Theory of electron capture from a hydrogenlike ion by a bare ion

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We have systematically developed a new approximation for the calculation of the cross section for electron capture from a hydrogenlike ion of large nuclear charge $Z_T e$ by a bare ion of charge $Z_P e$ moving with speed v. The amplitude in the wave treatment is obobtained through consistent expansion in the small parameters Z_P/Z_T and $Z_P e^2/\hbar v$; however, the ratio $Z_T e^2/\hbar v$ is not assumed small. Following a careful analysis of the approach to the energy shell, an off-shell factor is seen to arise which does not appear in the impulse approximation. The effects of this factor on the capture amplitude are explored. Using a peaking approximation, we derive a closed-form expression for the $1s \rightarrow ns$ capture amplitude which includes the effects of the off-shell factor and is accurate to order $(Z_P e^2/\hbar v)^2$. We tabulate the peaking-approximation cross section. The derivation of the asymptotic form of the cross section when $Z_P/Z_T << 1$ is justified. Using a realistic one-electron model, K-shell capture cross sections are calculated for protons on carbon, neon, and argon. These are seen to represent the data generally better than do the impulse approximation cross sections.

I. INTRODUCTION

Over the last ten years, electron capture has emerged as a process of great practical and fundamental significance.[1] For example, in determining the hydrogen escape flux from the earth's upper atmosphere, capture by protons from the plasmasphere provides an important nonthermal source of energetic hydrogen atoms.[2,3] Electron capture also gives rise to x-ray emission in the interstellar medium.[4,5] Moreover, as the medium is far from thermodynamic equilibrium, capture is an important factor in governing the level of ionization of the constituent ions and thus the state of the system. On the technological side, the capture process has been discussed as a possible mechanism for producing population inversion in an x-ray laer.[6] In neutral hydrogen beam injection into tokamak plasmas, beam attenuation, as a result of capture, seriously reduces the supplementary plasma heating derived from the beam.[7] These examples show the need for a more fundamental understanding of the capture mechanism.

Within the general area of electron capture there are many specific types. One may mention inner- or outer-shell capture from one-electron or many-electron atoms. On the other hand, one has symmetric or asymmetric capture depending on the relative charges of the target and projectile and also resonant or nonresonant capture depending on whether the initial and final bound energies of the captured electron are equal or not. This listing reflects the variety of the field and furthermore points out the limitations of present day theory: one often treats each type by a separate method. In addition, the picture is complicated by the present need for separate theories applicable at low and high relative projectile-target velocities.

A unified treatment for the whole spectral region has not yet emerged but a promising framework has been developed for capture in highly asymmetric systems where the projectile velocity v is much greater than the electron velocity in the bound state of the low-Z ion. This framework, which has evolved over the past few years through the efforts of Briggs[8] and other workers,[9–11] is

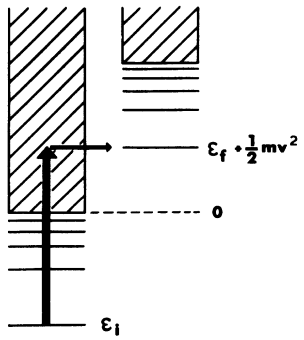

FIG. 1. Electronic energy-level diagram showing the two-step picture of capture: (1) ionization and (2) attachment. The target spectrum is on the left and the final-state spectrum is on the right.

most easily visualized in terms of an electronic energy-level diagram. Consider an asymmetric one-electron model with the target charge $Z_T e$ much larger than the projectile charge $Z_P e$. The electron is initially bound in the ground state of the target with binding energy ϵ_i. The energy-level diagram of the target is shown schematically in Fig. 1 with the ground-state energy noted explicitly. When the electron is captured by the projectile ion of velocity v, it acquires a binding energy ϵ_f and a kinetic energy $\frac{1}{2}mv^2$, with m the electron mass. Because the projectile, including the captured electron, is moving with velocity v relative to the nearly stationary target we add $\frac{1}{2}mv^2$ to ϵ_f to place the electron's energy in the final state on the same diagram. The key feature of the present formulation for interpreting capture dynamics is that capture reactions are mediated by target states centered around the most favorable energy $\epsilon_f + \frac{1}{2}mv^2$. Such states are represented by electron wave functions of momentum of the order of $m\vec{v}$. In this picture, virtual ionization provides the essential mechanism by which the electron acquires the kinetic energy $\frac{1}{2}mv^2$ and momentum $m\vec{v}$ of the final state. Because two steps are involved, this theory is intrinsically a second-Born-type theory.

This paper develops the theory in a time-independent framework by consistent expansion in the parameters Z_P/Z_T and $Z_P e^2/\hbar v$ where Z_P is a good measure of the final mean orbital velocity. It is not assumed that $(Z_T e^2/\hbar v)$ be small, i.e., the projectile velocity v need not be much larger than the initial mean orbital velocity. Hereafter we use atomic units ($m = e = \hbar = 1$) although m is retained in many equations for clarity.

It is now well established theoretically that the second Born theory gives the correct asymptotic velocity dependence of the cross section for asymmetric as well as symmetric captures.[12,13] Since this theory is second order, it provides for the double-scattering mechanism which is known to dominate at high velocities as was first derived by Thomas using a classical analysis.[1,14] The captured electron moves under the influence of two potentials deriving from the projectile and target nuclei. The second Born theory treats these two interactions on equal footing. From basic considerations an equal treatment of each potential[15] is well justified for symmetric and only moderately asymmetric captures. However, for the highly asymmetric case, the stronger potential has an appreciably greater effect on the electron's motion. Briggs has particularly stressed this point[8] in his impulse approximation (IA). Two important things to note about this theory are that it is obtained by retaining the lowest term of a consistent expansion of the total Green's function in the parameter Z_P/Z_T and it is not assumed that $Z_T/v << 1$. The electron-target interaction is included to all orders while the electron-projectile interaction (the weaker one) is included to first order. Briggs also pointed out the connection with ionization through the following picture. The electron initially bound to target T is ionized by its collision with projectile P leaving P essentially undeflected. The ionized state of the electron consists of a packet of incoming Coulomb spherical waves plus Coulomb plane wave traveling in the direction of P with approximately the same velocity. Thus, far from the target one has the system $(P+e)$ traveling with velocity $\vec{v}$. The weighting of each term of the packet is determined by the final-state distribution of momentum and is centered about $m\vec{v}$. The impulse approximation also leads to the correct asymptotic velocity dependence of the cross section.[16] The above discussion supports the conclusion that the impulse approximation is the lowest-order theory which is both derivable from a natural and consistent scheme and at the same time satisfies the known general characteristics of the capture process.

But the theory does not adequately represent experiment for velocities $Z_P << v \lesssim Z_T$ which is where the cross section reaches a maximum and then decreases again. For inner-shell capture from argon by protons this peak is at $v = 12$ a.u. or $E = 3.5$ MeV and here the parameter $(Z_P/v)^2$ equals 0.01 which is much less than 1. Macek and Taulbjerg have pointed out the cause for this discrepancy as being the neglect of a certain factor of the order of $(Z_T/v)^2$, even though the theory is supposedly derived correctly to this order.[11]

The problem arises because, according to the above capture picture, we represent the outgoing electron as a packet of Coulomb plane waves with distribution of momentum determined by the final state and centered about $m\vec{v}$. That is, we have an electron traveling along with the projectile but not bound to it. The ratio of the difference in energy of the two states to the actual final-state energy is roughly equal to the ratio of the final-state binding energy to the traveling kinetic energy. This ratio is approximately $(Z_P/v)^2$. Since the above energy difference is neglected, this ratio indicates the basic limitation of the theory.

Because the final state is a bound electron-

projectile system, one must represent the ionized electron using off-energy-shell Coulomb waves. Off-energy shell means that the wave's energy is not equal to the energy of the plane-wave part as for on-energy-shell Coulomb waves. The ratio of the difference in energy of the two waves to the on-shell energy is $(Z_P/v)^2$, the same as that discussed above. If we approximate the off-energy-shell waves by the on-energy-shell waves, then we expect errors of the same order as this difference; this is how the IA is derived. Jakubassa-Amundsen and Amundsen were the first to clarify this point.[9]

Unfortunately, the limit to the shell is nonuniform in the complex energy plane[17]: a branch point exists at the limit point. Thus, one can never go to the limit exactly. Yet, very close to the branch point the off-energy-shell function is approximated by the on-energy-shell one multiplied by an extra factor containing the effects of the branch point. It is precisely this factor which is left out of the IA as pointed out by Macek and Taulbjerg.[11] The error produced by neglect of this term is of the order $(Z_T/v)^2$. Moreover, it is especially important to realize that inclusion of this factor does not lead to any kind of divergence in the cross section and contains, in particular, contributions from the bound states. We derive the capture amplitude incorporating the *exact* off-energy-shell wave function by treating the strong potential to all orders. The theory is called the strong potential Born theory. Later, we make approximations on the amplitude to gain a closed-form expression.

We can interpret all the second-Born-type theories in terms of the electronic energy-level diagram of Fig. 1. Clearly, the important feature characterizing the theories is their treatment of the target spectrum. The second Born theory with free Green's function treats the continuous part of this spectrum using plane waves, which, in general, results in an overestimate for the cross section.[18] The error involved is of the order $(Z_T/v)^2$. The strong potential Born (hereafter referred to as SPB), incorporates the correct target spectrum of intermediate states. Both discrete and continuum levels are represented by exact wave functions of the electron in the field of the strong potential. Because the strong potential is included to all orders, the errors in this approximation are of the order $(Z_P/v)^2$ or Z_P/Z_T. The impulse approximation neglects additional small energy differences of order $(Z_P/v)^2$ and is apparently accurate to the same order as the SPB. Macek and Taulbjerg[11] show, however, that the IA neglects terms of order $(Z_T/v)^2$. This is the same order of error as for the plane-wave second Born theory. The continuum-intermediate-state theory[19] (CIS) is obtained by making further approximations to the IA. These approximations introduce additional errors of the order $(Z_T/v)^2$. Thus, the IA, CIS, and the plane-wave second Born theories all contain errors of order $(Z_T/v)^2$. The eikonal theory neglects part of the second Born terms and is accordingly of lower order than the second Born theory.[20] From an *a priori* standpoint, all of these theories except the SPB are inapplicable when Z_T/v is non-negligible. The SPB theory, since it requires only that Z_P/v be small, is applicable when Z_T/v is large provided that $(Z_P/v)^2 \ll 1$.

An even greater difference between the SPB theory and the others appears in the manner of inclusion of the target discrete spectrum. Here the SPB is unique since contributions from the bound states are provided for correctly by using the off-energy-shell wave function. These contributions are more important for the lower velocities. The other theories, however, do not give an adequate treatment of the bound states. The second Born, CIS, and eikonal theories do not include them at all. The IA treatment of the bound states is incorrect. Because the Coulomb waves appear in a final-state momentum integral, the wave's energy can become negative. The corresponding bound-state functions have exponentially *increasing* terms in coordinate space. Although other factors tend to compensate for this problem, the bound-state treatment is nonetheless wrong. The conclusion to be drawn from the analysis of the second-Born-type theories is that the SPB theory offers a more comprehensive framework and that it is the only theory which can be extended into the intermediate velocity region.

