorted by the *strong* projectile field. It is seen from Eq. (3.9) that a consistent theory for target excitation by a highly charged ion is of first order in the small parameter λ. Comparing Eq. (2.21) with (3.9) shows that the double-scattering term must be retained as for electron capture. This is to be contrasted with the much simpler situation in case of excitation by a weak perturbation where the ordinary first Born approximation provides a consistent first-order theory.

IV. STRONG-POTENTIAL WAVE FUNCTIONS

To obtain a physically transparent interpretation of the strong-potential Born expansion it is useful to examine the channel distorted SPB wave functions in some detail. The original work of Macek and Taulbjerg[3] demonstrated how the SPB approximation relates to the impulse approximation and it was emphasized that off-energy-shell effects play an essential role in this connection. In this section we analyze the channel-distorted SPB wave functions introduced in the previous section, and find that the distortion plays an equally important role.

By definition, the channel-distorted SPB wave function is given in two equivalent forms in Eq. (3.7). The compact version is most useful in the following derivation. The distorted initial state is written as a product of a plane wave $\phi_{\mathbf{K}_i}$ and a distortion factor $D_{\mathbf{K}_i}^+$,

$$\langle\mathbf{r}_T,\mathbf{R}_T|\Phi_i^+\rangle=\varphi_i(\mathbf{r}_T)\phi_{\mathbf{K}_i}(\mathbf{R}_T)D_{\mathbf{K}_i}^+(\mathbf{R}_T)\ . \tag{4.1}$$

To evaluate Eq. (3.7) we introduce the Fourier transforms $\tilde{\varphi}_i(\mathbf{k})$ and $\tilde{D}_{\mathbf{K}_i}^+(\mathbf{S})$ of the initial electron wave function and the distortion factor and use the Schrödinger equation in momentum space to write the Fourier transform of the product $V(\mathbf{r}_T)\varphi_i(\mathbf{r}_T)$ as

$$\widetilde{V_T\varphi_i}(\mathbf{k})=(\varepsilon_i-\tfrac{1}{2}k^2)\tilde{\varphi}_i(\mathbf{k})\ . \tag{4.2}$$

We then obtain

$$\begin{aligned}&\Psi_i^{+\mathrm{DSPB}}(\mathbf{r}_P,\mathbf{R}_P)\\&\quad=(2\pi)^{-3/2}\int d\mathbf{k}(\varepsilon_i-\tfrac{1}{2}k^2)\tilde{\varphi}_i(\mathbf{k})\\&\qquad\times\int d\mathbf{S}\,\tilde{D}_{\mathbf{K}_i}^+(\mathbf{S})G_P^+\phi_{\mathbf{Q}+\mathbf{S}}(\mathbf{R}_P)\phi_{\mathbf{q}}(\mathbf{r}_P)\ .\end{aligned} \tag{4.3}$$

Here the two complimentary sets of wave vectors $(\mathbf{q},\mathbf{Q})$ and $(\mathbf{k},\mathbf{K}_i)$ are related according to Eq. (2.7) as

$$\mathbf{q}=\mathbf{k}-\mathbf{v},\quad \mathbf{Q}=\alpha\mathbf{K}_i+\mathbf{k}\ , \tag{4.4}$$

where $\mathbf{v}=\mathbf{K}_i/\mu_i$ is the incident velocity vector and terms of order $1/M$ have been ignored. The operation of the Green's operator on the product of plane waves in Eq. (4.3) is now readily evaluated since the interatomic kinetic energy operator in G_P^+ may be replaced by $(\mathbf{Q}+\mathbf{S})^2/2\mu_f$. The remaining part of the operator only acts in the electron coordinate space. The result is

$$\Psi_i^{+\mathrm{DSPB}}(\mathbf{r}_P,\mathbf{R}_P)=(2\pi)^{-3/2}\int d\mathbf{k}\,\tilde{\varphi}_i(\mathbf{k}) \times\int d\mathbf{S}\tilde{D}^{+}_{\mathbf{K}_i}(\mathbf{S})\frac{\varepsilon_i-\frac{1}{2}k^2}{\varepsilon_S-\frac{1}{2}q^2} \times\psi^{c+}_{\mathbf{q},\varepsilon_S}(\mathbf{r}_P)\phi_{\mathbf{Q}+\mathbf{S}}(\mathbf{R}_P)\ , \tag{4.5}$$

where ε_S is given by the relation

$$\varepsilon_S=\tfrac{1}{2}q^2+\varepsilon_i-\tfrac{1}{2}k^2-\mathbf{v}\cdot\mathbf{S} \tag{4.6}$$

and where terms of order $1/\mu_i$ have been neglected. Note that terms of this order have implicitly been ignored already in the eikonal approximation, which we have used to remove the internuclear potential. The electron wave function in Eq. (4.5) is given by

$$\psi^{c+}_{\mathbf{q},\varepsilon_S}(\mathbf{r}_P)=[1+(\varepsilon_S+\tfrac{1}{2}\nabla^2_{\mathbf{r}_P}-V_P+i\eta)^{-1}V_P]\phi_{\mathbf{q}}(\mathbf{r}_P)\ , \tag{4.7}$$

and is off-the-energy shell according to Eq. (4.6).

Assuming that $v\gg Z_T$, and using that $\mathbf{q}\approx\mathbf{v}$ it is seen from Eq. (4.6) that the off-shell wave function in Eq. (4.5) is near the energy shell provided that the momentum distribution of the distorted interatomic wave is sharply peaked about $\mathbf{K}_i$. We may then introduce the near-shell approximation

$$\psi^{c+}_{\mathbf{q},\varepsilon}(\mathbf{r}_P)\approx g^{+}(q,\varepsilon)\psi^{c+}_{\mathbf{q}}(\mathbf{r}_P)\ , \tag{4.8}$$

where $\psi^{c+}_{\mathbf{q}}(\mathbf{r}_P)$ is an ordinary Coulomb wave and the off-shell factor $g^{+}(q,\varepsilon)$ is given by

$$g^{+}(q,\varepsilon)=\Gamma(1+i\nu)\exp(\pi\nu/2)[(\tfrac{1}{2}q^2-\varepsilon)/2q^2]^{-i\nu}\ , \tag{4.9}$$

where $\nu=Z_P/q$ is the Sommerfeld parameter corresponding to momentum $\mathbf{q}$.

