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# Distorted wave Born approximation for inelastic collisions: Application to electron capture by positrons from hydrogen atoms

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# Distorted-wave Born approximation for inelastic collisions: Application to electron capture by positrons from hydrogen atoms

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We have re-examined the distorted-wave Born approximation for inelastic collisions. We find that the distortion in the relative motion of the collision partners cannot be neglected even for high-energy ion-atom collisions. Furthermore, if the distortion in the relative motion is not treated exactly, post-prior discrepancies will occur. We have applied the distorted-wave Born approximation, with distortion included through first order, to ground-state-to-ground-state electron capture by positrons from hydrogen atoms. The results are presented in this paper. We have also examined the nonrelativistic asymptotic behavior of the cross section for electron capture from hydrogen by positrons incident with a speed $v \sim \infty$. We find that, for $e^2/\hbar v \ll 1$, capture occurs primarily to states of positronium that have an odd orbital-angular-momentum quantum number. It follows that the cusp signifying charge transfer to the continuum will, for positron impact, be symmetric when $e^2/\hbar v \ll 1$.

## I. INTRODUCTION

Let $M_P$ be the mass of a projectile P impinging on a one-electron ion or atom $(e+T)$, where $e$ is the electron of mass $m$ and T is the target nucleus of mass $M_T$. Neglecting a correction of order $m/M_T$, the interaction $V_{PT}$ between P and T depends only on the coordinate connecting P to the center of mass of the atom $(e+T)$. To this extent, therefore, $V_{PT}$ alone cannot induce a transition in the internal state of the atom. In other words, if the primary interaction $V_{Pe}$—the interaction between P and $e$—were turned off, the internal state of the target atom would remain essentially unchanged throughout the collision. $V_{PT}$ does indirectly influence the probability of a transition since the effect of $V_{Pe}$ depends on the trajectory of P and $V_{PT}$ influences this trajectory. If $m/M_P \ll 1$, however, P is (for all but very low projectile velocities) barely scattered and $V_{PT}$ plays almost no role. In this case it follows that in the calculation of the transition cross section, *integrated* over all scattering angles, the inclusion of $V_{PT}$ introduces only small corrections of orders $m/M_T$ and $m/M_P$. This well-known result[1] is sometimes thought to imply that in the Born expansion of the fully quantum-mechanical scattering amplitude, those Born terms involving $V_{PT}$ should sum to zero, or rather to a small quantity of the order of the larger of $m/M_T$ and $m/M_P$. In general this is incorrect, but for electron capture at high projectile velocities the first- and second-order Born terms involving $V_{PT}$ do very nearly cancel[2] if $m/M_T$, and $m/M_P \ll 1$. The reason for this peculiar cancellation is given in Appendix A.

For electron *capture* by *ions* the first Born matrix element of $V_{PT}$ gives a spuriously large contribution to the integrated cross section, and higher Born terms must be added to ensure a net contribution from $V_{PT}$ of the order of the larger of $m/M_T$ and $m/M_P$. As first recognized by Bassel and Gerjuoy,[3] this can be achieved by using the distorted-wave Born approximation. They chose the distortion potential in the initial channel to be the average, with respect to the initial internal state of $(e+T)$, of the actual perturbation in the initial channel. Analogously, the final channel distortion potential was chosen to be the average, with respect to the final internal state of $(e+P)$, of the final channel perturbation. Then $V_{PT}$ almost disappears from the effective perturbation, which is the difference of the actual perturbation and the distortion potential. However, in their numerical calculation of the scattering amplitude for $p + H(1s) \rightarrow H(1s) + p$ Bassel and Gerjuoy neglected the distortion of the relative motion of the collision partners, approximating the distorted waves by plane waves. Later Grant and Shapiro[4] included the corrections to the plane-wave relative motion through first order in the distortion potentials. They should have obtained (but did not) essentially the same numerical results as Bassel and Gerjuoy, for, as we show below, if a reaction is symmetric and if $m \ll M_P$, and $m \ll M_T$, as in $p + H(1s) \rightarrow H(1s) + p$, the net effect of including the first-order corrections to the plane-wave relative motion in both the initial and final channels is zero. In general, however, the net effect of including these first-order corrections is nonzero. Furthermore, the distortion in the relative motion of the collision partners must be treated exactly if post-prior discrepancies are to be avoided.

Note that the distortion potentials need not be of the Bassel-Gerjuoy form. Indeed, Geltman,[5]

 

Kleber and Nagarajan,[6] and Halpern[7] have taken the distortion potentials to be pure Coulomb potentials in their application of the distorted-wave Born approximation to electron capture by ions. This has the advantage that the distorted waves are readily calculated, being simply the known Coulomb wave functions.