The structure of the paper is as follows: In Sec. II we derive the exact SPB capture amplitude by retaining only the lowest term in an expansion in the small parameter Z_P/Z_T. A parameteric integral in the amplitude is then evaluated by making order-of-magnitude estimates of the size of certain parameters. A major part of the amplitude is seen to come from a pole contribution. In Sec. III the relation of the off-energy-shell wave function to the on-energy-shell wave function is found. An explicit form for the off-shell factor is exhibited and the on-energy-shell function is seen to result from a pole contribution of the integral representa-

tion of the off-energy-shell function. In Sec. IV we explore the relation of certain on- and off-shell matrix elements. In Sec. V the $1s \rightarrow ns$ capture cross section is derived using a peaking approximation. In Sec. VI the effects of the off-shell factor are determined and the derivation of the asymptotic form the cross section is justified. The $1s \rightarrow ns$ universal capture cross section is tabulated. Finally, the theory is extended to treat inner-shell capture for asymmetric systems and the capture cross sections are calculated for protons on carbon, neon, and argon. We use the notation of Macek and Shakeshaft.[10] Our plane-wave functions are represented as $\phi_{\vec{k}}(\vec{r}) = (2\pi)^{-3/2} e^{i\vec{k}\cdot\vec{r}}$. The reduced masses are $\nu_i = M_P M_T/[\alpha(m + M_T + M_P)]$ and $\nu_f = M_P M_T/[\beta(m + M_T + M_P)]$ with $\alpha = M_T/(m + M_T)$, $\beta = M_P/(m + M_P)$, and with M_T the target nuclear mass and M_P the projectile mass. The initial and final bound-state energies are ϵ_i and ϵ_f.

II. THE SPB AMPLITUDE

We are interested in the amplitude, exact within the framework of the SPB, for the capture of an electron from the bound state $\phi_i(\vec{r}_T)$ of $(e+T)$ by P to the bound state $\phi_f(\vec{r}_P)$ of $(e+P)$. The target charge Z_T is assumed to be much larger than the projectile charge Z_P. The theory will thus be developed using V_{Te} as the strong potential. We neglect errors of the order of m/M_T and m/M_P in the following analysis, and in accord with the arguments of Wick,[21] omit the internuclear potential. This implies that effects due to projectile deflection in the internuclear field are neglected.

The Hamiltonian for the system in the total center-of-mass frame is given by

$$H = -\frac{1}{2\nu_i}\nabla^2_{\vec{R}_T} - \frac{1}{2m}\nabla^2_{\vec{r}_T} + V_{Te} + V_{Pe}$$

$$\equiv H_0 + V_{Te} + V_{Pe} , \tag{2.1}$$

where $V_{Te} = -Z_T/r_T$ and $V_{Pe} = -Z_P/r_P$. The Green's function corresponding to the complete Hamiltonian H is defined by the equation

$$G^+ \equiv 1/(E - H + i\eta) ,$$

with E the total system energy and the limit $\eta \rightarrow 0_+$ being always implied. The scattering amplitude is expressed by the relation

$$A = \langle \psi_f \mid V_{Pe} + V_{Te} G^+ V_{Pe} \mid \psi_i \rangle \tag{2.2}$$

with

$$\psi_i(\vec{r}_T, \vec{R}_T) = (2\pi)^{3/2} \phi_{\vec{K}_i}(\vec{R}_T) \phi_i(\vec{r}_T) ,$$

$$\psi_f(\vec{r}_P, \vec{R}_P) = (2\pi)^{3/2} \phi_{\vec{K}_f}(\vec{R}_P) \phi_f(\vec{r}_P) ,$$

and

$$E = K_i^2/2\nu_i + \epsilon_i = K_f^2/2\nu_f + \epsilon_f .$$

If we scale all the coordinates by Z_T: $\vec{r}_T \rightarrow Z_T \vec{r}_T$, $\vec{R}_T \rightarrow Z_T \vec{R}_T$, etc., then V_{Te} has a strength of 1 whereas V_{Pe} has a strength of Z_P/Z_T which is much less than 1. Defining the Hamiltonian of the bound $(e+T)$ system plus free particle P as $H_0 + V_{Te}$ and the Green's function as

$$G_c^+ \equiv 1/(E - H_0 - V_{Te} + i\eta) ,$$

we see that the Neumann series of G^+ in terms of G_c^+ is

$$G^+ = G_c^+ + G_c^+ V_{Pe} G_c^+ + G_c^+ V_{Pe} G_c^+ V_{Pe} G_c^+ + \cdots . \tag{2.3}$$

Noting that G_c^+ is independent of Z_P and Z_T, we observe that Eq. (2.3) represents an expansion in the small parameter Z_P/Z_T. To obtain the SPB amplitude, we retain only the first term of Eq. (2.3):

$$G^+ \approx G_c^+ .$$

The Green's function G_c^+ has the property that

$$G_c^+ \mid \phi_{\vec{K}}(\vec{R}_T)\rangle = \mid \phi_{\vec{K}}(\vec{R}_T)\rangle (\epsilon - H_c + i\eta)^{-1} , \tag{2.4}$$

where $\epsilon = E - K^2/2\nu_i$ and H_c is a one-electron Coulomb Hamiltonian. It follows that our G_c^+ is closely related to the Coulomb Green's function. This property of G_c^+ plays an important role in the reduction of the SPB amplitude.

Our approximate amplitude is now given by

$$A_{\mathrm{SPB}} = \langle \psi_f \mid V_{Pe} + V_{Te} G_c^+ V_{Pe} \mid \psi_i \rangle . \tag{2.5}$$

Note that this amplitude, while it incorporates first and second Born terms, actually represents a zeroth-order amplitude in the small parameter Z_P/Z_T. For asymmetric collisions, this is the only amplitude that represents a consistent lowest-order approximation. In particular, the Brinkman-Kramers (BK) approximation[22] takes just the first

term in Eq. (2.5). The second term, however, is of the same order as the BK term and frequently of comparable magnitude.

In order to evaluate Eq. (2.5), we insert a complete set of plane-wave states

$$\langle \vec{R}_P,\vec{r}_P \mid \phi_{\vec{K}'}\phi_{\vec{k}}\rangle=(2\pi)^{-3}e^{i\vec{K}'\cdot\vec{R}_P}e^{i\vec{k}\cdot\vec{r}_P}$$

to give

$$A_{\rm SPB}=\int d^3k\,d^3K'\langle\psi_f(\vec{r}_P,\vec{R}_P)\mid\phi_{\vec{K}'}(\vec{R}_P)\phi_{\vec{k}}(\vec{r}_P)\rangle\langle\phi_{\vec{K}'}(\vec{R}_P)\phi_{\vec{k}}(\vec{r}_P)\mid(1+V_{Te}G_c^+)V_{Pe}\mid\psi_i(\vec{r}_T,\vec{R}_T)\rangle\ . \tag{2.6}$$

We have the relation

$$\langle\psi_f\mid\phi_{\vec{K}'}\phi_{\vec{k}}\rangle=(2\pi)^{3/2}\phi_f^*(\vec{k})\delta(\vec{K}'-\vec{K}_f) \tag{2.7}$$

and using Eq. (2.4) we have

$$\begin{aligned}(1+G_c^-V_{Te})\mid\phi_{\vec{K}'}(\vec{R}_P)\phi_{\vec{k}}(\vec{r}_p)\rangle&=\mid\phi_{\beta\vec{K}'-\vec{k}}(\vec{R}_T)\rangle[1+(\epsilon-H_c-i\eta)^{-1}V_{Te}]\mid\phi_{\vec{k}_2}(\vec{r}_T)\rangle\\&\equiv\mid\phi_{\beta\vec{K}'-\vec{k}}(\vec{R}_T)\rangle\mid\psi^{(-)}_{\vec{k}_2,\epsilon}(\vec{r}_T)\rangle\ ,\end{aligned} \tag{2.8}$$

where $\vec{k}_2\equiv\alpha\vec{k}+(1-\alpha\beta)\vec{K}'$, and $\epsilon\equiv E-(\beta\vec{K}'-\vec{k})^2/2\nu_i$. Since, in general, $\epsilon\neq k_2^2/2m$, Eq. (2.8) defines $\psi^{(-)}_{\vec{k}_2,\epsilon}(\vec{r}_T)$ as the off-energy-shell Coulomb wave function with ingoing wave-boundary condition. Because of the off-energy-shell nature of $\psi^{(-)}_{\vec{k}_2,\epsilon}$, we note that its expansion in a complete set of states for the Coulomb problem will necessarily include bound-state terms. This fact is very significant as pointed out in the Introduction.

We define the "average" momentum transfer vectors

$$\vec{K}=\beta\vec{K}_f-\vec{K}_i\ \text{ and }\ \vec{J}=\alpha\vec{K}_i-\vec{K}_f\ . \tag{2.9}$$

Carrying through the $\vec{R}_T$ integration, we obtain the result

$$\langle\phi_{\beta\vec{K}'-\vec{k}}(\vec{R}_T)\mid V_{Pe}(\alpha\vec{r}_T-\vec{R}_T)\mid\phi_{\vec{K}_i}(\vec{R}_T)\rangle=-\frac{Z_P\alpha^2}{2\pi^2\mid\vec{p}-\vec{K}\mid^2}e^{i(\vec{p}-\vec{K})\cdot\vec{r}_T}\ , \tag{2.10}$$

where $\vec{p}\equiv\alpha\vec{k}+(1-\alpha)\vec{K}$ and we have used the delta function of Eq. (2.7) to replace $\vec{K}'$ by $\vec{K}_f$. Inserting Eqs. (2.8) and (2.10) into Eq. (2.6) and writing $\tilde{\phi}_f^*(\vec{p}/\alpha-\vec{K}/\alpha+\vec{K})\approx\tilde{\phi}_f^*(\vec{p})$, since $\alpha\approx1$, our amplitude becomes

$$A_{\rm SPB}=-4\pi Z_P\int d^3p\,\tilde{\phi}_f^*(\vec{p})\frac{1}{\mid\vec{p}-\vec{K}\mid^2}\langle\psi^{(-)}_{\vec{p}+m\vec{v},\epsilon}(\vec{r})\mid e^{i(\vec{p}-\vec{K})\cdot\vec{r}}\mid\phi_i(\vec{r})\rangle\ . \tag{2.11}$$

We have used the momentum conservation equation[10]

$$\vec{K}+\vec{J}+m\vec{v}=0\ , \tag{2.12}$$

which is valid to order m/M_T and m/M_P. Also, we have the relations

$$\vec{v}\cdot\vec{K}=-\tfrac{1}{2}mv^2+(\epsilon_i-\epsilon_f)\ , \tag{2.13}$$

$$K^2+2m\epsilon_i=J^2+2m\epsilon_f\ . \tag{2.14}$$

Equation (2.13) is useful in reducing ϵ to the form

$$\epsilon=\tfrac{1}{2}mv^2+\vec{v}\cdot\vec{p}+\epsilon_f\ . \tag{2.15}$$

Equation (2.11) involves two three-dimensional integrals over momentum and coordinate space. Moreover, the $\vec{r}$ integrand contains the off-energy-shell Coulomb wave $\psi^{(-)}_{\vec{p}+m\vec{v},\epsilon}(\vec{r})$ whose properties and explicit form are not commonly known.