In this approximation, valid for

$$r_P|\sqrt{2\varepsilon}-q|\ll 1\ , \tag{4.10}$$

we obtain

$$\Psi_i^{+\mathrm{DSPB}}(\mathbf{r}_P,\mathbf{R}_P)=\int d\mathbf{k}\,\tilde{\varphi}_i(\mathbf{k})\gamma^{+}(q,\varepsilon)\psi^{c+}_{\mathbf{q}}(\mathbf{r}_P)\phi_{\mathbf{Q}}(\mathbf{R}_P)\ , \tag{4.11}$$

where ε is the value of ε_S for $\mathbf{S}=0$, i.e.,

$$\varepsilon-\tfrac{1}{2}q^2=\varepsilon_i-\tfrac{1}{2}k^2\ . \tag{4.12}$$

The parameter $\gamma^{+}(q,\varepsilon)$ is given by

$$\gamma^{+}(q,\varepsilon)=(2\pi)^{-3/2}\int d\mathbf{S}\,\tilde{D}^{+}_{\mathbf{K}_i}(\mathbf{S})\frac{\varepsilon-\frac{1}{2}q^2}{\varepsilon_S-\frac{1}{2}q^2}g^{+}(q,\varepsilon_S)\ . \tag{4.13}$$

In the derivation of this expression we have ignored a factor $\exp(i\mathbf{S}\cdot\mathbf{R}_P)$. This approximation is valid if Eq. (4.10) is fulfilled for $\mathbf{R}_P$, i.e., if $\mathbf{R}_P$ is restricted to the same region of space around the origin as required for the validity of the near-shell approximation Eq. (4.8).

It is readily seen from Eq. (4.13) that if the channel distortion is ignored, i.e., if the momentum distribution of the internuclear wave is a δ function, $\gamma^{+}(q,\varepsilon)$ is identical to $g^{+}(q,\varepsilon)$. The ordinary SPB wave function is, accordingly, properly identified from Eq. (4.11) in this limit. Similarly, the impulse approximation is obtained from Eq. (4.11) if γ^{+} is unity. More generally, γ^{+} in Eq. (4.13) appears as a suitable average of the off-shell factor g^{+} over the momentum distribution in the elastic channel.

To evaluate this modified off-shell factor γ^{+} we insert Eq. (4.9) into Eq. (4.13) to obtain

$$\gamma^{+}(q,\varepsilon)=(2q^2)^{i\nu}\exp(\pi\nu/2) \times\Gamma(1+i\nu)(\tfrac{1}{2}q^2-\varepsilon)(2\pi)^{-3/2} \times\int d\mathbf{S}\,\tilde{D}^{+}_{\mathbf{K}_i}(\mathbf{S})[\tfrac{1}{2}q^2-\varepsilon+\mathbf{v}\cdot\mathbf{S})]^{-1-i\nu}\ . \tag{4.14}$$

Using the representation

$$A^{-b}=i^b\frac{1}{\Gamma(b)}\int_0^\infty x^{b-1}\exp(-ixA)dx\ , \tag{4.15}$$

with $A=(\frac{1}{2}q^2-\varepsilon-\mathbf{v}\cdot\mathbf{S})$ in Eq. (4.14), the $\mathbf{S}$ integral can be expressed in terms of the distortion factor $D^{+}_{\mathbf{K}_i}(\mathbf{R})$ in coordinate space, and we find

$$\gamma^{+}(q,\varepsilon)=(2q^2)^{i\nu}(\tfrac{1}{2}q^2-\varepsilon)i \times\int_0^\infty dx\,x^{i\nu}e^{-ix[(1/2)q^2-\varepsilon]}D^{+}_{\mathbf{K}_i}(-x\mathbf{v})\ . \tag{4.16}$$

It was already noted in connection with Eq. (4.13) that the original off-shell factor g^{+} is obtained from γ^{+} if the distortion is ignored. This result is also obtained from Eq. (4.16) if $D^{+}_{\mathbf{K}_i}(\mathbf{R})=1$ everywhere. Alternatively, if a pure Coulomb potential is used for the distortion potential in all space the distortion factor is a confluent hypergeometric function. Equation (4.16) may also be evaluated analytically for this case and we find $\gamma^{+}(q,\varepsilon)=1$ to an excellent approximation. In this way, we recover the impulse approximation, which as previously been obtained by the *ad hoc* omission of g^{+} in the SPB approximation. Note that the impulse approximation is obtained even though the Coulomb form at large distances of all two-body potentials is retained. The essential feature is that the residual potential V_P-U_i in Eq. (3.7), when operating on $|\Phi_i^{+}\rangle$, vanishes faster than $1/R_T$ for finite values of r_T. Then, our factor $\gamma^{+}(q,\varepsilon)$ generally extracts a residual influence of off-shell propagation characteristic of intermediate states of an effective short-range potential in the electronic coordinate $\mathbf{r}_P$.

To evaluate γ^{+} for more realistic distortion potentials we again employ the eikonal approximation for the distorted nuclear wave $D^{+}_{\mathbf{K}_i}$. Note that the forward cone, where the eikonal approximation is inaccurate, is avoided in the integral in Eq. (4.16). In the present case $U_i(R)$ is asymptotic to $-Z_P/R$. Since the eikonal phase is logarithmically divergent, it is most appropriate to write the distortion factor as a product of a pure Coulomb term and a term due to the residual short-range potential. The eikonal approximation is then given by

$$D^{+}_{\mathbf{K}_i}(\mathbf{R})=(vR-\mathbf{v}\cdot\mathbf{R})^{-i\nu_P} \times\exp\left[-\frac{i}{v}\int_{-\infty}^{Y}\left[U_i(R')+\frac{Z_P}{R'}\right]dY'\right], \quad (4.17)$$

where Y is the coordinate of $\mathbf{R}$ along the asymptotic velocity vector $\mathbf{v}=\mathbf{K}_i/\mu_i$, and where ν_P is the Sommerfeld parameter corresponding to momentum $\mathbf{v}$, $\nu_P=Z_P/v$. The overall phase is chosen for later convenience. Inserting in Eq. (4.16) and replacing q by v in all slowly varying functions in anticipation of a peaking approximation in the integration over the momentum distribution of the initial electron state in Eq. (4.11), we find

$$\gamma^{+}(q,\varepsilon)=i\int_0^{\infty}dx\, e^{-ix}\exp\left[-\frac{i}{v}\int_{xv/(\frac{1}{2}q^2-\varepsilon)}^{\infty}\left[U_i(R)+\frac{Z_P}{R}\right]dR\right]. \quad (4.18)$$

Equations (4.11) and (4.18) represent the main result of this section. We recall that the derivation was based on the near-shell approximation for the electron motion in intermediate states and on the eikonal approximation for the internuclear motion. As in previous developments[22,23] of the SPB approximation, the near-shell approximation is considered valid for high velocities in symmetric collisions and also for intermediate velocities in asymmetric collisions. The eikonal approximation is valid for high wave numbers, i.e., in general, for ion-atom collisions, but not for positrons or positronium species.