We have applied the distorted-wave Born approximation to electron capture by a positron from a hydrogen atom. We used the Bassel-Gerjuoy form of the distortion potentials and included these potentials consistently through first order. The results are presented below. Note that since, in our application, $m/M_T = \frac{1}{1836} \ll 1$, $V_{PT}$ alone cannot induce transitions—its role is to scatter P and thereby modify the effect of $V_{Pe}$. This modification is substantial since, with $m/M_P = 1$, P undergoes appreciable scattering.

In Sec. II we introduce some notation. In Sec. III we outline the distorted-wave Born approximation, with distortion included consistently through first order. We do this for an arbitrary inelastic collision, but our application is to ground-state-to-ground-state electron capture from hydrogen by positrons. In Sec. IV we present some results. We also comment in Sec. V on the asymptotic behavior of the cross section for electron capture from hydrogen by positrons incident with a very high speed.

## II. SOME NOTATION

As stated above, the masses of the electron $e$, target nucleus T, and projectile P are denoted by $m$, $M_T$, and $M_P$. We define the mass ratios

$$\alpha \equiv M_T/(m+M_T), \quad \beta \equiv M_P/(m+M_P), \tag{2.1}$$

and the reduced masses

$$\mu_T = \alpha m, \quad \mu_P = \beta m, \tag{2.2a}$$

$$\nu_i = M_P(m+M_T)/(m+M_T+M_P), \tag{2.2b}$$

$$\nu_f = M_T(m+M_P)/(m+M_T+M_P). \tag{2.2c}$$

Let $\vec{r}_T$ and $\vec{r}_P$ be the coordinates of the electron relative to T and to P, respectively. Let $\vec{R}_T$ be the coordinate of P relative to the center of mass of $(e+T)$ and let $-\vec{R}_P$ be the coordinate of T relative to the center of mass of $(e+P)$. Let $\vec{R}$ be the coordinate of P relative to T. The coordinate system is shown in Fig. 1. We have

$$\begin{aligned} &\vec{r}_P = -\vec{R}_T + \alpha\vec{r}_T, \quad \vec{R}_P = \beta\vec{R}_T + (1-\alpha\beta)\vec{r}_T, \\ &\vec{R} = \vec{R}_T + (1-\alpha)\vec{r}_T. \end{aligned} \tag{2.3}$$

Let $-e$ denote the electron charge, and let $Z_T e$ and $Z_P e$ be the charges of T and P, respectively. Let $\epsilon_i$ be the internal energy of $(e+T)$ in the initial state $i$ and let $\epsilon_f$ be the internal energy of $(e+P)$ in the final state $f$. The characteristic radii of $(e+T)$ and $(e+P)$ are $a_T$ and $a_P$, respectively, where

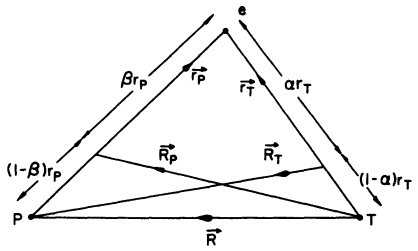


FIG. 1. Coordinate system.

$$a_T = \hbar^2/(Z_T\mu_T e^2), \quad a_P = \hbar^2/(Z_P\mu_P e^2). \tag{2.4}$$

Unless stated otherwise, we work in the center-of-mass frame of all three particles. In this frame the total energy $E$ of the system is

$$E = (\hbar^2/2\nu_i)K_i^2 + \epsilon_i = (\hbar^2/2\nu_f)K_f^2 + \epsilon_f, \tag{2.5}$$

where $\hbar\vec{K}_i$ is the initial momentum of P and $\hbar\vec{K}_f$ is the final momentum of $(e+P)$ with $K_i = |\vec{K}_i|$ and $K_f = |\vec{K}_f|$. If $\vec{v}$ is the incident velocity of P relative to the center of mass of $(e+T)$, we have $\hbar\vec{K}_i = \nu_i\vec{v}$. We define the "average" momentum-transfer vectors

$$\vec{K} = \beta\vec{K}_f - \vec{K}_i, \quad \vec{J} = \alpha\vec{K}_i - \vec{K}_f. \tag{2.6}$$

Here $\hbar\vec{K}$ is the momentum transferred to P, averaged over the internal motion of $(e+P)$ in state $f$, and $\hbar\vec{J}$ is the momentum transferred to T, averaged over the internal motion of $(e+T)$ in state $i$.