Kelsey and Macek have derived an integral representation for the related function $\chi^{(-)}_{\vec{k},\epsilon}(r)$ defined as[23]

$$\chi^{(-)}_{\vec{k},\epsilon}(\vec{r})\equiv\psi^{(-)}_{\vec{k},\epsilon}(\vec{r})-\phi_{\vec{k}}(\vec{r})\ . \tag{2.16}$$

They were then able to reduce the matrix element involving $\chi^{(-)}_{\vec{p}+m\vec{v},\epsilon}$ in Eq. (2.11) to a one-dimensional in-

tegral. Substituting their expression Eq. (25) into Eq. (2.11), defining $\vec{k}_1 \equiv \vec{p} - \vec{K}$ and noting that now $\vec{k}_2 = \vec{p} + m\vec{v}$, we find

$$A_{SPB} = -4\pi Z_P \int d^3p\, \tilde{\phi}_f^*(\vec{p}) k_1^{-2} \left[\langle \phi_{\vec{k}_2} | e^{i\vec{k}_1 \cdot \vec{r}} | \phi_i \rangle + Z_T \frac{2^4\pi}{(2\pi)^{3/2}} N_i m X [-ie^{i\pi\tau}/(2\sin\pi\tau)] \right.$$

$$\left. \times \frac{\partial}{\partial \mu} \int_C d\rho \rho^{-\tau} [D_1 D_2 - 2(E_1 E_2 + 4X^2 \vec{k}_1 \cdot \vec{k}_2)\rho + D_2 F_1 \rho^2]^{-1} \right], \quad (2.17)$$

where with $\mu_1 = \mu$ and $\mu_2 = 0$,

$$\phi_i(\vec{r}) = N_i e^{-\mu r}, \quad \mu = Z_T, \quad N_i = Z_T^{3/2}/\pi^{1/2}, \quad (2.18)$$

$$X = [-2m(\epsilon + i\eta)]^{1/2}, \quad \mathrm{Re}X > 0 \quad (2.19)$$

$$\tau = mZ_T/X, \quad (2.20)$$

$$D_i = (X + \mu_i)^2 + k_i^2, \quad (2.21)$$

$$E_i = X^2 - \mu_i^2 - k_i^2, \quad (2.22)$$

$$F_1 = (X - \mu)^2 + k_1^2. \quad (2.23)$$

The contour C starts at $1 + i0$, encircles the origin within the unit circle, and ends at $1 - i0$.

Equation (2.17) gives the fundamental result of the SPB theory. We emphasize that the order of the errors involved are m/M_T, m/M_P, and Z_P/Z_T. Equation (2.17) is further simplified by evaluating the ρ integral and by making a peaking approximation to the $\vec{p}$ integral. Both of these simplifications introduce errors of the order of $(Z_P/v)^2$. We now effect the ρ integration; the peaking approximation is carried through in Secs. IV and V.

Using a partial fraction decomposition, we can rewrite the ρ integral as

$$\int_C d\rho \rho^{-\tau} [F_1 D_2 (\rho^2 - 2B\rho + + C)]^{-1} = [2F_1 D_2 (B^2 - C)^{1/2}]^{-1} \int_C d\rho \rho^{-\tau} \left[\frac{1}{\rho - \rho_+} - \frac{1}{\rho - \rho_-} \right], \quad (2.24)$$

with

$$B = (E_1 E_2 + 4X^2 \vec{k}_1 \cdot \vec{k}_2)/F_1 D_2, \quad C = D_1/F_1 \quad (2.25)$$

$$\rho_\pm = B \pm (B^2 - C)^{1/2}. \quad (2.26)$$

Equation (2.24) contains two pole terms at $\rho = \rho_+$ and $\rho = \rho_-$. In consideration of the derivation of the ρ integral by Macek and Kelsey as used in Eq. (2.17), we note that the contour C does not enclose either of these poles. To gain information on their location, observe that D_2 *exactly* equals $p^2 + Z_P^2/n^2$ and that Eqs. (2.19), (2.22), and (2.23) give the order-of-magnitude estimates $|E_1 E_2 + 4X^2 \vec{k}_1 \cdot \vec{k}_2| \approx v^4$ and $|F_1| \approx |D_1| \approx v^2$, provided $p^2 << (mv)^2$ and $p \lesssim Z_P$. We are anticipating a peaking approximation here; nevertheless, when these relations hold we estimate the magnitudes of the moduli to be $|\rho_+| \approx (v/Z_P)^2 >> 1$ and $|\rho_-| \approx (Z_P/v)^2 << 1$.

Since ρ_+ is outside the unit circle, we immediately evaluate the first term in Eq. (2.24) to give

$$\int_C d\rho \rho^{-\tau} \frac{1}{\rho - \rho_+} = \frac{2i \sin\pi\tau}{e^{i\pi\tau}(1-\tau)\rho_+} {}_2F_1(1, 1-\tau; 2-\tau; 1/\rho_+). \quad (2.27)$$

To integrate the second term of Eq. (2.24), form the closed contour Γ by adding the unit circle to the contour C. The contour Γ contains the pole at $\rho = \rho_-$ and thus we can write

$$\int_C d\rho\rho^{-\tau}\frac{1}{\rho-\rho_-}=\int_\Gamma d\rho\rho^{-\tau}\frac{1}{\rho-\rho_-}-\int_{|\rho|=1}d\rho\rho^{-\tau}\frac{1}{\rho-\rho_-}$$
$$=-2\pi i\rho_-^{-\tau}+\frac{2i\sin\pi\tau}{\tau e^{i\pi\tau}}{}_2F_1(1,\tau;1+\tau;\rho_-)\ . \tag{2.28}$$

Substituting Eqs. (2.27) and (2.28) into Eq. (2.24) and then substituting this into Eq. (2.17), we have

$$A_{\rm SPB}=-4\pi Z_P\int d^3p\,\tilde{\phi}_f^*(\vec{\rm p})k_1^{-2}\left[\langle\phi_{\vec{\rm k}_2}|e^{i\vec{\rm k}_i\cdot\vec{\rm r}}|\phi_i\rangle+Z_T\frac{2^4\pi}{(2\pi)^{3/2}}N_imX\frac{\partial}{\partial\mu}[2F_1D_2(B^2-C)^{1/2}]^{-1}\right.$$
$$\times\left[\frac{1}{(1-\tau)\rho_+}{}_2F_1(1,1-\tau;2-\tau;1/\rho_+)\right.$$
$$\left.\left.-\frac{1}{\tau}{}_2F_1(1,\tau;1+\tau;\rho_-)+\frac{e^{i\pi\tau}}{\sin\pi\tau}\pi\rho_-^{-\tau}\right]\right]. \tag{2.29}$$

Additional simplifications of Eq. (2.29) will be made in the peaking approximation of Secs. IV and V. We point out, however, that $\tilde{\phi}_f^*(\vec{\rm p})$ determines the condition $p\lesssim Z_P$ which was needed for estimating $|\rho_+|>>1$ and $|\rho_-|<<1$.

The impulse approximation amplitude is derived from Eq. (2.29) by neglecting the first term within the large parentheses, approximating ${}_2F_1\ (1,\tau;1+\tau;\rho_-)$ by unity, and disregarding a certain multiplicative factor in ρ_- in the pole term. This last factor arises from the off-energy-shell function. Its form and affect on the amplitude is treated in the following sections. There, the pole contribution to the amplitude will be seen to result from the on-energy-shell Coulomb wave and the second term will be derived from a plane wave.

III. OFF-ENERGY-SHELL WAVE FUNCTION

We have seen how the capture amplitude as expressed in Eq. (2.11) involves $\psi^{(-)}_{\vec{\rm k},\epsilon}(\vec{\rm r})$, the off-energy-shell ($\epsilon\neq\frac{1}{2}k^2$) scattering solution of the Coulomb problem with ingoing wave-boundary condition. As previously stated, the IA is derived by approximating $\psi^{(-)}_{\vec{\rm k},\epsilon}$ with the on-energy-shell Coulomb wave $\psi^{(-)}_{\vec{\rm k}}$. Since the limit to the shell is nonuniform, an extra factor representing the branch point in the complex energy plane multiplies $\psi^{(-)}_{\vec{\rm k}}$. The inclusion of this factor is crucial to a proper treatment of the relative errors involved.

We now give a closed-form expression for $\psi^{(-)}_{\vec{\rm k},\epsilon}(\vec{\rm r})$ and then find the correct limiting value. This value has been obtained by Mapleton using a lengthy partial-wave analysis.[17] Because a thorough understanding of the mathematical properties of the off-energy-shell function is necessary to use the SPB theory, we present a shorter and more transparent derivation of Mapleton's result. In particular, the method of derivation implies that in the limit to shell the cancellation (as shown in Sec. IV) of the plane-wave term in Eq. (2.29) by the second ${}_2F_1$ term originates in the structure of $\psi^{(-)}_{\vec{\rm k},\epsilon}$.

The function

$$\chi^{(-)}_{\vec{\rm k},\epsilon}(\vec{\rm r})\equiv\langle\vec{\rm r}|(\epsilon-H_c-i\eta)^{-1}V_{Te}|\phi_{\vec{\rm k}}\rangle$$

satisfies the inhomogeneous equation with $\epsilon\neq\frac{1}{2}k^2$:

$$(H_c-\epsilon+i\eta)\chi^{(-)}_{\vec{\rm k},\epsilon}(\vec{\rm r})=\frac{Z_T}{r}\phi_{\vec{\rm k}}(\vec{\rm r})\ . \tag{3.1}$$

Kelsey and Macek solved Eq. (3.1) finding the closed-form integral representation[23]

$$\chi^{(-)}_{\vec{\rm k},\epsilon}(\vec{\rm r})=\frac{\tau}{(2\pi)^{3/2}}\left[\frac{ie^{i\pi\tau}}{2\sin\pi\tau}\right]\int_C d\rho\rho^{-\tau}\frac{(1-s)(1-t)}{(1-s\rho)(1-t\rho)}$$
$$\times\exp\left[\left[\frac{s\rho}{s\rho-1}-\frac{1}{2}\right]X(r-z)+\left[\frac{t\rho}{t\rho-1}-\frac{1}{2}\right]X(r+z)\right], \tag{3.2}$$

where

$$s=-\frac{X-ik}{X+ik}, \quad t=1/s \ , \tag{3.3}$$

and the z axis is parallel to $\vec{k}$. Here we still have $\mathrm{Re}X>0$ but with X defined according to

$$X=[-2m(\epsilon-i\eta)]^{1/2} \ . \tag{3.4}$$

Note that $+i\eta$ appears in Eq. (2.19) because $\psi^{(-)}_{\vec{k},\epsilon}$ is complex conjugated in Eq. (2.11). The contour C is defined as in Sec. II and any singularities of the integrand must not be inside the contour.

From the definition Eq. (2.8) we have

$$\psi^{(-)}_{\vec{k},\epsilon}(\vec{r})=\phi_{\vec{k}}(\vec{r})+\chi^{(-)}_{\vec{k},\epsilon}(\vec{r}) \ . \tag{3.5}$$

This $\psi^{(-)}_{\vec{k},\epsilon}(\vec{r})$ has a form similar to that for the on-energy shell function $\psi^{(-)}_{\vec{k}}(\vec{r})$ which has the integral representation

$$\psi^{(-)}_{\vec{k}}(\vec{r}) \propto e^{ikz}{}_1F_1[-i\nu,1;-ik(r+z)]$$

$$=\frac{i}{\pi}\sinh\pi\nu\int_{-1}^{+1}du\,(1-u)^{i\nu-\delta}(1+u)^{-i\nu+\delta-1}e^{ik[u(r+z)+(r-z)]/2} \ , \tag{3.6}$$

where δ is a convergence factor and $\nu\equiv Z_T/k$. The on-energy-shell function is a solution of the homogeneous form of Eq. (3.1), viz.,

$$(H_c-\epsilon+i\eta)\psi^{(-)}_{\vec{k}}(\vec{r})=0 \ .$$

Equation (3.6) is used to evaluate a matrix element in the next section. As shown also in the next section, such use represents an alternative to the use of Eq. (3.2) in Eq. (2.11) to give Eq. (2.17).