The γ^{+} factor in Eq. (4.18) is evaluated numerically below for the static channel potential pertaining to a $1s$ initial target state. For more qualitative purposes we first examine a model potential for which the γ^{+} factor can be evaluated analytically, namely the Hulthen potential

$$U_H(R)=-\frac{Z_P}{R}+\frac{Z_P}{R_0}\frac{1}{\exp(R/R_0)-1}, \quad (4.19)$$

where R_0 is a range parameter. This potential is, in fact, a realistic approximation to the proper channel potential and provides—as documented below— an accurate approximation to the γ^{+} factor. Introducing the parameter

$$x_0=R_0(\tfrac{1}{2}q^2-\varepsilon)/v, \quad (4.20)$$

we find in the Hulthen case

$$\gamma^{+}=\frac{\Gamma(1+ix_0)\Gamma(1+i\nu_P)}{\Gamma(1+i\nu_P+ix_0)}. \quad (4.21)$$

It is seen that the limit $R_0=0$ in Eq. (4.21) recovers the impulse approximation and the limit $R_0\to\infty$ recovers the original off-shell factor. Equation (4.21) interpolates between these two limits. Generally, it is seen that γ^{+} approaches unity for small values of x_0, i.e., if the deviation from the energy shell is sufficiently small or if the collision velocity is high enough. It is realistic to assume that R_0 is of order $1/Z_T$, while $(\frac{1}{2}q^2-\varepsilon)$ is positive and of order $(Z_T)^2$ according to Eq. (4.12). This implies that x_0 is of order $\nu_T=Z_T/v$, which is generally assumed to be smaller than unity under conditions where strong-potential expansions are considered valid. The parameter x_0 is accordingly effectively restricted to the range between zero and unity.

The static channel potential defined by Eq. (2.22) is readily evaluated for hydrogenic wave functions, but the integrals in Eq. (4.18) must be evaluated numerically to obtain the corresponding γ^{+} factor. In fact, special care is required in the numerical integration because of the logarithmic divergence of the phase factor in Eq. (4.18) in the limit of small-x values. In case of a $1s$ initial state the channel potential appears as

$$U_{1s}(R)=-\frac{Z_P}{R}+\frac{Z_P}{R}(1+Z_TR)\exp(-2Z_TR). \quad (4.22)$$

Notice that the static channel potential in Eq. (4.22) is very well approximated by the Hulthen potential in Eq. (4.19) if the screening radius R_0 is determined by the radius of the initial state, $R_0=1/2Z_T$.

We have evaluated the γ^{+} factor numerically for the static channel potential in Eq. (4.22) for a sequence of velocities and found that the resulting γ^{+} factor is well approximated by the analytic result [Eq. (4.21)] derived from the Hulthen potential. The comparison of the two factors is illustrated for a representative case in Fig. 1 where an extended region of the parameter x_0 is shown to document the quality of the Hulthen factor Eq. (4.21) even far off the energy shell. Our conclusion is that the Hulthen potential for all practical purposes, may be applied in place of the static channel potential. Note that an analytic expression is important for most applications in order to complete the integration over the momentum distribution in Eq. (4.11).

The modified γ^{+} factor in Fig. 1 converges towards the original off-shell factor g^{+} at large (positive or negative) values of the parameter x_0, i.e., far off the energy shell. However, x_0 is small in the physically relevant region and γ^{+} is close to unity and analytic in x_0,

$$\gamma^{+}\approx 1+\alpha x_0+\cdots, \quad (4.23)$$

where α is a suitable complex parameter. An expression for α is readily derived from Eq. (4.21),

$$\alpha=i[\Psi(1)-\Psi(1+i\nu_P)], \quad (4.24)$$

where $\Psi(z)=\Gamma'(z)/\Gamma(z)$ is the digamma function. For high velocities, i.e., for small values of the Sommerfeld's parameter ν_P, α may be approximated as

$$\alpha \underset{\nu_P\to 0}{\approx} \pi^2\nu_P/6. \quad (4.25)$$

This implies that γ^+ is unity to second order in the deviation from the energy shell at high velocities. The pure impulse approximation is accordingly obtained in this limit. At low velocities, on the other hand, it is found that α becomes purely imaginary and diverges as

$$\alpha \underset{v_P \to \infty}{\approx} -i \ln v_P \ . \tag{4.26}$$

A more careful analysis is accordingly needed in this limit. The correct result

$$\gamma^+ \underset{v_P \to \infty}{\approx} \exp(-ix_0 \ln v_P) \tag{4.27}$$

is, however, readily derived directly from Eq. (4.21). Note that the factor $\ln v_P$ is never large for realistic values of v_P. Equation (4.27) shows that γ^+, for strongly asymmetric systems at intermediate velocities, is well represented by a simple phase factor. A qualitatively similar result has been derived elsewhere[8] in the case where the distortion potential was modeled by a cutoff Coulomb potential. The analytic properties of γ^+ should be contrasted with the highly singular behavior of the original off-shell factor in the on-shell limit.

The modified γ^+ factor is shown in Fig. 2 for various model potentials for which it may be evaluated analytically. In addition to the Hulthen potential, this includes model potentials that are constant inside and Coulombic outside a certain cutoff radius R_0. The case where the potential is continuous across R_0 was considered in Ref. 8. In a similar way a simple expression for γ^+ may be derived[25] when the potential vanishes inside R_0. We note that while the Hulthen parameter is accurately determined by a comparison with the static channel potential, there is no reason to expect that the cutoff radius can be uniquely determined. In the figure the cutoff radius is equated to the screening radius of the Hulthen potential, but it appears that a suitable scale factor might be more appropriate in the sense that common curves for magnitude and phase could be derived by a judicious choice. Since, however, the analytic expression in Eq. (4.21) for γ^+ is simple to work with, and since the Hulthen potential is physically well justified, it is preferred in practical applications. Figure 2 is presented here primarily to illustrate that a strong variation in the magnitude of γ^+ is generally accompanied by a strong variation in the phase of γ^+. Noting that the x_0 parameter is restricted to positive values where the magnitude of γ^+ is larger than unity, it is seen that there is a cancellation effect between