Let $\phi_i(\vec{r}_T)$ represent the initial internal state of $(e+T)$ and let $\phi_f(\vec{r}_P)$ represent the final internal state of $(e+P)$. The initial and final wave functions of the complete system are

$$\psi_i = \exp(i\vec{K}_i\cdot\vec{R}_T)\phi_i(\vec{r}_T), \tag{2.7a}$$

and

$$\psi_f = \exp(i\vec{K}_f\cdot\vec{R}_P)\phi_f(\vec{r}_P), \tag{2.7b}$$

respectively. The perturbations in the initial and final channels are, respectively,

$$V_i \equiv V_{Pe}(r_P) + V_{PT}(R) \equiv -Z_P e^2/r_P + Z_P Z_T e^2/R, \tag{2.8a}$$

$$V_f \equiv V_{Te}(r_T) + V_{PT}(R) \equiv -Z_T e^2/r_T + Z_P Z_T e^2/R. \tag{2.8b}$$

The scattering amplitude for the transition $i \to f$ is

$$T = \langle\psi_f|V_f|\Psi_i^+\rangle \tag{2.9a}$$

$$= \langle\Psi_f^-|V_i|\psi_i\rangle, \tag{2.9b}$$

where $\Psi_i^+$ and $\Psi_f^-$ are the exact wave functions of the

complete system satisfying incoming and outgoing boundary conditions, respectively. The total cross section is

$$\sigma=\frac{1}{2\pi\beta\hbar^2v^2}\left(\frac{\nu_f}{\nu_i}\right)\int_{K_{\min}}^{K_{\max}}|T|^2K\,dK\,, \tag{2.10}$$

where $K_{\max}=\beta K_f+K_i$ and $K_{\min}=|\beta K_f-K_i|$. The differential cross section is

$$\frac{d\sigma}{d\Omega}=\frac{\nu_i\nu_f}{(2\pi)^2\hbar^4}\frac{K_f}{K_i}|T|^2\,. \tag{2.11}$$

The Fourier transform $\tilde f(\vec k)$ of any function $f(\vec r)$ is defined as

$$\tilde f(\vec k)=\left(\frac{1}{2\pi}\right)^{3/2}\int d^3r\exp(-i\vec k\cdot\vec r)f(\vec r)\,. \tag{2.12}$$

## III. ANALYSIS

Bassel and Gerjuoy[3] defined the distortion potentials

$$U_i(\vec R_T)=\int d^3r_T\,|\phi_i(\vec r_T)|^2V_i\,, \tag{3.1a}$$

$$U_f(\vec R_P)=\int d^3r_P\,|\phi_f(\vec r_P)|^2V_f\,, \tag{3.1b}$$

where the integrations are carried out with $\vec R_T$ fixed in Eq. (3.1a) and $\vec R_P$ fixed in Eq. (3.1b). The distorted waves $\chi_i^+$ and $\chi_f^-$ are defined by the equations

$$[-(\hbar^2/2\nu_i)\nabla_{\vec R_T}^2-(\hbar^2/2\mu_T)\nabla_{\vec r_T}^2+U_i+V_{Te}]\chi_i^+ =(E+i\eta)\chi_i^+\,, \tag{3.2a}$$

$$[-(\hbar^2/2\nu_f)\nabla_{\vec R_P}^2-(\hbar^2/2\mu_P)\nabla_{\vec r_P}^2+U_f+V_{Pe}]\chi_f^- =(E-i\eta)\chi_f^-\,, \tag{3.2b}$$

where $\eta$ is an infinitesimally small but positive quantity. The effective perturbations in the initial and final channels are, respectively, $V_i-U_i$ and $V_f-U_f$. With some manipulation it can be shown[8] (noting that $U_i$ and $U_f$ alone cannot induce transitions) that

$$T=\langle\chi_f^-|(V_f-U_f)|\Psi_i^+\rangle \tag{3.3a}$$

$$=\langle\Psi_f^-|(V_i-U_i)|\chi_i^+\rangle\,. \tag{3.3b}$$

In the distorted-wave Born approximation we approximate $\Psi_i^+$ by $\chi_i^+$ and $\Psi_f^-$ by $\chi_f^-$, and obtain

$$T\simeq\langle\chi_f^-|(V_f-U_f)|\chi_i^+\rangle \tag{3.4a}$$

$$=\langle\chi_f^-|(V_i-U_i)|\chi_i^+\rangle\,. \tag{3.4b}$$

We will, in fact, derive Eqs. (3.4) below.