Rewriting the integral in Eq. (3.2) as

$$I\equiv e^{-Xr}\int_C d\rho\,\rho^{-\tau}\frac{(1-t)(1-s)}{t-s}\left[\frac{1}{\rho-t}-\frac{1}{\rho-s}\right]\exp\{X\rho[(r-z)/(\rho-t)+(r+z)/(\rho-s)]\} \ , \tag{3.7}$$

we see that it has two singularities at $\rho=s$ and $\rho=t$. From Eq. (3.3), we have $|s|\to 0$ and $|t|\to\infty$ as $\epsilon\to\frac{1}{2}k^2$. Therefore, when going to the shell we can write

$$I\approx e^{-Xr}\int_C d\rho\,\rho^{-\tau}\frac{1}{\rho-s}\exp[X\rho(r+z)/(\rho-s)] \ . \tag{3.8}$$

To evaluate this, form the closed contour Γ by adding the unit circle to C:

$$\int_\Gamma d\rho\cdots=\int_C d\rho\cdots+\int_{|\rho|=1}d\rho\cdots \ .$$

The integral on the unit circle is easily found since $|\rho|>>|s|$. The result is

$$\int_{|\rho|=1}d\rho\cdots=-\left[\frac{2\sin\pi\tau}{-ie^{i\pi\tau}}\right]\frac{1}{\tau}e^{X(r+z)} \ . \tag{3.9}$$

We evaluate the integral along Γ by noting that the contour encloses the pole at s. If one expands the exponential in a power series in $X\rho(r+z)/(\rho-s)$ and integrates term by term using Cauchy's integral formula for the nth derivative, one obtains

$$\int_\Gamma d\rho\,\rho^{-\tau}\frac{1}{\rho-s}e^{X\rho(r+z)/(\rho-s)}=-2\pi i s^{-\tau}e^{X(r+z)}{}_1F_1[\tau,1;-X(r+z)], \quad 0\le\arg(s)<2\pi \ . \tag{3.10}$$

On combining Eqs. (3.7)–(3.10), we have the result

$$\chi^{(\mp)}_{\vec{k},\epsilon}(\vec{r})=\frac{\tau}{(2\pi)^{3/2}}\left[\frac{ie^{i\pi\tau}}{2\sin\pi\tau}\right]I$$

$$\approx-\frac{1}{(2\pi)^{3/2}}e^{Xz}-\frac{2\pi i\tau}{(2\pi)^{3/2}}\left[\frac{ie^{i\pi\tau}}{2\sin\pi\tau}\right]s^{-\tau}e^{Xz}{}_1F_1[\tau,1;-X(r+z)]\,, \tag{3.11}$$

for $\epsilon\approx\frac{1}{2}k^2$. From Eq. (3.4), we observe that $X=i\sqrt{2\epsilon}$ and thus

$$\psi^{(\mp)}_{\vec{k},\epsilon}(\vec{r})=\phi_{\vec{k}}(\vec{r})+\chi^{(\mp)}_{\vec{k},\epsilon}(\vec{r})$$

$$\approx\frac{1}{(2\pi)^{3/2}}s^{i\nu}e^{\pi\nu}\frac{\pi\nu}{\sinh\pi\nu}e^{ikz}{}_1F_1[-i\nu,1;-ik(r+z)]\,, \tag{3.12}$$

for $\epsilon\approx\frac{1}{2}k^2$, where we have set $\tau=Z_T/ik\equiv-i\nu$ and $s^{i\nu}$ is equal to

$$s^{i\nu}=\left[\frac{1-2\epsilon/k^2}{4}\right]^{i\nu},\quad 2\epsilon<k^2\,. \tag{3.13}$$

Using the definition of the on-energy-shell function

$$\psi^{(\mp)}_{\vec{k}}(\vec{r})\equiv\frac{1}{(2\pi)^{3/2}}e^{\pi\nu/2}\Gamma(1+i\nu)e^{ikz}{}_1F_1[-i\nu,1;-ik(r+z)]\,, \tag{3.14}$$

we gain the desired relation

$$\psi^{(\mp)}_{\vec{k},\epsilon}(\vec{r})\approx\left[\frac{1-2\epsilon/k^2}{4}\right]^{i\nu}e^{\pi\nu/2}\Gamma(1-i\nu)\psi^{(\mp)}_{\vec{k}}(\vec{r})\,, \tag{3.15}$$

for $\epsilon\approx\frac{1}{2}k^2$, where we have also used $|\Gamma(1+i\nu)|^2=\pi\nu/\sinh\pi\nu$.

Pradhan,[24] and later Mapleton,[17] have previously derived the result Eq. (3.15). Since the derivation presented here works with the full wave function, and not a partial-wave decomposition, it is conceptually more direct. The on-energy-shell Coulomb wave of Eq. (3.15) arises from the pole term in the evaluation of Eq. (3.7) while the unit-circle integration gives rise to a plane wave which cancels the plane-wave term of $\psi^{(\mp)}_{\vec{k},\epsilon}$. Equation (3.15) shows also how the impulse approximation must be modified for Coulomb interactions. Since the branch cut factor is integrated over, and gives a well-defined result, the multiplicative factor must not be arbitrarily dropped as done by Pradhan, Mapleton, and later workers.[25,8,9,32]

The deletion of the multiplicative factor originates with the work of Okubo and Feldman on the scattering of two bare charged particles. They noted that the multiplicative factor $s^{i\nu}e^{\pi\nu/2}\Gamma(1-i\nu)$ of Eq. (3.15) distorts the elastic-scattering T matrix so that the expected Rutherford cross section is not obtained in the correct form. Since the latter must hold the method for obtaining the T matrix must be modified when dealing with the Coulomb problem. Okubo and Feldman renormalized their wave functions such that the asymptotic form was correct. Their procedure is acceptable when the wave functions represent entrance or exit channels. Alternatively, Dettmann showed that a wave-packet treatment[26] of elastic Coulomb scattering with the T matrix incorporating the multiplicative factor of Eq. (3.15) leads to the correct Rutherford cross section. In essence Dettman's analysis shows that for the Coulomb problem the particles always propagate off the shell.

For the problem of interest in this paper, $\psi^{(\mp)}_{\vec{k},\epsilon}$ always enters under a momentum integral, i.e., as an intermediate state. Thus, we are not justified in requiring $\psi^{(\mp)}_{\vec{k},\epsilon}$ to satisfy a particular asymptotic form in coordinate space. The extra factor must also be retained since it represents, in the limit to the shell, the fact that the particle in reality always propagates off shell. Finally, we note that the cross section is altered in a finite way even though $s^{i\nu}$ is undefined at the branch point.

It is our intention in this paper to take special care in delimiting the errors in the approximations made. Since $\vec{r}$ and $\vec{p}$ are arbitrary, it is difficult to keep track of the errors in the derivation leading to Eq. (3.15); in particular, when t is large but not infinite, terms of order $1/t$ are neglected. Because

these occur in an exponential in Eq. (3.2), their contribution to the matrix elements of Eq. (2.11) is not immediately obvious. To analyze the errors, we first carry out the $\vec{r}$ integration using Eq. (2.29) and then go to the shell following a procedure similar to the one used for $\psi^{(-)}_{\vec{k},\epsilon}$. The approach of the matrix element to the shell is made in the next section.

IV. APPROXIMATE EVALUATION OF $A_{\rm SPB}$

Having found the proper limit of $\psi^{(-)}_{\vec{k},\epsilon}(\vec{r})$, we proceed to evaluate the matrix element under the $\vec{p}$ integral in Eq. (2.11). From Eqs. (2.11) and (3.15) and the relations $\vec{k}_1=\vec{p}-\vec{K}$ and $\vec{k}_2=\vec{p}+m\vec{v}$, we have the following integral:

$$\langle\psi^{(-)}_{\vec{k}_2}|e^{i\vec{k}_1\cdot\vec{r}}|\phi_i\rangle=\frac{e^{\pi\nu/2}}{(2\pi)^{3/2}}\Gamma(1-i\nu)N_i\int d^3r\,e^{i\vec{J}\cdot\vec{r}}e^{-\mu r}{}_1F_1[i\nu,1;ik_2(r+z)]\,, \tag{4.1}$$

where $\vec{J}=\vec{k}_1-\vec{k}_2$. Substituting Eq. (3.6) into Eq. (4.1) and performing the $\vec{r}$ integration and some other reductions, we have the result

$$\langle\psi^{(-)}_{\vec{k}_2}|e^{i\vec{k}_1\cdot\vec{r}}|\phi_i\rangle=-\frac{4iN_i}{(2\pi)^{3/2}}e^{\pi\nu/2}\Gamma(1-i\nu)\sinh\pi\nu$$
$$\times\frac{\partial}{\partial\mu}\int_0^1 du\,u^{i\nu+\delta-1}(1-u)^{-i\nu-\delta}[\mu^2+J^2-2(ik_2\mu-\vec{k}_2\cdot\vec{J})u]^{-1}\,, \tag{4.2}$$

where δ is a convergence factor.

If we change variables to $t=u/(1-u)$, Eq. (4.2) becomes

$$\langle\psi^{(-)}_{\vec{k}_2}|e^{i\vec{k}_1\cdot\vec{r}}|\phi_i\rangle=\frac{-4iN_ie^{\pi\nu/2}\Gamma(1-i\nu)\sinh\pi\nu}{(2\pi)^{3/2}(\mu^2+J^2)}$$
$$\times\frac{\partial}{\partial\mu}\int_0^\infty dt\,t^{i\nu+\delta-1}\{1-[1-2(ik_2\mu-\vec{k}_2\cdot\vec{J})/(\mu^2+J^2)]t\}^{-1}\,. \tag{4.3}$$

Equation (4.3) allows us to more easily determine the phase convention on

$$Z\equiv 2(ik_2\mu-\vec{k}_2\cdot\vec{J})/(\mu^2+J^2)\,.$$

The branch cut of $1-Z$ is along the real axis from $Z=1$ to $-\infty$ so that $-\pi<\arg(1-Z)\leq+\pi$. Further reduction of Eq. (4.3) and use of Eq. (3.15) gives the desired matrix element

$$\langle\psi^{(-)}_{\vec{k}_2,\epsilon}|e^{i\vec{k}_1\cdot\vec{r}}|\phi_i\rangle\approx e^{\pi\nu/2}\Gamma(1+i\nu)\left[\frac{1-2\epsilon/k_2^2}{4}\right]^{-i\nu}$$
$$\times\left[-\frac{4\pi N_i}{(2\pi)^{3/2}}e^{\pi\nu/2}\Gamma(1-i\nu)\frac{\partial}{\partial\mu}\frac{(K^2-v^2+\mu^2+2\vec{p}\cdot\vec{J}-2ik_2\mu)^{-i\nu}}{(\mu^2+J^2)^{1-i\nu}}\right], \tag{4.4}$$

for $\epsilon\approx\frac{1}{2}k_2^2$. Note that ν here is defined as Z_T/k_2.

This derivation is straightforward, but as stated before it does not allow us to keep track of the relative errors involved in the approximations used in arriving at it, yet this is exactly what we must do in order to assess the consistency of the whole development. Indeed, the later peaking approximation of Sec. V would be suspect if the errors introduced here were larger. We are led then to derive Eq. (4.4) by other means which permit a clearer estimation of the approximation error.