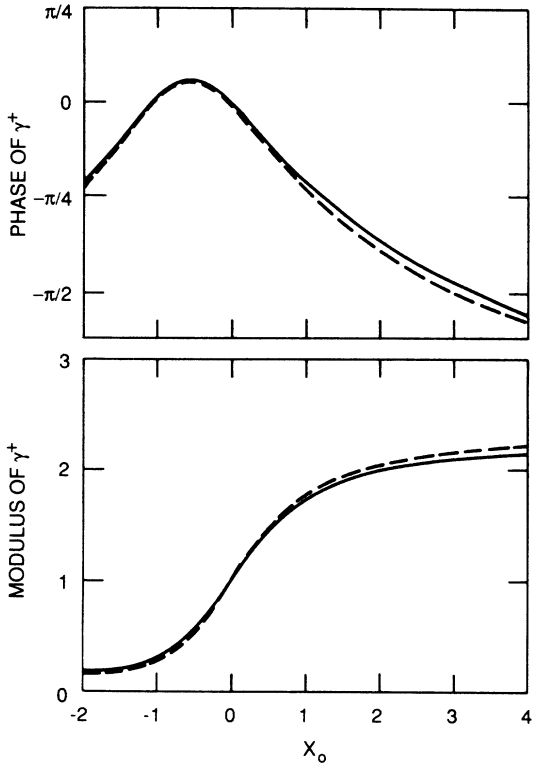

FIG. 1. Off-shell factor γ^+ for the static channel potential pertaining to a 1s initial target state as a function of the off-energy-shell parameter $x_0 = R_0(q^2/2 - \varepsilon)/v$ with $R_0 = 1/2Z_T$. The corresponding factor for the Hulthen potential is included (dashed line) for comparison. The Sommerfeld parameter is $v_P = 1$.

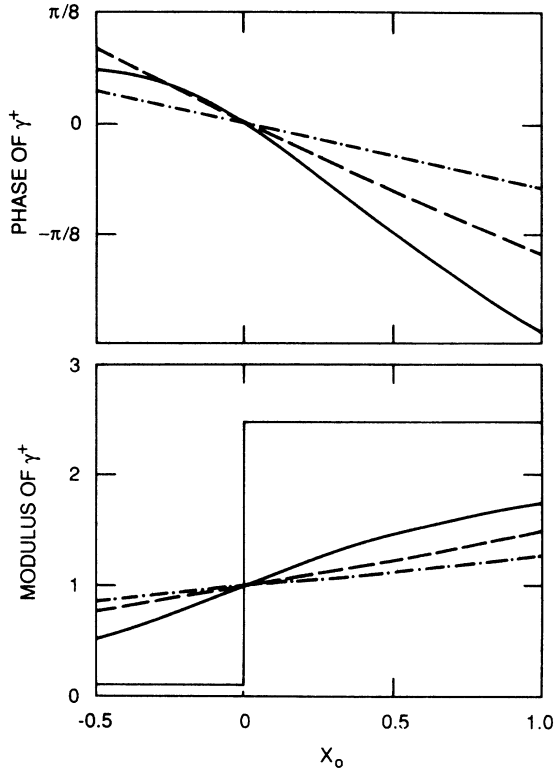

FIG. 2. Off-shell factor γ^+ as a function of the off-energy-shell parameter $x_0 = R_0(q^2/2 - \varepsilon)/v$, for different model channel potentials: (——) Hulthen, (— — —) discontinuous cutoff Coulomb, (—·—·—·) continuous cutoff Coulomb. The discontinuous absolute value of the Coulomb off-shell factor g^+ is included for comparison. The Sommerfeld parameter is $v_P = 1$.

magnitude and phase when the integral over the momentum space wave function of the initial state is performed. This effect was already noted[3] in connection with the original SPB theory for electron capture where the combined effect of magnitude and phase of the off-shell factor g^+ at low velocities was found to give rise to a reduction of the cross section in spite of the fact that the magnitude of g^+ was much larger than unity. The general implication is that the detailed choice of the distortion potential is less important in such cases. A more critical dependence in the choice of the distortion potential appears if selective components of the momentum distribution dominate the considered process. This is the case for radiative electron capture discussed in Sec. VI.

V. ELECTRON CAPTURE IN ASYMMETRIC COLLISIONS

In this section we complete the analysis of the electron-capture cross section in the channel-distorted SPB approximation. A peaking approximation is applied to connect directly with previous results and to compare with experimental data.

The T-matrix element for electron capture is given by Eq. (3.8) in the channel-distorted SPB approximation. Introducing the Fourier transform $\tilde{V}_T$ of the target potential and the expression given by Eq. (4.5) for the channel-distorted SPB wave function, we integrate over the internuclear coordinate $\mathbf{R}_P$ to obtain

$$T_{fi}^{\mathrm{DSPB}}=(2\pi)^{-3/2}\int d\mathbf{k}\,\tilde{\varphi}_i(\mathbf{k})\int d\mathbf{S}\,\tilde{D}^{+}_{\mathbf{K}_i}(\mathbf{S})\langle\varphi_f(\mathbf{r}_P)|e^{-i(\mathbf{J}+\mathbf{k}+\mathbf{S})\cdot\mathbf{r}_P}|\psi^{c+}_{\mathbf{q},\varepsilon_S}(\mathbf{r}_P)\rangle\frac{\varepsilon_i-k^2/2}{\varepsilon_S-q^2/2}\tilde{V}_T(-\mathbf{J}-\mathbf{k}-\mathbf{S})\,, \tag{5.1}$$

where $\mathbf{J}$ is the average momentum transfer vector defined in Eq. (2.8) and Ψ^{c+} is the off-energy-shell Coulomb wave function given by Eq. (4.7) with $\mathbf{q}=\mathbf{k}-\mathbf{v}$ as in Eq. (4.4). The energy parameter ε_S is given by Eq. (4.6). The expression in Eq. (5.1) is the most general form of the channel-distorted strong-potential Born approximation for electron capture. The original SPB T matrix in a similar form is readily identified if the channel distortion is ignored, i.e., if $\tilde{D}_{\mathbf{K}_i}$ is replaced by a δ function. Note that while Eq. (5.1) properly includes pole contributions from the spectrum of bound states it is understood that the pole contribution corresponding to the final state is explicitly excluded as discussed in Sec. III.

The general form of the DSPB T matrix in Eq. (5.1) is not easily computed without further simplifications. A more tractable form may be obtained if the approximate form of the DSPB wave function Eq. (4.11) is used in Eq. (3.8). We then obtain

$$T_{fi}^{\mathrm{DSPB}}=(2\pi)^{-3/2}\int d\mathbf{k}\,\tilde{\varphi}_i(\mathbf{k})\gamma^{+}(\mathbf{q},\varepsilon)\tilde{V}_T(-\mathbf{J}-\mathbf{k})\times\langle\varphi_f(\mathbf{r}_P)|e^{i(\mathbf{J}+\mathbf{k})\cdot\mathbf{r}_P}|\Psi^{c+}_{\mathbf{q}}(\mathbf{r}_P)\rangle\,. \tag{5.2}$$

It is also easy to derive this form directly from the exact DSPB T matrix in Eq. (5.1). One makes the near-shell approximation for the off-shell electron wave function and a peaking approximation in which $\mathbf{S}$ is set to zero in $\tilde{V}_T$ and in the factor $\exp(-i\mathbf{S}\cdot\mathbf{r}_P)$. These latter approximations presume that $\tilde{D}^{+}_{\mathbf{K}_i}(\mathbf{S})$ is sharply peaked on an atomic scale, and this is in accord with the restriction of the off-shell DSPB wave function in the matrix element in Eq. (5.2) to values of $\mathbf{r}_P$ of the order of the spatial extent of φ_f.