Writing

$$\chi_i^+=\phi_i(\vec r_T)[e^{i\vec K_i\cdot\vec R_T}+g_i^+(\vec R_T)]\,, \tag{3.5a}$$

$$\chi_f^-=\phi_f(\vec r_P)[e^{i\vec K_f\cdot\vec R_P}+g_f^-(\vec R_P)]\,, \tag{3.5b}$$

and taking the Fourier transform of Eq. (3.2a) we find that the Fourier transform $\tilde g_i^+(\vec k)$ of $g_i^+(\vec R_T)$ is given by the equation

$$(\hbar^2/2\nu_i)(k^2-K_i^2-i\eta)\tilde g_i^+(\vec k)+\left(\frac{1}{2\pi}\right)^{3/2}\int d^3p\,\tilde U_i(|\vec k-\vec p|)\tilde g_i^+(\vec p)+\tilde U_i(|\vec k-\vec K_i|)=0\,. \tag{3.6}$$

The solution of this equation in first-order perturbation theory (with perturbation $U_i$) is

$$\tilde g_i^+(\vec k)\simeq-\left(\frac{2\nu_i}{\hbar^2}\right)\frac{\tilde U_i(|\vec k-\vec K_i|)}{k^2-K_i^2-i\eta}\,. \tag{3.7a}$$

Similarly, in first-order perturbation theory, we have

$$\tilde g_f^-(\vec k)\simeq-\left(\frac{2\nu_f}{\hbar^2}\right)\frac{\tilde U_f(|\vec k-\vec K_f|)}{k^2-K_f^2+i\eta}\,. \tag{3.7b}$$

With $g_i^+(\vec R_T)$ and $g_f^-(\vec R_P)$ calculated from Eqs. (3.7) we use Eq. (3.4b) to obtain

$$T\simeq T_1+T_2^++T_2^-\,, \tag{3.8}$$

where

$$T_1=\langle\psi_f|(V_i-U_i)|\psi_i\rangle\,, \tag{3.9}$$

$$T_2^+=\langle\psi_f|(V_i-U_i)|g_i^+\phi_i\rangle\,, \tag{3.10}$$

$$T_2^-=\langle g_f^-\phi_f|(V_i-U_i)|\psi_i\rangle\,; \tag{3.11}$$

we have neglected the cross term containing $g_f^-g_i^+$, this term being of the order of $(V_i-U_i)U_fU_i$.

We have used the prior-collision interaction $V_i-U_i$ in obtaining Eqs. (3.9)–(3.11). If we were to use the post-collision interaction $V_f-U_f$, these equations would be replaced by

$$T_1=\langle\psi_f|(V_f-U_f)|\psi_i\rangle\,, \tag{3.12}$$

$$T_2^+=\langle\psi_f|(V_f-U_f)|g_i^+\phi_i\rangle\,, \tag{3.13}$$

$$T_2^-=\langle g_f^-\phi_f|(V_f-U_f)|\psi_i\rangle\,. \tag{3.14}$$

There is, in general, a "post-prior discrepancy", that is, Eqs. (3.9)–(3.11) yield a different estimate of $T$ from Eqs. (3.12)–(3.14). In our application to positronium formation by electron capture from hydrogen we used the post form, which is especially simple since (see below) $U_f\equiv0$. The post-prior discrepancy is removed when terms of all orders in $U_i$ and $U_f$ are included, as indicated by Eqs. (3.4). It should be noted that, except in special circumstances, the "post" and "prior" forms of $T_1$ are different, that is,

$$\langle\psi_f|(V_i-U_i)|\psi_i\rangle\neq\langle\psi_f|(V_f-U_f)|\psi_i\rangle\,; \tag{3.15}$$

for while we always have

$$\langle\psi_f|V_i|\psi_i\rangle=\langle\psi_f|V_f|\psi_i\rangle,$$

we usually have

$$\langle\psi_f|U_i|\psi_i\rangle\neq\langle\psi_f|U_f|\psi_i\rangle.$$

For example, for positron impact on hydrogen we have $U_i\neq 0$, but (see below) $U_f\equiv 0$. An exception arises when $m\ll M_T$, and $M_P$, and the reaction is highly symmetric so that $U_i=U_f$, as in the reaction $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p$. There would, however, be post-prior discrepancies for the reactions $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(2s)+p$ and $\mathrm{He}^{++}+\mathrm{H}(1s)\rightarrow\mathrm{He}^{+}(1s)+p$.