From Eq. (2.29), we have the quantity under the $\vec{p}$ integral within the large square brackets

$$\langle\psi^{(-)}_{\vec{k},\epsilon}|e^{i\vec{k}_1\cdot\vec{r}}|\phi_i\rangle=\langle\phi_{\vec{k}_2}|e^{i\vec{k}_1\cdot\vec{r}}|\phi_i\rangle+\frac{2^4\pi}{(2\pi)^{3/2}}mN_iZ_TX\frac{\partial}{\partial\mu}[2F_1D_2(B^2-C)^{1/2}]^{-1}$$
$$\times\left[\frac{1}{(1-\tau)\rho_+}{}_2F_1(1,1-\tau;2-\tau;1/\rho_+)-\frac{1}{\tau}{}_2F_1(1,\tau;1+\tau;\rho_-)+\frac{\pi e^{i\pi\tau}}{\sin\pi\tau}\rho_-^{-\tau}\right]. \tag{4.5}$$

Comparison of Eqs. (2.11) and (2.29) implies that Eq. (4.5) equals Eq. (4.4) for $\epsilon \approx \frac{1}{2}k^2$. In order to demonstrate this equality, we first must justify the derivation of Sec. II which led to Eq. (4.5). Since we assume $(Z_P/v)^2 \ll 1$ and because Eq. (4.5) appears within a $\vec{p}$ integral containing $\tilde{\phi}_f^*(\vec{p})$, which implies that the major contribution to $A_{\rm SPB}$ comes from $\vec{p}$ values such that $p \lesssim Z_P$, we have

$$D_1 \approx (\mu - imv)^2 + K^2 + 2\vec{p}\cdot(\vec{J} - i\mu\hat{v}) , \tag{4.6}$$

$$D_2 \approx p^2 + Z_P^2/n^2 , \tag{4.7}$$

$$E_1E_2 + 4X^2\vec{k}_1\cdot\vec{k}_2 \approx 2(\mu^2+J^2)[(mv)^2 + 2m\vec{v}\cdot\vec{p}] , \tag{4.8}$$

$$F_1 \approx (\mu + imv)^2 + K^2 + 2\vec{p}\cdot(\vec{J} + i\mu\hat{v}) , \tag{4.9}$$

$$X \approx -i[(mv)^2 + 2m\vec{v}\cdot\vec{p}]^{1/2} , \tag{4.10}$$

$$\tau \approx Z_T m/X . \tag{4.11}$$

Thus, the conditions under which (4.5) were derived, specifically

$$|C| = \frac{|D_1|}{|F_1|} = 1 + O(Z_P^2/v^2) \quad \text{and} \quad B = \frac{E_1E_2 + 4X^2\vec{k}_1\cdot\vec{k}_2}{F_1D_2} \approx \left[\frac{v}{Z_P}\right]^2 \gg 1 , \tag{4.12}$$

are seen to be satisfied. Moreover, we can approximate $\rho_\pm$ using their definitions Eqs. (2.26) and (4.12). The results are

$$\rho_+ \approx 2B \quad \text{and} \quad \rho_- \approx C/2B . \tag{4.13}$$

Equations (4.6)–(4.13) are used to reduce Eq. (4.5) where we neglect terms of order $(Z_P/v)^2$. The first term in the large parentheses is neglected since it contains the $1/\rho_+$ factor and the second term is approximated by $-1/\tau$. We see that Eq. (4.5) reduces to the form

$$\langle \psi^{(-)}_{\vec{k}_2,\epsilon} | e^{i\vec{k}_1\cdot\vec{r}} | \phi_i \rangle \approx \langle \phi_{\vec{k}_2} | e^{i\vec{k}_1\cdot\vec{r}} | \phi_i \rangle + \frac{2^4\pi}{(2\pi)^{3/2}} mN_iZ_TX \frac{\partial}{\partial\mu}[4(\mu^2+J^2)(m^2v^2+2m\vec{v}\cdot\vec{p})]^{-1}$$
$$\times \left[-\frac{1}{\tau} + \frac{\pi e^{i\pi\tau}}{\sin\pi\tau} e^{-2\pi i\tau} \left[\frac{[(\mu - imv)^2 + K^2 + 2\vec{p}\cdot(\vec{J} - i\mu\hat{v})](p^2 + Z_P^2/n^2)}{4(\mu^2+J^2)(m^2v^2+2m\vec{v}\cdot\vec{p})} \right]^{-\tau} \right] . \tag{4.14}$$

Note that the factor $e^{-2\pi i\tau}$ arises because the phase of ρ_- was defined with the branch cut along the positive real axis whereas Eq. (4.4) was derived taking the branch cut of $1-Z$ along the negative real axis.

The first term of Eq. (4.14) gives the first Born amplitude when substituted into the full amplitude Eq. (2.29). It is readily verified that

$$\langle \phi_{\vec{k}_2} | e^{i\vec{k}_1\cdot\vec{r}} | \phi_i \rangle = -\left[\frac{2}{\pi}\right]^{1/2} N_i \frac{\partial}{\partial\mu}(\mu^2+J^2)^{-1} . \tag{4.15}$$

Comparison of the second term of Eq. (4.14) with Eq. (4.15), employing Eqs. (4.10) and (4.11), shows that they cancel. Therefore, we are left with the result

$$\langle \psi^{(-)}_{\vec{k}_2,\epsilon} | e^{i\vec{k}_1\cdot\vec{r}} | \phi_i \rangle = -\frac{4\pi^2}{(2\pi)^{3/2}} mN_i\tau \left[\frac{e^{i\pi\tau}}{\sin\pi\tau}\right]$$
$$\times \frac{\partial}{\partial\mu}\frac{e^{-2\pi i\tau}}{\mu^2+J^2} \left[\frac{[(\mu - imv)^2 + K^2 + 2\vec{p}\cdot(\vec{J} - i\mu\hat{v})](p^2 + Z_P^2/n^2)}{4(\mu^2+J^2)(m^2v^2+2m\vec{v}\cdot\vec{p})} \right]^{-\tau} . \tag{4.16}$$

Equation (4.16) is equivalent to Eq. (4.4) when terms of order $(Z_P/v)^2$ are neglected.

The approximate amplitude is obtained by substituting Eq. (4.16) back into Eq. (2.29) in the place of the large square bracket quantity. We have

$$A_{\mathrm{SPB}}=-4\pi Z_P\int d^3p\,\tilde{\phi}_f^*(\vec{p})\,|\,\vec{p}-\vec{K}\,|^{-2}\times\left[\frac{4\pi^2}{(2\pi)^{3/2}}mN_i\tau\left[\frac{e^{-i\pi\tau}}{\sin\pi\tau}\right]\times\frac{\partial}{\partial\mu}(\mu^2+J^2)^{-1}\left[\frac{[(\mu-imv)^2+K^2+2\vec{p}\cdot(\vec{J}-i\mu\hat{v})](p^2+Z_p^2/n^2)}{4(\mu^2+J^2)(m^2v^2+2m\vec{v}\cdot\vec{p})}\right]^{-\tau}\right]. \quad (4.17)$$

Recall that τ is defined by Eqs. (4.10) and (4.11). It is to be emphasized that when $(Z_P/v)^2<<1$, Eq. (4.12) provides the conditions justifying the simplification of Eq. (2.11) to (4.17) and $(Z_P/v)^2$ also indicates the order of the errors involved in applying Eq. (4.17).

V. PEAKING APPROXIMATION FOR FINAL s STATES

The amplitude in Eq. (4.17) involves a three-dimensional integral. If we restrict the final electronic states to isotropic ones, i.e., to final s states, Eq. (4.17) can be simplified further. The momentum integral can then be evaluated analytically reducing the amplitude to a closed-form expression.

The simplification is achieved by neglecting all terms linear in $\vec{p}$ in the integrand. This approximation introduces errors of the same order as before, viz., $(Z_P/v)^2$, though apparently it should result in errors of the order Z_P/v. The reason there are no Z_P/v errors is seen on expanding the slowly varying part of the integrand in a Taylor series about $\vec{p}=0$. The slowly varying part is assumed to be everything except $\tilde{\phi}_f^*(\vec{p})(p^2+Z_P^2/n^2)^{-\tau}$. On integrating the linear term of the series, we see it gives no contribution since $\tilde{\phi}_f^*(\vec{p})(p^2+Z_P^2/n^2)^{-\tau}$ is taken as an even function of $\vec{p}$. Thus, the quadratic term is the first to contribute beyond the constant term and is of the order $(Z_P/v)^2$.

Results of Refs. 9 and 31 show that application of the peaking approximation to the IA is not valid for low energies. This means that the matrix element draws large contributions from large $\vec{p}$ where $\epsilon-\frac{1}{2}k^2$ is not necessarily small. Since this energy difference is assumed small in the IA, these results imply that the IA itself is invalid. This raises the question as to the validity of applying the peaking approximation to the SPB theory. To see that it can apply, consider the ratio R of the $\vec{p}$ integrands in the SPB and IA amplitudes. From Eqs. (4.17) and (3.15) we have

$$R\equiv\left[\frac{p^2+Z_P^2/n^2}{v^2+2\vec{p}\cdot\vec{v}}\right]^{-\tau}e^{-i\pi\tau/2}\Gamma(1+\tau)\,,$$

where $\tau=iZ_T/(v^2+2\vec{p}\cdot\vec{v})^{1/2}$. When $\vec{p}\approx-\vec{v}/2$ and $v^2+2\vec{p}\cdot\vec{v}>0$, τ is imaginary and R oscillates rapidly. This rapid oscillation reduces the resulting contributions in the SPB theory. Alternatively, when $\vec{p}\approx-\vec{v}/2$ and $v^2+2\vec{v}\cdot\vec{p}<0$, τ is real and positive and R is of the order

$$|\,R\,|\approx\sqrt{2\pi\tau}e^{-\tau}(p^2\tau/Z_T^2)^{-\tau}\,,$$

which is much less than unity. For other large $\vec{p}$ values, the quantity $|\,R\,|$ is of the order of unity. It follows that the integrand is more strongly peaked in the SPB approximation than in the IA. In this connection, Shakeshaft and Macek[10] have shown that the peaking approximation is valid for the plane-wave second Born amplitude when $Z_P<<Z_T$ and $v>>Z_P$. This supports our observation that the failure of the peaking approximation is peculiar to the IA.

To show that the factor $D_1^{-\tau}$ of Eq. (4.17):

$$D_1^{-\tau}=[K^2+(\mu-iv)^2+2\vec{p}\cdot(\vec{J}-i\mu\hat{v})]^{-\tau}$$

is slowly varying, we rewrite it taking the z axis of $\vec{p}$ along $\vec{v}$ and use $\mu=Z_T$, $K_z=-\frac{1}{2}(v+Z_T^2/v)$, and Eq. (2.12). We have

$$D_1=K^2-2\vec{p}_\perp\cdot\vec{K}_\perp+(Z_T-iv)^2(1+p_z/v)\,.$$

Since the major contribution to the amplitude comes from the region of small $K_\perp$ and $p\lesssim Z_P<<v$, one has $|\,\vec{p}_\perp\cdot\vec{K}_\perp\,|<<K^2$ and $p_z/v<<1$. Our expression for D_1 becomes

$$D_1\approx K^2+(Z_T-iv)^2$$

and the minimum magnitude it attains is $2Z_Tv$. Therefore, we conclude that $D_1^{-\tau}$ can be taken as slowly varying.

Neglecting the linear terms in $\vec{p}$ of Eq. (4.17), our amplitude becomes

$$A_{\mathrm{SPB}}=\frac{16\pi^2}{(2\pi)^{3/2}}\frac{Z_P}{K^2}N_i(4v^2)^{iv}e^{\pi\nu}\,|\,\Gamma(1+iv)\,|^2$$

$$\times\int d^3p\,\tilde{\phi}_f^*(\vec{\mathrm{p}})(Z_P^2/n^2+p^2)^{-iv}\frac{\partial}{\partial\mu}\frac{1}{\mu^2+J^2}\left[\frac{K^2+(\mu-iv)^2}{\mu^2+J^2}\right]^{-iv}. \tag{5.1}$$

Now ν equals Z_T/v.