The expression in Eq. (5.2) may be reduced to a transparent form by the further application of the so-called full peaking (FP) approximation which is valid at sufficiently high velocities. In this approximation $\mathbf{k}$ is ignored compared to $\mathbf{v}$ in the ionization matrix element in Eq. (5.2) to obtain

$$T_{fi}^{\mathrm{DSPB\text{-}FP}}=\tilde{V}_T(-\mathbf{J})\langle\varphi_f(\mathbf{r}_P)|e^{-i\mathbf{J}\cdot\mathbf{r}_P}|\Psi^{c+}_{\mathbf{v}}(\mathbf{r}_P)\rangle\times(2\pi)^{-3/2}\int d\mathbf{k}\,\tilde{\varphi}_i(\mathbf{k})\gamma^{+}(\mathbf{q},\varepsilon)\,. \tag{5.3}$$

Comparing with the corresponding form of the impulse approximation, i.e., the case where $\gamma^+=1$, we obtain

$$T_{fi}^{\mathrm{DSPB\text{-}FP}}=MT_{fi}^{\mathrm{IA\text{-}FP}}\,, \tag{5.4}$$

where

$$M=\frac{\int d\mathbf{k}\,\tilde{\varphi}_i(\mathbf{k})\gamma^{+}(\mathbf{q},\varepsilon)}{\int d\mathbf{k}\,\tilde{\varphi}_i(\mathbf{k})}\,. \tag{5.5}$$

The original M factor[3] of the SPB theory is obtained when γ^+ in Eq. (5.5) is replaced by the complete off-shell factor g^+.

The M factor is readily evaluated numerically when the γ^+ factor is available in closed form. As discussed in Sec. IV, the Hulthen potential provides an accurate representation of the channel potential pertaining to an initial $1s$ state. Using the expression given by Eq. (4.21), it is easy to see that the M factor depends only on the parameters $\rho=R_0Z_T^2/Z_P$ and $\nu_P=Z_P/v$.

The magnitude of M is shown in Fig. 3 for a sequence of values of ρ. In conformity with our previous notion it is seen that $|M|^2$ interpolates between the impulse approximation and the original form of the SPB when ρ (or R_H) varies from zero to infinity. In the $1s$ case considered here R_0 is given by $R_0=1/2Z_T$, which implies that $\rho=Z_T/2Z_P$, i.e., that ρ is proportional to the asymmetry parameter λ. Generally, it is seen that inclusion of the channel potential implies that the capture cross sections at fixed ν_P tends towards the impulse approximation as the asymmetry is increased. The deviation from the IA is, however, not insignificant for practical values of λ. This is illustrated in Fig. 4, which shows the cross

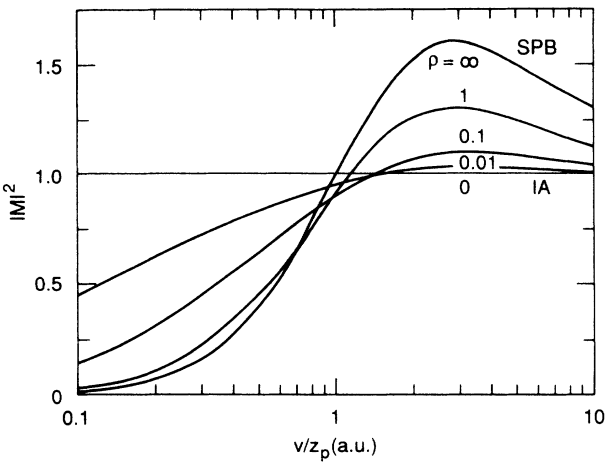

FIG. 3. Ratio of DSPB to IA cross sections for $1s$ to $1s$ capture. The channel potential is of the Hulthen form. The parameter ρ is given by $\rho = R_0 Z_T^2 / Z_P$.

section for electron capture from the K shell in proton-argon collisions. The theoretical curves represent the full-peaking results for the cross section for $1s$ to $1s$ capture in a standard one-electron model for ion-atom collisions involving inner-shell processes (see, for example, the review by Madison and Merzbacher[26]). The SPB and the IA cross sections were adopted form Alston's work.[6] The channel-distorted SPB cross section was obtained using Eq. (5.4). The experimental data[27] represent the total cross section for capture from the K shell. The perfect agreement between the theory and the experimental data at high energies is somewhat misleading since the data include contributions—on the order of 20% according to a simple n^{-3} estimation—from excited states. It remains an open question to what extent the more pronounced deviation at lower energies is due to inaccuracies of the full-peaking approximation. Note in this connection that the FP was found to be accurate in this energy range in the original SPB calculations,[6] but not in the corresponding IA calculations. The evaluation of the DSPB T matrix under less restrictive conditions is needed to clarify this point.

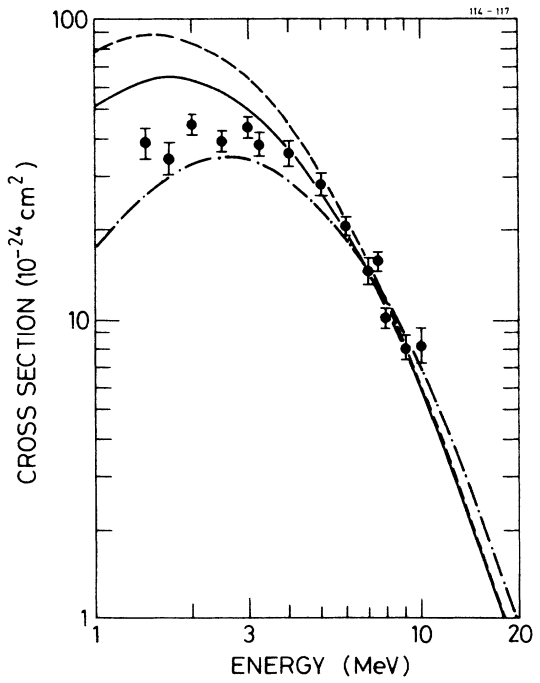

FIG. 4. K-shell capture cross sections for protons on argon: (— — —) impulse approximation, (—·—·—·) strong-potential Born approximation, (——) channel-distorted strong-potential Born approximation. Experimental data are ● Horsdal-Pedersen (Ref. 27).