In calculating the differential cross section $d\sigma/d\Omega$ we prefer to work consistently through first order in $U_i$ and $U_f$ and discard corrections of higher order, but this is somewhat a matter of taste. Let $\zeta$ be the parity of $\phi_f^*(\vec{r}_P)\phi_i(\vec{r}_T)$. We may have $\zeta=\pm 1$, but for definiteness we assume $\zeta=1$. Without loss in generality we may assume $\phi_i$ and $\phi_f$ are real. Then $T_1$ is real and we have through first order in $U_i$ and $U_f$

$$\frac{d\sigma}{d\Omega}\simeq\frac{\nu_i\nu_f}{(2\pi\hbar^2)^2}\frac{K_f}{K_i}[T_1^2+2T_1\,\mathrm{Re}(T_2^++T_2^-)]. \tag{3.16}$$

Note that the right-hand side of Eq. (3.16) and hence our estimate of $d\sigma/d\Omega$ is not necessarily positive. If $m\ll M_T$, and $M_P$, and if $U_i=U_f$ we have $\mathrm{Re}(T_2^++T_2^-)=0$. To see this, note that if $U_i=U_f\equiv U$ the problem of the relative motion of P and T reduces essentially to the problem of potential scattering with a potential $U$. If $m\ll M_T$, and $M_P$, the eikonal approximation[9] may be used and we have, neglecting corrections of order $m/M_T$ and $m/M_P$,

$$\chi_i^+=\phi_i e^{i\vec{K}_i\cdot\vec{R}_T+iS_+/\hbar}, \tag{3.17a}$$

$$\chi_f^-=\phi_f e^{i\vec{K}_f\cdot\vec{R}_P+iS_-/\hbar}, \tag{3.17b}$$

where $S_+$ and $S_-$ are the eikonal phases, defined by

$$S_+=-\frac{1}{v}\int_{-\infty}^{z}U(R')dZ', \tag{3.18a}$$

$$S_-=-\frac{1}{v}\int_{\infty}^{z}U(R')dZ', \tag{3.18b}$$

where $v=|\vec{v}|$ with $\vec{v}=\hbar\vec{K}_i/\nu_i\approx\hbar\vec{K}_f/\nu_f$, and where in a coordinate system $(X,Y,Z)$ with the $Z$ axis chosen to be parallel to $\vec{v}$ we have $R'=(X^2+Y^2+Z'^2)^{1/2}$. Expanding the exponentials in Eqs. (3.17) we have, through first order in $U$,

$$g_i^+=(iS_+/\hbar)e^{i\vec{K}_i\cdot\vec{R}_T}, \tag{3.19a}$$

$$g_f^-=(iS_-/\hbar)e^{i\vec{K}_f\cdot\vec{R}_P}. \tag{3.19b}$$

Using Eqs. (3.10) and (3.11), we obtain

$$T_2^++T_2^-=(i/\hbar)\langle\psi_f|(V_i-U_i)|S\psi_i\rangle, \tag{3.20}$$

where

$$S=S_+-S_-=-\frac{1}{v}\int_{-\infty}^{\infty}U(R')dZ'. \tag{3.21}$$

Now, under an inversion of coordinates, i.e., $\vec{R}_T\rightarrow-\vec{R}_T$, $\vec{r}_T\rightarrow-\vec{r}_T$, the expression $\langle\psi_f|V_i|S\psi_i\rangle$ transforms to its complex conjugate multiplied by $\zeta$ $(=1)$ and hence $\langle\psi_f|V_i|S\psi_i\rangle$ is purely real so that $T_2^+$ $+T_2^-$ is purely imaginary, as we set out to prove. (However, $T_2^+$ and $T_2^-$ each have nonzero real parts.) It follows from Eq. (3.16) that in this case

$$\frac{d\sigma}{d\Omega}\simeq\frac{\nu_i\nu_f}{(2\pi\hbar^2)^2}\frac{K_f}{K_i}T_1^2, \tag{3.22}$$

and the inclusion of distortion in the relative motion of P and T introduces no correction to the differential cross section through first order in the distortion potential $U$.

Equation (3.22) should be compared to the expression used by Grant and Shapiro[9] to study the reaction $p+\mathrm{H}(1s)\rightarrow\mathrm{H}(1s)+p$:

$$\frac{d\sigma}{d\Omega}\simeq\frac{\nu_i\nu_f}{(2\pi\hbar^2)^2}\frac{K_f}{K_i}(T_1^2+4T_1\,\mathrm{Re}T_2^-).$$

This expression follows from the incorrect statement $T_2^+=T_2^-$. (That $T_2^+\neq T_2^-$ follows from above; we have also verified this computationally.)