To evaluate the $\vec{\mathrm{p}}$ integral in Eq. (5.1), substitute[27] $\tilde{\phi}_{ns}(\vec{\mathrm{p}})$ for $\tilde{\phi}_f^*(\vec{\mathrm{p}})$ to give

$$S_n\equiv\int d^3p\,\tilde{\phi}_{ns}(\vec{\mathrm{p}})(Z_P^2/n^2+p^2)^{-iv}$$

$$=\frac{2}{\pi}\left[\frac{2}{n}\right]^{1/2}Z_P^{5/2}\int d^3p\,n^{2+2iv}(n^2p^2+Z_p^2)^{-2-iv}C_{n-1}^1\left[\frac{n^2p^2-Z_P^2}{n^2p^2+Z_P^2}\right], \tag{5.2}$$

where $C_{n-1}^1(x)$ is a Gegenbauer polynomial. If we change variables to $u=Z_P^2/[(np)^2+Z_P^2]$ and use the relation $C_{n-1}^1(1-2u)=n\,{}_2F_1(n+1,-n+1;\frac{3}{2};u)$, Eq. (5.2) becomes[28]

$$S_n=4Z_P^{3/2-2iv}n^{2iv}\left[\frac{2}{n}\right]^{1/2}\int_0^1 du\,u^{-1/2+iv}(1-u)^{1/2}\,{}_2F_1(n+1,-n+1,\tfrac{3}{2};u)$$

$$=4Z_p^{3/2-2iv}n^{2iv}\left[\frac{2}{n}\right]^{1/2}\frac{\Gamma(\frac{1}{2}+iv)\Gamma(\frac{3}{2})}{\Gamma(2+iv)}\,{}_3F_2(n+1,-n+1,\tfrac{1}{2}+iv;\tfrac{3}{2},2+iv;1). \tag{5.3}$$

Using Saalschutz's theorem[29]

$${}_3F_2(\alpha,\beta,-m;\gamma,1+\alpha+\beta-m-\gamma;1)=\frac{(\gamma-\alpha)_m(\gamma-\beta)_m}{(\gamma)_m(\gamma-\alpha-\beta)_m},$$

where $(a)_n\equiv\Gamma(a+n)/\Gamma(a)$, we can reduce Eq. (5.3) to

$$S_n=4Z_P^{3/2-2iv}n^{2iv}\left[\frac{\pi}{2n}\right]^{1/2}\frac{\Gamma(\frac{1}{2}+iv)}{\Gamma(2+iv)}(-1)^{n-1}\frac{(n-1-iv)(n-2-iv)\cdots(1-iv)}{(n+iv)(n-1+iv)\cdots(2+iv)}. \tag{5.4}$$

Since S_n will appear as $|\,S_n\,|^2$ in the cross section, we have from Eq. (5.4),

$$|\,S_n\,|^2=(2Z_P)^3\pi\frac{|\,\Gamma(\frac{1}{2}+iv)\,|^2}{|\,\Gamma(1+iv)\,|^2}\frac{1}{n(n^2+v^2)}. \tag{5.5}$$

The expression for $|A_{\mathrm{SPB}}|^2$ is readily obtained by performing the differentiation in Eq. (5.1), multiplying by the complex conjugated expression and using Eq. (5.5). The total cross section is given by integrating $|A_{\mathrm{SPB}}|^2$ over the transverse momentum transfer $K_\perp$:

$$\sigma_{\mathrm{SPB}}=(2\pi v^2)^{-1}\int_0^\infty |A_{\mathrm{SPB}}|^2K_\perp dK_\perp, \tag{5.6}$$

where $K_\perp$ is defined $K_\perp^2\equiv K^2-K_z^2$. We define the quantity

$$|\,M_n(v)\,|^2\equiv\frac{n^2}{\pi}e^{\pi\nu}\frac{|\,\Gamma(\frac{1}{2}+iv)\,|^2}{(n^2+v^2)}=\frac{2n^2}{(1+e^{-2\pi\nu})(n^2+v^2)} \tag{5.7}$$

and recall $N_i=(Z_T^3/\pi)^{1/2}$ and $|\,N(v)\,|^2=e^{\pi\nu}|\,\Gamma(1+iv)\,|^2$. Then Eq. (5.6) becomes

$$\sigma^n_{\mathrm{SPB}}=\left[\frac{Z_P^5}{Z_T^7}\right]|M_n(v)|^2\frac{1}{n^3}$$
$$\times\left\{2^8\pi v^{12}|N(v)|^2\int_{x_m}^{\infty}dx\left[\frac{1+v^2}{x^6}+\frac{1}{(x-x_0)^2+4v^2}\left[\frac{1+v^3}{x^4}+\frac{2x_0(x-x_0)-8v^2}{x^5}\right]\right]\right.$$
$$\left.\times\exp\left[-2v\tan^{-1}\left[\frac{2v}{x-x_0}\right]\right]\right\}, \tag{5.8}$$

where we have set $x=K^2/v^2$, $x_m=\frac{1}{4}(1+v^2)^2$, and $x_0=1-v^2$.

This cross section for $1s\rightarrow ns$ captures is valid to order $(Z_P/v)^2$. Equation (5.8) is the expression obtained by Briggs with the exception of the factor $|M_n(v)|^2$. Therefore, we can attribute the factor $2n^2/[(1+e^{-2\pi v})(n^2+v^2)]$ to a proper treatment of the approach to the shell. In the next section, we discuss what effects $|M_n(v)|^2$ has on the cross section.

VI. RESULTS AND DISCUSSION

In the cross section given in Eq. (5.8), we have separated three factors. The factor in braces depends only on the ratio v, but not on Z_T and v separately. This factor then presents the cross section σ_{SPB} as proportional to a universal curve which is a function of v. The other factors are the constant Z_P^5/Z_T^7 which provides a scaling of the universal curve dependent on the given projectile and target charges and $|M_n(v)|^2 n^{-3}$ which provides the dependence on the final-state quantum number n.

Recently much work[9,30,31] has been done concerning improvements to the so called "severe peaking" approximations of Sec. V leading to Eq. (5.8). These attempts are based, however, on the impulse approximation which does not take the

TABLE I. Universal capture cross sections in units of (Z_P^5/Z_T^7) a.u. as a function of $v=Z_T/v$ from Eq. (5.8). To obtain the SPB cross section in a.u. for $1s\rightarrow ns$ captures, multiply the table value by $(Z_P^5/Z_T^7)|M_n(v)|^2 n^{-3}$. The number in parentheses is the power of ten multiplying the corresponding table entry.

v (a.u.)	σ $[(Z_P^5/Z_T^7)$ a.u.]	$\log_{10}(\sigma)$	v (a.u.)	σ $[(Z_P^5/Z_T^7)$ a.u.]	$\log_{10}(\sigma)$
0.01	1.729 90(−19)	−18.762 0	0.90	67.9323	1.832 08
0.05	1.597 64(−11)	−10.796 5	0.95	88.1022	1.944 99
0.10	4.556 70(−8)	−7.341 35	1.00	110.478	2.043 28
0.15	4.525 95(−6)	−5.344 29	1.20	209.923	2.322 06
0.20	1.108 86(−4)	−3.955 12	1.40	296.492	2.472 01
0.25	0.001 245 33	−2.904 72	1.60	346.933	2.540 25
0.30	0.008 465 17	−2.072 36	1.80	358.989	2.555 08
0.35	0.040 438 2	−1.393 21	2.00	342.121	2.534 18
0.40	0.148 546	−0.828 138	2.20	308.268	2.488 93
0.45	0.445 061	−0.351 580	2.40	267.237	2.426 90
0.50	1.133 02	0.054 237 5	2.60	225.553	2.353 25
0.55	2.525 01	0.402 263	2.80	186.892	2.271 59
0.60	5.038 29	0.702 283	3.00	152.932	2.184 50
0.65	9.160 51	0.961 920	3.20	124.117	2.093 83
0.70	15.390 2	1.187 24	3.40	100.220	2.000 95
0.75	24.165 0	1.383 19	3.60	70.7008	1.906 88
0.80	35.793 6	1.553 81	3.80	64.9162	1.812 35
0.85	50.406 6	1.702 49	4.00	52.2329	1.171 94

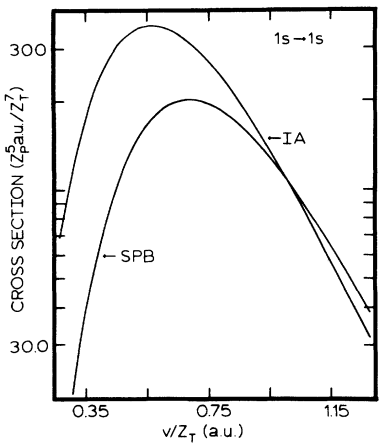

FIG. 2. Universal curve for $1s \rightarrow 1s$ capture from Eq. (5.8).

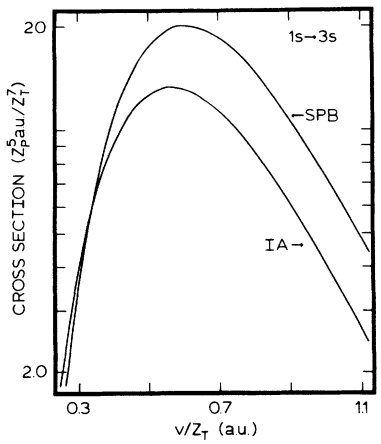

FIG. 3. Universal curve for $1s \rightarrow 3s$ capture from Eq. (5.8).

proper limit to shell. We have seen that a correct treatment in the severe peaking case results in a factor $|M_n(v)|^2$. Clearly then, neglect of this term leads to an error of order $(Z_T/v)^2$. Moreover, since the *origin* of this term, in general, is independent of the peaking approximation, although the specific form here is dependent on it, we can expect this error to persist. That is, one cannot validly go beyond the severe-peaking approximation without first incorporating the off-shell factor. Indeed, the basic result of Briggs contains errors of order v^2, which will be large for $v \lesssim Z_T$.

From the foregoing considerations, we think it useful to present the universal curve, except for $|M_n(v)|^2$, in tabular form. Table I lists these values in the range $v=0.01$ to 4.0. For ease of reference we also list the base 10 logarithms of these values. The numbers in the table were obtained from Eq. (5.8) after numerical integration of the integral. The code was checked against an explicit analytic evaluation $v=1$, where the integrand simplifies considerably, and against the asymptotic formula Eq. (6.1). One can easily calculate the cross section in a.u. for the desired charge states by multiplying the table value by $(Z_P^5/Z_T^7)|M_n(v)|^2 n^{-3}$.

A. Effects of the off-shell factor

Consider the effects of $|M_n(v)|^2$ on the capture cross sections. First note its effect when multiplying the n-independent universal curve. In the limit $v \rightarrow 0$, $|M_n(v)|^2 \approx (1+\pi v) > 1$. Then, when $v \approx n$ we have $|M_n(v)|^2 \approx 1$ and for $v > n$ the factor $n^2/(n^2+v^2)$ dominates giving $|M_n(v)|^2 < 1$. For v very large, the factor $(Z_P/v)^2$ is not small and the theory is invalid, thus $|M_n(v)|^2$ passes through unity in the range of validity only for the smallest n values. For these n values, $|M_n(v)|^2$ enhances the capture cross section when $0 < v \lesssim n$ and reduces it when $n \lesssim v$. The effect is clearly shown in Figs. 2 and 3 for $n=1$ and 3, respectively. For higher n values, $|M_n(v)|^2$ always increases the cross section in the allowed range of v.

The off-shell factor also influences the excited-state capture probability. The total cross section for capture into excited s states, which is defined as

$$\sigma^{n>1} = \sum_{n>1} \sigma^n \ ,$$

is given in the IA by

$$\sigma_{\mathrm{IA}}^{n>1} \approx 0.202 \sigma_{\mathrm{IA}}^{1} \ ,$$

while for SPB one has

$$\sigma_{\mathrm{SPB}}^{n>1} = F(v) \sigma_{\mathrm{SPB}}^{1}$$

with $F=0.204$, 0.242, 0.344, and 0.615 for $v=0.1$, 0.5, 1.0, and 2.0, respectively. For the IA, about 17% of the s-state capture is into excited states. In the SPB this percentage increases as v increases. It is 17%, 19%, 26%, and 38% for $v=0.1$, 0.5, 1.0, and 2.0, respectively. This behavior is in accord with the qualitative idea that as the velocity decreases the interaction time increases allowing the final excited states to play a more important role in the exchange process.