VI. RADIATIVE ELECTRON CAPTURE

The amplitude for radiative electron capture of a loosely bound electron by a highly charged ion is given by

$$A = \langle \Phi_f | \hat{\mathbf{e}} \cdot \nabla_{\mathbf{r}_P} | \Psi_i^+ \rangle \ . \tag{6.1}$$

The energy of the emitted photon is determined by the energy-conservation condition

$$\omega = \frac{v^2}{2} + \varepsilon_i - \varepsilon_f + \mathbf{v} \cdot \mathbf{J} \ , \tag{6.2}$$

where $\mathbf{J}$ is the momentum transfer vector defined in Eq. (2.8). Note that the transition operator in this matrix element only depends on the electron coordinate $\mathbf{r}_P$. The integral over the complementary Jacobi coordinate $\mathbf{R}_P$ is therefore readily done if the distorted wave of relative motion is suitably approximated. When the channel-distorted wave function, given by Eq. (4.11), is used the $\mathbf{R}_P$ integral provides a δ function with the argument $\mathbf{k}+\mathbf{J}$ so that the integral over the momentum distribution of the initial electron state is trivial. The result is

$$A \approx \tilde{\varphi}_i(-\mathbf{J}) \gamma^+(q,\varepsilon) \langle \varphi_f(\mathbf{r}_P) | \hat{\mathbf{e}} \cdot \nabla_{\mathbf{r}_P} | \psi_{\mathbf{q}}^{c+}(\mathbf{r}_P) \rangle \ , \tag{6.3}$$

where the vector $\mathbf{q} = -\mathbf{J} - \mathbf{v}$ is determined by the general relation given by Eq. (4.4) with $\mathbf{k} = -\mathbf{J}$, and ε is given by Eq. (4.12).

As discussed in Sec. III, γ^+ is generally close to unity at high velocities. At intermediate velocities γ^+ is better represented by the phase factor given by Eq. (4.27). Since phase factors may be ignored when the absolute square of the amplitude is formed, to obtain the differential cross section γ^+ may be omitted in this approximation, and Eq. (6.3) is therefore essentially equivalent to the impulse approximation for REC. This is particularly satisfactory since the IA reflects the physically transparent picture of REC as a free-bound radiative transition in the projectile frame.

In previous evaluations of REC the original form of the SPB wave function was used.[16] Then Eq. (6.3) is also obtained, but with the complete off-shell factor g^+ in place of γ^+. Since $|g^+|$ is typically much larger than unity (see Fig. 2 for positive values of the argument), it appears that the inclusion of the channel distortion is absolutely essential for a proper description of the REC process.

The elimination of the off-shell factor was already indicated in Jakubassa-Amundsen's work.[15] She realized that

the theory of radiative electron capture and radiative recombination of free electrons must merge in the zero-energy limit, i.e., that a genuine free-bound description of REC should apply in the limit of a vanishing binding energy of the initial electron state. To test that this limiting procedure is strictly valid in the channel-distorted SPB theory, we note that the modified factor γ^+ incorporates the channel radius R_0 and the binding energy ε_i in the combination $x_0=(k^2/2-\varepsilon_i)R_0/v\approx|\varepsilon_i|R_0/v$. As the binding energy vanishes, the corresponding bound-state wave function, and hence the channel radius R_0, increase without limit. Then $\varepsilon_i R_0/V$ is indeterminate and further considerations are needed. For a wide class of states, however, the mean radius of bound-state functions relates to the binding energy according to $R_0\approx 1/\sqrt{\varepsilon_i}$, so that $x_0\approx\varepsilon_i R_0\approx\sqrt{\varepsilon_i}\to 0$ as the binding energy vanishes. It follows that the bound-free transition matrix element is indeed the limiting form of the REC amplitude as the binding vanishes. Note that this result requires the simultaneous use of the off-energy-shell electron wave function and the channel-distorted wave functions for relative motion. We recognize that the situation is more complex when the limit $\varepsilon_n\to 0$ is taken along a Rydberg series $n\to\infty$, since then $R\propto n^2$. In this instance high velocity components remain as $\varepsilon_n\to 0$, and the IA may not represent the appropriate picture.

The expression given by Eq. (6.3) is based upon the approximate DSPB wave function given by Eq. (4.11). It is, accordingly, not the most general form of the REC amplitude in the channel-distorted SPB theory. To derive a more accurate expression we may use the complete DSPB wave function given by Eq. (4.5) to approximate the exact scattering state in the ket of Eq. (6.1). As above, the integral over $\mathbf{R}_P$ is readily evaluated since the radiative transition operator is independent of this coordinate. We then obtain

$$A=(2\pi)^{-3/2}\int \tilde{D}^{\,+}_{\mathbf{K}_i}(\mathbf{S})\tilde{\varphi}_i(\mathbf{k}) \times\langle\varphi_f(\mathbf{r}_P)|\hat{\mathbf{e}}\cdot\nabla_{\mathbf{r}_P}|\Psi^{c\,+}_{\mathbf{q},\varepsilon_S}(\mathbf{r}_P)\rangle \times\frac{\varepsilon_i-k^2/2}{\varepsilon_S-q^2/2}d\mathbf{S}\,, \tag{6.4}$$

where

$$\mathbf{k}=-\mathbf{J}-\mathbf{S},\quad \mathbf{q}=-\mathbf{J}-\mathbf{v}-\mathbf{S}\,, \tag{6.5}$$

and where ε_S is given by Eq. (4.6). This is the most general form of the DSPB amplitude for radiative electron capture. The special case where the distortion factor was omitted was evaluated in Ref. 15. To insure that the amplitude approached the free-bound amplitude, i.e., the proper radiative recombination limit as the binding of the initial state vanishes, a term corresponding to the free-bound amplitude was split off in Jakubassa-Amundsen's work[15] and the off-energy shell factor omitted in that term. With our more general form, it is now possible to justify this procedure as a first approximation.

Our previous form Eq. (6.3) is obtained if the near-shell approximation Eq. (4.8) is applied to the off-energy-shell wave function and if the peaking approximation $\mathbf{S}\approx 0$ is applied in the resulting free-bound transition element and in the initial-state wave function. Notice that while the near-shell approximation becomes better as the binding energy of the initial state is reduced, this is not the case when $\tilde{\varphi}_i(\mathbf{k})$ is approximated by $\tilde{\varphi}_i(-\mathbf{J})$ since the momentum space wave function becomes more sharply peaked in this limit. In a more careful evaluation where $\varphi_i(\mathbf{k})$ is kept under the integral, it can be shown that the general DSPB amplitude given by Eq. (6.4) indeed reduces to the proper radiative recombination limit when the binding of the initial state is reduced to zero ($Z_T\to 0$). Details are given in Appendix B. This justifies the procedure used in Ref. 15 where the off-shell-factor was omitted in the pole term of the REC amplitude. Presumably, exact evaluation of Eq. (6.4) would yield an REC amplitude very nearly equal to the amplitude obtained by splitting off the pole term for special treatment, but would be applicable over the entire REC spectrum.