In Appendix B we express $T_1$, $T_2^+$, and $T_2^-$ in Eqs. (3.9)–(3.11) as integrals over momentum space. In Appendix C we describe the evaluation of these integrals for the case when $Z_P=Z_T=1$ and $i$ and $f$ are ground states. For $i$ and $f$ both ground states we have

$$U_i(R_T)=(Z_PZ_T-Z_P)\frac{e^2}{R_T}+Z_Pe^2\left(\frac{1}{R_T}+\frac{1}{\alpha a_T}\right)\exp\left(\frac{-2R_T}{\alpha a_T}\right)$$
$$-Z_PZ_Te^2\left(\frac{1}{R_T}+\frac{1}{\gamma a_T}\right)\exp\left(\frac{-2R_T}{\gamma a_T}\right), \tag{3.23}$$

where $\gamma=1-\alpha$. The expression for $U_f(R_P)$ has a similar form but with $Z_P$ and $Z_T$ interchanged, and $R_T$, $\alpha$, $\gamma$, and $a_T$ replaced by $R_P$, $\beta$, $1-\beta$, and $a_P$, respectively, in the right-hand side of Eq. (3.23). Note that when P is a positron we have $U_f(R_P)\equiv 0$. This can be easily understood by noting that because the positron and electron have the same mass and equal but opposite charges there is no preferred sign of $U_f$.

In units in which $\hbar=e=1$ the Fourier transform of $U_i(R_T)$ is given by

$$\left(\frac{\pi}{2}\right)^{1/2}\tilde{U}_i(k)=\frac{Z_P Z_T - Z_P}{k^2} + \frac{Z_P}{(4Z_T^2m^2+k^2)}\left(1+\frac{4Z_T^2m^2}{(4Z_T^2m^2+k^2)}\right) - \frac{Z_P Z_T}{(4Z_T^2M_T^2+k^2)}\left(1+\frac{4Z_T^2M_T^2}{(4Z_T^2M_T^2+k^2)}\right). \tag{3.24}$$

The Fourier transform of $U_f(R_P)$ has a similar form but with $Z_P$ and $Z_T$ interchanged and $M_T$ replaced by $M_P$ in the right-hand side of Eq. (3.24).

We now demonstrate that the distorted-wave Born amplitude is a *variational* estimate of the exact amplitude. Let $H$ denote the Hamiltonian of all three particles, $\Psi_{it}^+$ and $\Psi_{ft}^-$ the trial approximations to $\Psi_i^+$ and $\Psi_f^-$, respectively, and let $\delta\Psi_i^+ = \Psi_i^+ - \Psi_{it}^+$ and $\delta\Psi_f^- = \Psi_f^- - \Psi_{ft}^-$ denote the errors in the trial wave functions. The exact (on-shell) amplitude $T$ satisfies the Kohn-type variational principle[10]

$$T = T_v + \epsilon\,, \tag{3.25}$$

where

$$T_v = \langle\psi_f|V_f|\Psi_{it}^+\rangle + \langle\Psi_{ft}^- - \psi_f|(H-E-i\eta)|\Psi_{it}^+\rangle\,, \tag{3.26}$$

$$\epsilon = -\langle\delta\Psi_f^-|(H-E-i\eta)|\delta\Psi_i^+\rangle\,. \tag{3.27}$$

Since the error term $\epsilon$ is of second order in the errors in the trial wave functions, $T_v$ is a variational estimate of $T$. We choose $\Psi_{it}^+ = \chi_i^+$ and $\Psi_{ft}^- = \chi_f^-$. Note that

$$(H-E)|\psi_i\rangle = V_i|\psi_i\rangle\,, \tag{3.28}$$

$$(H-E)|\psi_f\rangle = V_f|\psi_f\rangle\,, \tag{3.29}$$

$$(H-E-i\eta)|\chi_i^+\rangle = (V_i-U_i)|\chi_i^+\rangle\,, \tag{3.30}$$

$$(H-E+i\eta)|\chi_f^-\rangle = (V_f-U_f^*)|\chi_f^-\rangle\,. \tag{3.31}$$

Combining Eqs. (3.26) and (3.30) we have

$$T_v = \langle\psi_f|V_f|\chi_i^+\rangle - \langle\psi_f|(V_i-U_i)|\chi_i^+\rangle + \langle\chi_f^-|(V_i-U_i)|\chi_i^+\rangle\,. \tag{3.32}$$

Using Eqs. (3.29) and (3.30) we have

$$\langle\psi_f|V_f|\chi_i^+\rangle = \langle\psi_f|(H-E)|\chi_i^+\rangle = \langle\psi_f|(V_i-U_i)|\chi_i^+\rangle\,; \tag{3.33}$$

we have used the Hermiticity of $H$, which follows from the fact that surface terms vanish since $\chi_i^+$ has only an elastic scattering component—recall that $U_i(\vec{R}_T)$ cannot induce transitions. Therefore the first two terms on the right-hand side of Eq. (3.32) cancel and we obtain

$$T_v = \langle\chi_f^-|(V_i-U_i)|\chi_i^+\rangle \tag{3.34}$$

$$= \langle\chi_f^-|(H-E-i\eta|\chi_i^+\rangle = \langle\chi_f^-|(V_f-U_f)|\chi_i^+\rangle\,. \tag{3.35}$$

Hence the distorted-wave Born amplitude is a variational estimate.