The effects of the off-shell factor have been treated previously in the calculations of Macek and Shakeshaft.[10] Their method implicitly included this factor without the explicit factorization

TABLE II. Comparison of the cross sections σ_{2c} of Macek and Shakeshaft from Ref. 10 with the SPB cross sections derived from Eq. (5.8). The charge scaling of the SPB results is evidently not present in the σ_{2c} values.

Z_T	E_{lab} (MeV)	Z_T/v (a.u.)	σ_{2c} (a.u.)	σ_{SPB} (a.u.)
20	2.5	2.003	130	136.3
20	5.0	1.419	210	201.1
10	2.5	1.005	110	111.9
20	10.0	1.005	92	111.9
10	5.0	0.7097	26	22.20
10	10.0	0.5038	2.0	1.850

achieved in this paper and in Macek and Taulbjerg.[11] The calculations made use of a peaking approximation similar to that employed here though part of the term

$$ {}_2F_1(1,1-\tau;2-\tau;1/\rho_+)/[\rho_+(1-\tau)] $$

in Eq. (2.29) was retained. This term was neglected in the present work. Table II shows a comparison of the $1s\rightarrow 1s$ capture cross sections of Macek and Shakeshaft with those derived from Eq. (5.8). The differences between the two sets of values are everywhere less than 20%; however, the lack of charge scaling in the earlier results is apparent in the two cross sections for $v=1.005$. This lack of scaling is consistent with keeping the ${}_2F_1$ term which destroys the dependence of the cross section on v only.

B. Asymptotic form of the capture cross section

In the limit $v\rightarrow 0$, that is for large velocities, the IA cross section σ_{IA} (we drop the superscript on σ here) for $1s\rightarrow 1s$ capture takes the form (in a.u.)

$$ \sigma_{\text{IA}}=\sigma_{\text{BK}}(0.295+5\pi v/2^{11}Z_T)\ , \tag{6.1} $$

where $\sigma_{\text{BK}}=2^{18}\pi Z_P^5 Z_T^5/(5v^{12})$ is the asymptotic Brinkman-Kramers cross section. The coefficient of the v^{-11} term in Eq. (6.1) differs by a factor of 2 from the coefficient of the v^{-11} term of the second Born approximation. Briggs has shown that this discrepancy is not inherent to the IA but is due to the peaking approximation.[8,32] Thus, the above asymptotic form Eq. (6.1) is strictly valid only for highly asymmetric captures.

In all previous derivations of Eq. (6.1), an approximation has been made that is not justified. Considering Eq. (5.8) except for $|M_1(v)|^2$, the incorrect derivation goes as follows: In the limit $v\rightarrow 0$ both $|N(v)|^2$ and the exponential term tend to unity. Setting them equal to one and using

$$ v/[(x-x_0)^2+4v^2]\rightarrow\frac{\pi}{2}\delta(x-1)\ , $$

the second term of $v\sigma_{\text{IA}}$ results in σ_{IA} $\rightarrow 2^7\pi^2 Z_P^5 Z_T^4/v^{11}$ and the v^{-12} term is gained from a straightforward evaluation of the integral as $v\rightarrow 0$. In effect, one writes

$$ \sigma_{\text{IA}}\propto\int_{x_m}^{\infty}dx\left[\frac{1+v^2}{x^6}+\frac{1}{(x-x_0)^2+4v^2}\left[\frac{1+v^2}{x^4}+\frac{2x_0(x-x_0)-8v^2}{x^5}\right]\right]=C_{-1}v^{-1}+C_0+C_1v+\cdots $$

with C_{-1}, C_0, etc., constants. One assumes that on retaining $|N(v)|^2 e^{-2v\tan^{-1}[2v/(x-x_0)]}$ only the coefficients C_n, $n>0$, are modified. But since the expansion has a $1/v$ term, $|N(v)|^2=1+\pi v+O(v^2)$, and the v dependence of the exponential factor is not clear, this assumption is not readily apparent.

To justify the derivation and to clarify the relative errors, consider the integral $L(v)$:

$$ \begin{aligned} L(v)&\equiv\int_{x_m}^{\infty}dx\,x^{-n}[(x-x_0)^2+4v^2]^{-1}e^{-2v\tan^{-1}[2v/(x-x_0)]}\\ &=\int_{x_m}^{\infty}dx\,x^{-n}(x-x_0+2iv)^{+iv-1}(x-x_0-2iv)^{-iv-1}\ , \end{aligned} $$

where the second form is true by definition. The integrand has two branch points at $x=x_0\pm 2i\nu$ and a pole at $x=0$ in the complex x plane. To evaluate $L(\nu)$, we close the contour in the upper half plane by adding the contour $\gamma=\{x=x_m+iy:0\le y<\infty\}$ and by going around the branch cut taken from $x_0+2i\nu$ to $x_0+i\infty$ as shown in Fig. 4. We can write $L(\nu)=J(\nu)+K(\nu)$ where

$$J(\nu)=-\int_{\text{branch cut}} dx\cdots$$

and

$$K(\nu)=-\int_{\gamma} dx\cdots .$$

The integration along the other parts of the closed contour gives zero contribution.

The branch point and thus the integration around the cut arises from the exponential factor and does not exist if the latter is set equal to one, instead, one has a pole contribution at $x=x_0+2i\nu$. When setting $|N(\nu)|^2=1$ and $e^{-2\nu\tan^{-1}[2\nu/(x-x_0)]}=1$, one assumes that $|N(\nu)|^2$ cancels the contribution from the branch cut. Actually, one has[28]

$$J(\nu)=-i[\pi/2\,|N(\nu)|^2(x_0+2i\nu)^n]\times\frac{\Gamma(-i\nu)\Gamma(n+1)}{\Gamma(n+1-i\nu)}{}_2F_1[n,-i\nu;n+1-i\nu;(x_0-2i\nu)/(x_0+2i\nu)] .$$

Since the pole contribution is $2\pi i(x_0+2i\nu)^{-n}(4i\nu)^{-1}$, we get equality because[33]

$$\frac{\Gamma(-i\nu)\Gamma(n+1)}{\Gamma(n+1-i\nu)}{}_2F_1[n,-i\nu;n+1-i\nu;(x_0-2i\nu)/(x_0+2i\nu)]=\frac{i}{\nu}+O(\nu) .$$

As the integrand of $K(\nu)$ is analytic everywhere along γ, we immediately deduce that the leading term of $K(\nu)$ is a constant independent of ν [$K(\nu)$ and $J(\nu)$ have imaginary constant terms of equal magnitude but opposite sign so that $L(\nu)$ is real as it must be]. The x^{-6} term of σ_{IA} can be integrated by parts with the integrated part giving σ_{BK}; the remaining integral is of the form $\nu^2 L(\nu)$ and does not contribute to order less than ν^2. $K(\nu)$ provides the modification of the σ_{BK} coefficient from 1 to 0.295. The above observations validate the derivation of Eq. (6.1).

Now we consider the effect of $|M_n(\nu)|^2$ on Eq. (6.1). The asymptotic form for $1s\rightarrow 1s$ capture in the SPB is derived from $\sigma_{\text{SPB}}=|M_1(\nu)|^2\sigma_{\text{IA}}$,

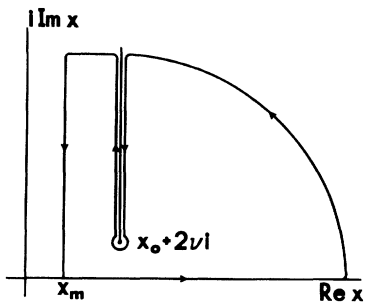

FIG. 4. Integration contour used in justifying the derivation of the asymptotic form for the capture cross section Eq. (6.1).

which on approximating $|M_1(\nu)^2\approx 1+\pi\nu$ and using Eq. (6.1), becomes

$$\sigma_{\text{SPB}}=\sigma_{\text{BK}}(0.319+5\pi\nu/2^{11}Z_T) . \tag{6.2}$$

Here we have a constant change in the v^{-12} term of about 8%. This is apparently rather small considering that the v^{-11} term remains unchanged. But for large v, $(Z_P/v)^2<<0.08$ and we conclude that this 8% change is meaningful and greater than the error limitations of the SPB approximation. The nonuniform approach to the energy shell of $\psi^{(-)}_{\vec{k},\epsilon}$ has affected even the large velocity behavior of the cross section. This difference of asymptotic forms between the second Born theory (free Green's function) and the SPB theory (Coulomb Green's function) implies that third-order effects of one theory are needed to gain equality with the other. Shakeshaft has considered the problem of third Born contributions to the asymptotic cross section.[34] If we use his cross section Eq. (4.21) which contains contributions from the first three Born terms, keeping in mind that for asymmetric processes terms of the order Z_P/Z_T can be neglected, we arrive at exactly Eq. (6.2). But Eq. (6.2) does not contain contributions from the third Born term $V_{Te}G_0^+V_{Pe}G_0^+V_{Pe}$ which are of higher order than the SPB theory. Here G_0^+ is the free Green's function.

C. Application to inner-shell capture

We have thus far considered only capture from a hydrogenlike atom. To apply the theory to inner-shell capture, we need to introduce a more realistic atomic model. We want to incorporate this model into the present framework and Eq. (5.8), in particular, without major modification. Several restrictions on the model allow this to be done. (1) Take the captured inner-shell electron's motion as independent of the other electrons. (2) Represent the electron's wave function by an unmodified hydrogen wave function of effective charge Z_S. (3) Use the experimental binding energy ϵ_B for the initial bound state.

Restriction (1) is the approximation of considering a single active electron in the process. For the initial state, the use of this independent-particle model is justified by the wide separation of binding energies for the inner subshell electrons.[35] And since the exit velocity of the active electrons in the final state is large, the "core" of inactive electrons can be taken as frozen in the initial configuration. Thus, we take the active electron as moving in a potential of the Hartree-Fock type, e.g., a Hartree-Fock-Slater (HFS) potential for the K shell.[36]

The complete inclusion of this HFS potential $V_{\rm HFS}$ within the present framework would be quite difficult to execute. However, following the lead of previous calculations on ionization,[37,38] we represent $V_{\rm HFS}$ by a scaled hydrogenic potential V_S which is shifted by a constant amount V_0:

$$V_{\rm HFS} \approx V_S \equiv -\frac{Z_S}{r} + V_0 \ .$$

The value of Z_S is obtained following Slater's empirically derived rules, viz., Z_S equals $Z_T - 0.3$. Preferably, the experimental binding energy ϵ_B should agree with the ground-state energy of V_S. This condition gives V_0 equal to $\epsilon_B + \frac{1}{2}Z_S^2$. For large radial distances, V_S is not a good representation of $V_{\rm HFS}$. Because $\phi_i(\vec{r})$ appears in the coordinate integral of Eq. (2.11), which implies that the major contribution to the capture amplitude comes from radial distances of the order of $1/Z_S$ or less, this deficiency is not a major flaw. Comparison of $V_{\rm HFS}$ and V_S in the inner region shows good agreement, in fact, at $r = 1/Z_S$ the fractional error between V_S and $V_{\rm HFS}$ for the K shell is 0.019 for carbon, 0.022 for neon, and 0.015 for argon.