VII. DISCUSSION

We have examined lowest-order approximations to transition matrices and associated wave functions for strongly interacting atomic species. We find that the lowest-order wave function for strong potentials involves the strong-potential Green's function to describe electron propagation in intermediate states and a distorted initial wave function to describe elastic scattering of the relatively massive projectile. Our calculations show that both aspects are essential and can be incorporated into a single factor $\gamma^+(q,\varepsilon)$. This factor has been evaluated using eikonal waves and it is shown that a relatively simple form derived from the Hulthen potential is quite accurate. With this new factor we have computed capture from inner shells and find improved agreement with experiment at high energies where the theory is expected to hold unequivocally.

Combining elastic scattering and off-shell propagation places the theory of radiative electron capture on a sound *ab initio* basis. Intuitive models that treat the bound electron as initially free yield the impulse approximation. Here we have correctly incorporated the structure of the initial bound state and shown how channel distortion and off-shell propagation combine to yield the impulse approximation which neglects both of these effects at the outset.

The strong-potential Born approximation derives from an expansion in powers of the parameter $\lambda=Z_T/Z_P$, which is independent of velocity. The expansion might therefore seem to apply over the whole velocity range just as the first Born approximation appears to apply to excitation or ionization of strongly bound systems by weak perturbations if no subsequent approximations are employed. It is, however, well known that the first Born approximation for excitation or ionization is inaccurate at low velocities unless it is amended to account for binding effects[28] which are exactly equivalent[8] to the channel distortion effects that we have identified in capture-type reactions. The binding corrections in first Born type excitation processes correspond, however, to the channel distortion of the initial and final states due to the weak per-

turbation. The implication is that a proper treatment of electron capture at low velocities involves the retention also of the weak channel distortion in the final state. Since this distortion has been omitted in the present formulation of the DSPB theory it appears that the corresponding Sommerfeld's parameter must be small for the theory to hold,

$$\nu_T = Z_T/v \ll 1 \ . \tag{7.1}$$

Note that this condition is usually implied in applications of various peaking approximations in practical evaluations. Here, the condition appears on more fundamental grounds. In addition to the limitations implied by the neglect of the distortion in the final channel, the condition in Eq. (7.1) should probably also be satisfied in order that the static channel approximation may provide a proper description of the strong elastic distortion in the initial channel. Further work is accordingly needed to develop the present formulation of the theory of electron capture in asymmetric collisions to a level that may compare with the binding corrected versions of the first Born approximation for inner-shell ionization by low-charged projectiles.[29]

ACKNOWLEDGMENTS

This research has been sponsored by the U.S. Department of Energy, Office of Basic Energy Science, Division of Chemical Sciences, under Contract No. DE-AC05-84OR21400 with Martin Marietta Energy System, Inc.

APPENDIX A: REMOVAL OF THE INTERNUCLEAR POTENTIAL

It has been customary to ignore the internuclear potential from the outset in perturbation treatments of ion-atom collisions. This is usually justified in a distorted-wave formulation by retaining the internuclear potential in initial and final channels and by applying the eikonal approximation for the corresponding distorted waves. More generally, it is readily seen that any distortion potential $U(R)$ *common* to the initial and final channels can be ignored in so far as total cross sections are concerned. In this appendix we consider more generally the eikonal approximation when different distortion potentials U_i and U_f are employed in the initial and final channels.

Writing the distorted channel functions as

$$|\Phi_c^{\pm}\rangle = D_c^{\pm}|\Phi_c\rangle \ , \tag{A1}$$

$D_c^{\pm}$ is a simple phase factor in the eikonal approximation

$$D_c^{\pm}(\mathbf{R}) = (vR + \mathbf{v}\cdot\mathbf{R})^{i\nu} \times \exp\left[-\frac{i}{v}\int_{-\infty}^{Y}\left[U_c(R') + \frac{Z}{R'}\right]dY'\right] , \tag{A2}$$

where Y is the coordinate of $\mathbf{R}$ along the asymptotic velocity vector $\mathbf{v}$. The potential U_C is considered to be asymptotic to the Coulomb form $-Z/R$ and ν is the corresponding Sommerfeld parameter $\nu = Z/v$. Now we may write the identity

$$\frac{1}{2\mu_i}\nabla^2_{\mathbf{R}_T} D_i^+|\Phi_i\rangle = D_i^+\frac{1}{2\mu_i}\nabla^2_{\mathbf{R}_T}|\Phi_i\rangle + D_i^+ U_i|\Phi_i\rangle + \frac{1}{2\mu_i}(\nabla^2_{R_T} D_i^+)|\Phi_i\rangle \ , \tag{A3}$$

and recognize that the three terms on the right-hand side are of the order $(\mu_i)^1$, $(\mu_i)^0$, and $(\mu_i)^{-1}$, respectively. The last term in Eq. (A3) may, accordingly, be ignored in ion-atom collisions. We then obtain

$$|\Psi_i^+\rangle = D_i^+\{1 + [E - (H - U_i) + i\eta]^{-2} W_i\}\Phi_i\rangle \ . \tag{A4}$$

The eikonal form of the distorted-wave T-matrix element is correspondingly given by

$$T_{fi} = \langle \Phi_f | D_f^{-*} D_i^+ W_f \{1 + [E - (H - U_i) + i\eta]^{-1} W_i\}|\Phi_i\rangle \ . \tag{A5}$$

Since $H - U_i = H_T + W_i$, it is seen that the residual effect of long-range forces is combined in the product of two eikonal phase factors while the remaining components in Eq. (A5) exhibit simple short-range properties.