Halpern[11] has examined the variational correction to a variety of approximate amplitudes. For a specific choice of trial wave functions $\Psi_{it}^+$ and $\Psi_{ft}^-$, Halpern determines whether the asymptotic form of, e.g., $\Psi_{it}^+$ generates an amplitude correct to second order in the errors of the trial wave functions. If not, he shows how to obtain a second-order accurate estimate by either adding a correction term or finding a more suitable trial wave function.

Finally, we would like to comment briefly on an approximation introduced by Band[12] and referred to by him as the "full first-order perturbation-theory" approximation. Recurrent attention is paid to this approximation and yet we believe it has no firm foundation. In the derivation of his approximate scattering amplitude using time-dependent perturbation theory Band overlooked the fact that this amplitude was obtained by projection onto a final-state wave function that is not orthogonal to the initial-state wave function even in the limit $t\to\infty$ (where $t$ is the time), since the coordinates $\vec{R}_T$ and $\vec{R}_P$ are treated as time independent.

## IV. RESULTS AND DISCUSSION

We have applied the distorted-wave Born approximation in the *post* form, with distortion included in the relative motion through first order, to the reaction

$$e^+ + H(1s) \to Ps(1s) + p\,.$$

Recall that $U_f \equiv 0$ so that Eqs. (3.8) and (3.12)–(3.14) simplify to

$$T \simeq T_{JS} + \langle\psi_f|V_f|g_i^+\phi_i\rangle\,,$$

where $T_{JS} = \langle\psi_f|V_f|\psi_i\rangle$ is the Jackson-Schiff amplitude. Thus, for the above reaction, the present estimate and the Jackson-Schiff estimate differ only by the inclusion through first order of the distortion in relative motion. Note that, for the above reaction, $T_{JS}$ is identical to the *post* form of $T_1$.

Very recently Mandal *et al.*[13] calculated the differential cross section for the above reaction using the distorted-wave Born approximation with $U_i$ taken into account through all orders. This involved the solution of a coupled set (infinite in number, in principle) of one-dimensional integral equations. Our results (SW) for the differential cross section, at impact energies of 20, 100, and

TABLE I. Differential cross section, in units of $a_0^2$, as a function of scattering angle, for the reaction $e^+ + H(1s) \rightarrow Ps(1s) + p$, at an impact energy of 20 eV. The symbols JS, SW, and MGS refer to "post-form" versions of the distorted-wave Born approximation in which the distortion in the relative motion is included through zeroth, first, and infinite order, respectively. The symbol MG refers to an approximation applied to this reaction by Mandal and Guha (Ref. 17). The notation $a(b)$ means $a \times 10^{-b}$.

| Angle (deg) | JS | SW | MGS | MG |
|---|---|---|---|---|
| 0 | 3.2(1) | 4.2(1) | 4.0(1) | 4.1(1) |
| 5 | 2.9(1) | 3.8(1) | 3.6(1) | 3.7(1) |
| 10 | 2.1(1) | 2.8(1) | 2.7(1) | 2.8(1) |
| 15 | 1.2(1) | 1.8(1) | 1.7(1) | 1.7(1) |
| 20 | 5.5 | 9.3 | 8.8 | 9.2 |
| 25 | 1.9 | 4.0 | 3.8 | 4.1 |
| 30 | 3.5(−1) | 1.3 | 1.4 | 1.5 |
| 35 | 1.2(−3) | 5.3(−2) | 3.7(−1) | 4.5(−1) |
| 40 | 1.1(−1) | −3.8(−1) | 5.8(−2) | 8.0(−2) |

200 eV, are compared to those of Mandal *et al.* (MGS) in Tables I and II and Fig. 2. Also shown are results we have obtained using the Jackson-Schiff (JS) approximation, in which the differential cross section is computed from $|T_{JS}|^2$, and the approximation (MG) in which the differential cross section is computed from $|T_1|^2$ with the *prior* form of $T_1$. The latter approximation was applied by Mandal and Guha.[14] Note that the JS, SW, and MGS approximations are "post-form" approximations in which the distortion in the relative motion of the collision partners is included through zeroth, first, and infinite order, respectively. At small scattering angles our results for the differential cross sections are in rather good agreement with the MGS results, and are consistently an improvement over the JS results. However, the agreement worsens as the angle increases and our results become negative and stay negative. This is because the distortion in the relative motion of the positron and hydrogen atom, in the initial channel, increases with increasing scattering angle, of course, so that terms quadratic and higher order in the distortion potential become increasingly important. The MG results are in very good agreement with the MGS results at small angles.