The effects of the inclusion of V_0 in V_S needs some discussion. V_0 arises from the outer screening of the core in contrast to the 0.3 of Z_S which arises from inner screening. The undesirable consequence of V_0 is a shifting upward of the continuum threshold of V_S with respect to $V_{\rm HFS}$.[37,38] Thus, the lower-energy continuum states of $V_{\rm HFS}$ are represented by bound states of V_S. This bound-state modeling in effect would not even allow electronic escape. But here once again, only the large-r region is a problem; the wave functions of V_S must necessarily be of similar form to the wave functions of $V_{\rm HFS}$ for $r \lesssim 1/Z_S$, since the two potentials agree well in this region. Moreover, for the captures considered here the final electronic energy is relatively high in the continuum away from the threshold as shown schematically in Fig. 1. We conclude that restriction (2) does not seriously limit the theory and is well justified for our process. Note that the picture of capture as a momentum weighting of ionization is fundamental to the above discussion.

Since we have incorporated ϵ_B into V_S, we must also alter our kinematic relations. In particular, we replace Eqs. (2.13) and (2.14) by

$$\vec{v}\cdot\vec{K} = -\tfrac{1}{2}mv^2 + \epsilon_B - \epsilon_f \ , \tag{6.3}$$

$$K^2 + 2m\epsilon_B = J^2 + 2m\epsilon_f \ . \tag{6.4}$$

The amplitude squared appearing in the cross section Eq. (5.8) is steeply peaked near the minimum value x_m, thus, the correct minimum momentum transfer is critical for a proper treatment. Using Eq. (6.3) we get x_m equal to $(1-2\epsilon_B/v^2)^2/4$. Equation (6.4) is used to substitute for J^2 in Eq. (5.1) after the μ differentiation. Following the derivation of Sec. V with the above modifications and replacing Z_T with Z_S, we arrive at the $1s \rightarrow ns$ SPB peaking approximation for inner-shell capture. Formula (5.8) becomes

$$\sigma_{\rm SPB} = \frac{Z_P^5}{Z_S^7} 2^9 \pi v^{12} |N(v)|^2 |M_n(v)|^2 \frac{1}{n^3} \times \int_{x_m}^{\infty} dx \left[\frac{1+v^2}{(x+x_1)^4} + \frac{1}{(x-x_0)^2+4v^2} \left[\frac{1+v^2}{(x+x_1)^2} + \frac{2x_0(x-x_0)-8v^2}{(x+x_1)^3} \right] \right] \frac{1}{x^2} \times e^{-2v\tan^{-1}[2v/(x-x_0)]} \ , \tag{6.5}$$

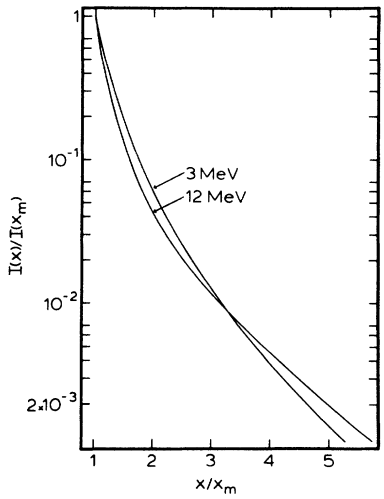

FIG. 5. Plot of the integrand of Eq. (6.5) for argon for two impact energies.

where $x_1=v^2+2\epsilon_B/v^2$ and v is given by Z_S/v. The extra factor of 2 arises because there are two K-shell electrons. The only alteration in the basic form of Eq. (5.8) as seen in Eq. (6.5) is the appearance of x_1. Because it is in the denominator, its presence acts to reduce the cross section. On the other hand, the lower limit of integration is smaller. This, coupled with the steep peaking of the integrand near the lower limit acts to overcome the reduction due x_1. The net effect of these two changes is to increase the value of the integral in Eq. (6.5) as compared to that in Eq. (5.8). Also, since Z_S is less than Z_T the multiplicative factors in Eq. (6.5) produce an additional increase in the cross section.

We use Eq. (6.5) to calculate the $1s\rightarrow 1s$ capture cross sections for protons on carbon, neon, and argon. For the K-shell binding energies ϵ_B, we use

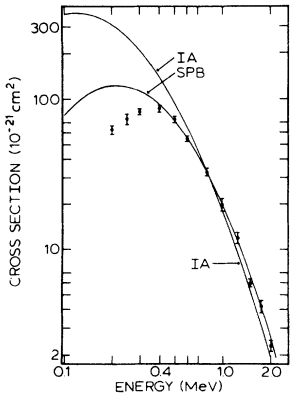

FIG. 6. SPB and IA cross sections for K-shell capture from carbon by protons. Data are from Rødbro *et al.* (Ref. 40).

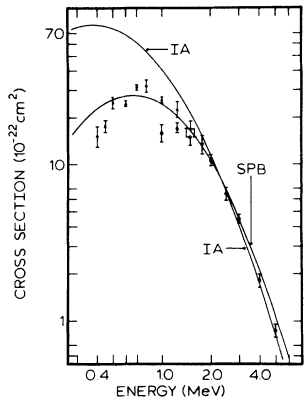

FIG. 7. SPB and IA cross sections for K-shell capture from neon by protons. Data are ●, Cocke *et al.* (Ref. 41); ▲, Rødbro *et al.* (Ref. 40).

the values taken from the compilation of Krause[39]: 288 eV for carbon; 870.2 eV for neon; and 3206.0 eV for argon. We checked the numerical evaluation of Eq. (6.5) against that used for Eq. (5.8) when $Z_S=Z_T$ and $\epsilon_B=-\frac{1}{2}Z_T^2$ in the former. Figure 5 shows a plot of the integrand of Eq. (6.5) for argon for v values of 0.8 and 1.6. These values correspond roughly to incident proton energies of 12 and 3 MeV. The lower energy is near the peak in the capture cross section and here the integrand is not as steeply peaked. This is in accord with the decreasing dominance in the capture amplitude of the "longitudinal" momentum transfer for lower velocities. From the smoothness of the integrand shown in Fig. 5, we are assured that numerical errors in the calculations are completely negligible.

In Figs. 6–8 we present the capture cross sections for protons on carbon, neon, and argon. The SPB theory is compared with the IA theory and with the experimental data.[40–43] It is seen that the

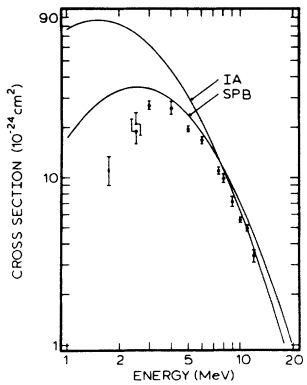

FIG. 8. SPB and IA cross sections for K-shell capture from argon by protons. Data are ●, Macdonald *et al.* (Ref. 42); ▲, Andriamonje *et al.* (Ref. 43).

SPB cross sections follow the data more consistently than do the IA ones up until the peak. For carbon, the agreement is quite good up to the peak, though the agreement is qualified somewhat since the carbon data were taken with CH_4 as the target. In neon, the scatter in the data around the peak makes comparison difficult, yet clearly the SPB curve follows the trend of the data better. The SPB curve for argon is roughly 5–10% above the data, but again the trend of the data is followed more closely.

In the energy range below the peak in the cross section, both the SPB and IA curves diverge considerably from the data. However, the SPB curve is much reduced compared to the IA one. In carbon the SPB peak is less than a factor of 2 too large whereas the IA peak is five times too large. Also, the calculated peak locations for SPB theory are closer to that of the data. For carbon again, the SPB peak is a factor of 2 too low while the IA peak is a factor of 3 too low.

Kocbach has also performed peaking approximation calculations under similar conditions to those used here.[31] He used the IA theory in the impact-parameter formalism. From his Eq. (3) we have the capture amplitude as

$$A_{\mathrm{IA}}(\vec{b},v)=\int d^3p\,\tilde{\phi}_f^*(\vec{p})e^{i\vec{p}\cdot\vec{b}}f(\vec{p},\vec{v},\vec{b})\ . \tag{6.6}$$

The peaking approximation is obtained from Eq. (6.6) by writing

$$e^{i\vec{p}\cdot\vec{b}}f(\vec{p},\vec{v},\vec{b})\approx f(0,\vec{v},\vec{b})$$

so one has

$$A_{\mathrm{IA}}^{P1}(\vec{b},v)=(2\pi)^{3/2}\tilde{\phi}_f(0)f(0,\vec{v},\vec{b})\ . \tag{6.7}$$

A less restrictive approximation used by Kocbach is

$$e^{i\vec{p}\cdot\vec{b}}f(\vec{p},\vec{v},\vec{b})\approx e^{i\vec{p}\cdot\vec{b}}f(0,\vec{v},\vec{b})$$

which gives

$$A_{\mathrm{IA}}^{P2}=(2\pi)^{3/2}\tilde{\phi}_f^*(\vec{b})f(0,\vec{b},\vec{v})\ . \tag{6.8}$$

The corresponding approximation in the wave treatment[44] sets $\vec{k}_2\approx m\vec{v}$ but retains $\vec{k}_1=\vec{p}-\vec{K}$ so that $\vec{J}$ in Eq. (4.1) is replaced by $\vec{J}+\vec{p}$. But since $\vec{J}=\vec{k}_1-\vec{k}_2$ is an exact result, retaining $\vec{p}$ is not justified and A_{IA}^{P2} is a worse approximation than A_{IA}^{P1}.

D. Symmetric capture

For $1s\rightarrow 1s$ capture in the forward direction by protons from hydrogen, it is well known that the second Born approximation to the cross section decreases more slowly than the BK approximation in the limit of large velocities. This behavior is true even for the second Born theory without inclusion of the internuclear potential, here called BK2. The BK2 cross section stays above the BK one as the velocity decreases down to as low as 2 a.u. But at the lower velocities the BK cross section generally gives an overestimate for the capture probability.[45] Miraglia *et al.*[46] have given exact values for the total cross section for the BK and BK2 theories. They find that for an incident energy of 1.0 MeV, where $v=6.3$ a.u., the total cross sections are 3.52×10^{-17} and 1.40×10^{-16} cm^2 for BK and BK2, respectively. For 0.1 MeV, where $v=2$ a.u., their values are 7.04×10^{-22} and 1.22×10^{-21} cm^2. This unrealistic increase of the BK2 cross section over the BK cross section can be ascribed to the use of plane waves for continuum target states in the BK2 theory and to the absence of a discrete target spectrum.

Macek and Shakeshaft[18] have noted that the use of the Coulomb Green's function substantially alters the situation. This is to be expected since the Coulomb Green's function provides a correct treatment of the target spectrum. At asymptotic velocities the SPB approximation to the capture cross section also decreases more slowly than the BK one.[8,32] Contrary to the behavior of the BK2 theory, though, the SPB cross section becomes

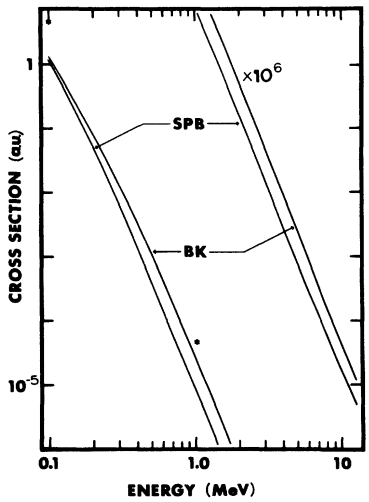

FIG. 9. Comparison of the BK, BK2, and SPB cross sections for capture from hydrogen by protons. BK2 denotes the second Born theory without inclusion of the internuclear potential. The BK2 values, the *'s, are from Ref. 46. For the BK curve, Ref. 45 was used. The SPB curve is derived from Eq. (5.8) with $Z_P=Z_T=1$.

smaller than the BK one. Figure 9 clearly verifies this behavior down to 0.1 MeV. Moreover, note that at the lower velocities, where the validity of the peaking approximation is questionable, a more accurate treatment of the SPB amplitude Eq. (4.17) may tend to pull the cross section down further. Figure 9 thus gives a clear indication of the results of incorporating a more accurate treatment of the target spectrum.

ACKNOWLEDGMENT

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