The Green's operator that appears in Eqs. (A4) and (A5) after the complete eikonal phase factor has been extracted from the initial state is generally rather complicated, from an analytical point of view, since a corresponding set of eigensolutions is not readily available. It is therefore more useful to extract only the eikonal phase factor that pertains to the common internuclear Coulomb potential. The product of the Coulomb phase factors is, in an excellent approximation, given by

$$D_f^{-*} D_i^+ = b^{2iZ_T Z_P/v} \ , \tag{A6}$$

where b is the component of the internuclear coordinate in the plane perpendicular to $\mathbf{K}_i$, i.e., the impact parameter. It is readily shown that this factor may be omitted in the T matrix and still provide the correct result for the total cross section

$$\sigma_{fi} = (2\pi)^4 \mu_i \mu_f \frac{K_f}{K_i}\int d\Omega |T_{fi}|^2 \ . \tag{A7}$$

The internuclear potential is therefore usually ignored with the understanding that the theory only applies for differential cross sections if a suitable eikonal transform is subsequently made to incorporate the internuclear scattering. More precisely, the transition matrix element, which is a function of momentum transfer $\mathbf{K}_\perp$ perpendicular to the initial momentum $\mathbf{K}_i$, may be transformed to the impact parameter representation via

$$A_{fi}(\mathbf{b}) = (2\pi)^{-1}\int T_{fi}(\mathbf{K}'_\perp) e^{i\mathbf{K}'_\perp\cdot\mathbf{b}} d^2\mathbf{K}'_\perp \ , \tag{A8}$$

multiplied by $b^{2iZ_P Z_T/v}$, and transformed back to obtain a T-matrix element which includes the internuclear scattering.

APPENDIX B: DETAILED ANALYSIS OF THE REC AMPLITUDE

Equation (6.3) is the most general form of the SPB amplitude for radiative electron capture. The special case

where the distortion factor was omitted was evaluated in Ref. 15. To insure that the amplitude approached the free-bound amplitude as the binding energy of the inital state vanishes, a term corresponding to the free-bound amplitude was split off and the off-energy-shell factor omitted in that term only. With our more general form, it is now possible to justify this procedure as a first approximation.

To see how this emerges we note that the pole term representing free-bound transitions just corresponds to the near-shell approximation for the off-shell wave function in Eq. (6.4). For REC the vector $\mathbf{K}=-\mathbf{J}-\mathbf{v}$ is large, of the order of $-\mathbf{v}$, while $\mathbf{J}$ is small. Indeed, at the peak of the REC cross section we have $\mathbf{J}=0$. It is then appropriate to neglect $\mathbf{S}$ compared with $\mathbf{K}$ and write

$$A=\langle\varphi_f|\hat{\mathbf{e}}\cdot\nabla_{\mathbf{r}_P}|\Psi_{\mathbf{K}}^{c+}\rangle I(\mathbf{J}) , \tag{B1}$$

where $I(\mathbf{J})$ is given by

$$I(\mathbf{J})=(2\pi)^{-3/2}\int \tilde{D}^{+}_{\mathbf{K}_i}(\mathbf{S})\frac{\varepsilon_i-k^2/2}{\varepsilon_S-q^2/2}g(q,\varepsilon_S)\tilde{\varphi}_i(\mathbf{k})d\mathbf{S} , \tag{B2}$$

and where $\mathbf{k}=-\mathbf{J}-\mathbf{S}$ and $\mathbf{q}=\mathbf{k}-\mathbf{v}$. Our previous derivation corresponds to neglecting $\mathbf{S}$ in $\tilde{\varphi}_i(-\mathbf{J}-\mathbf{S})$. Since $\tilde{\varphi}_i$ represents a loosely bound electron, the neglect of $\mathbf{S}$ is not obviously correct as the initial binding energy vanishes. We therefore evaluate the integral more exactly for capture from a hydrogen $1s$ state of the target near the cross-section peak at $\mathbf{J}=0$. To investigate the validity of the peaking approximation it is sufficient to examine the mathematically convenient case where the channel potential assumes the pure Coulomb form. Introducing $\tilde{\varphi}_i(\mathbf{k})=N_i(Z_T^2+k^2)^{-2}$ and Eq. (4.15) to represent the phase factor of g^{+} combined with the denominator in Eq. (B2), we have

$$I(0)=\tfrac{1}{2}i(2v^2)^{i\nu_P}N_i\int_0^\infty dx\, x^{i\nu_P}e^{-iZ_T^2x/2}(2\pi)^{-3/2}\times\int d\mathbf{S}\tilde{D}^{+}_{\mathbf{K}_i}(\mathbf{S})\frac{e^{-ix\mathbf{v}\cdot\mathbf{S}}}{Z_T^2+S^2} . \tag{B3}$$

We now return to coordinate space for the distortion factor and use the explicit form $D^{+}_{\mathbf{K}_i}(\mathbf{R})=(vR-\mathbf{v}\cdot\mathbf{R})^{-i\nu_P}$ to obtain

$$I(0)=\frac{i}{8\pi}N_i(2v^2)^{i\nu_P}\int_0^\infty dx\, x^{i\nu_P}e^{-iZ_T^2x/2}\int d\mathbf{R}\frac{e^{-Z_TR}}{R}[v|x\mathbf{v}+\mathbf{R}|+\mathbf{v}\cdot(x\mathbf{v}+\mathbf{R})]^{-i\nu_P} . \tag{B4}$$

Introducing the coordinate $\mathbf{r}=\mathbf{R}/xv$, and evaluating the x integral we find

$$I(0)=iN_i2^{i\nu_P}\mathbf{v}^2\int d\mathbf{r}\frac{1}{r}\frac{(1+|\hat{\mathbf{v}}+\mathbf{r}|+\hat{\mathbf{v}}\cdot\mathbf{r})^{-i\nu_P}}{(Z_Tvr+iZ_T^2/2)^3} , \tag{B5}$$

which may be expressed as

$$I(0)=\tilde{\varphi}(0)i\nu_T2^{i\nu_P}\int_0^\infty dr\, rf(r)(r+i\nu_T/2)^{-3} , \tag{B6}$$

where

$$f(r)=\tfrac{1}{2}\int_{-1}^{1}d\cos\theta[1+(1+r^2+2r\cos\theta)^{1/2}+r\cos\theta]^{-i\nu_P} . \tag{B7}$$

The remaining integral in Eq. (B6) peaks strongly at $r=0$ since $\nu_T=Z_T/v$ is small. The integral over r in Eq. (B6) divides into two regions $0\le r<1$ and $1\le r<\infty$, and the integral over the second region is easily seen to be bounded by a constant independent of ν_T. In the region $0\le r<1$ we expand $f(r)$ in a power series in r and evaluate the integral in terms of hypergeometric functions. It is seen that the lowest-order term dominates thus confirming the simple peaking approximation $f(r)\approx f(0)$ in Eq. (B6). Our result is

$$I(0)=\tilde{\varphi}_i(0)+O(\nu_T\ln\nu_T) . \tag{B8}$$

This confirms the approximation used in Eq. (6.3) where we omitted the $\mathbf{S}$ dependence of $\tilde{\varphi}(-\mathbf{J}-\mathbf{S})$ at the outset, and shows that the approximation becomes exact in the limit $\nu_T\to 0$.

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