TABLE II. Same as Table I but for an impact energy of 200 eV.

| Angle (deg) | JS | SW | MGS | MG |
|---|---|---|---|---|
| 0 | 1.0(−1) | 1.2(−1) | 1.3(−1) | 1.4(−1) |
| 5 | 7.1(−2) | 8.9(−2) | 9.8(−2) | 1.0(−1) |
| 10 | 2.6(−2) | 3.6(−2) | 4.2(−2) | 4.3(−2) |
| 15 | 5.1(−3) | 9.2(−3) | 1.3(−2) | 1.3(−2) |
| 20 | 3.6(−4) | 1.4(−3) | 3.2(−3) | 3.1(−3) |
| 25 | 2.7(−5) | −2.1(−4) | 8.0(−4) | 7.3(−4) |

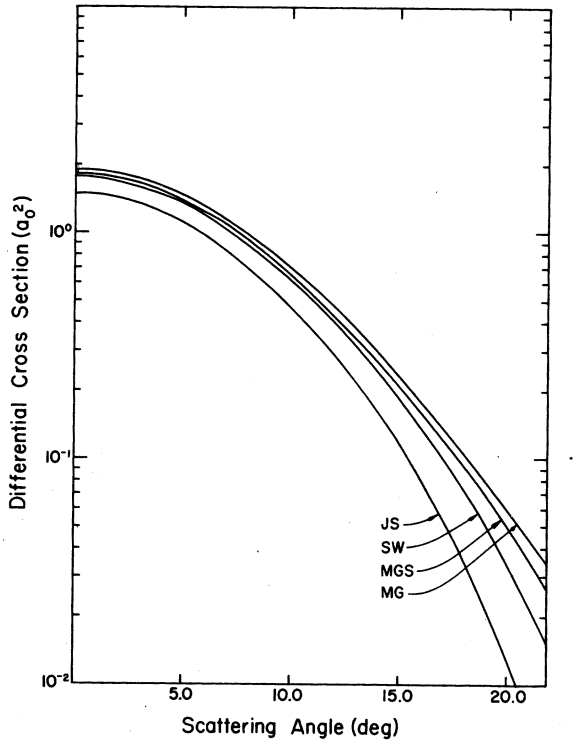


FIG. 2. Differential cross section as a function of scattering angle for the reaction $e^+ + H(1s) \rightarrow Ps(1s) + p$ at an impact energy of 100 eV. The symbols have the same meaning as in Table I.

The integrated cross sections versus impact energy are shown in Table III. Our results always lie below the MGS results, well below at low energies. The reason for this is that in our approximation the contribution to the integrated cross section from large angles is negative. The contribution from large angles becomes increasingly important as the energy decreases. For energies above about 70 eV our results for the integrated cross section are an improvement over the JS results. We are a little surprised that at 200 eV the agreement between our results and the MGS results is not better than shown—the disagreement is about 21%.

We conclude from the comparison of the JS, SW, and MGS results that the inclusion of distortion in the relative motion is essential even at small scattering angles. The inclusion of distortion through first order seems to be adequate at small angles, but at large angles, specifically at angles larger than the angle at which the JS differential cross section is zero, higher-order terms in the distortion potential must be taken into account. We expect these remarks to apply to electron capture by ions, not just by positrons.

TABLE III. Integrated cross section, in units of $(\pi a_0^2)$, as a function of impact energy, for the reaction $e^+ + H(1s) \rightarrow Ps(1s) + p$. The symbols have the same meaning as in Tables I and II.

| Energy (eV) | JS | SW | MGS | MG |
|---|---|---|---|---|
| 13.6 | 4.8 | 2.0 | 4.5 | 4.5 |
| 20.0 | 3.3 | 2.2 | 3.3 | 3.4 |
| 50.0 | 4.6(−1) | 4.3(−1) | 5.1(−1) | 5.5(−1) |
| 100.0 | 4.5(−2) | 4.8(−2) | 5.7(−2) | 6.1(−2) |
| 200.0 | 2.4(−3) | 3.0(−3) | 3.8(−3) | 3.8(−3) |

## V. SOME COMMENTS ON Ps FORMATION AT HIGH SPEEDS

Despite the fact that MGS take into account the distortion potential to all orders, their approximation is inadequate at high speeds ($e^2/\hbar v \ll 1$) because important terms of order $V_{Te}V_{Pe}$ and $V_{PT}V_{Pe}$ are omitted. These terms represent the following two mechanisms, which have been analyzed both classically[15] and quantum mechanically[16,17] and are illustrated in Fig. 3: (a) The positron, incident with a high speed $v$ (velocity $\vec{v}$) strikes the electron and knocks it toward the target proton with a speed $v/\sqrt{2}$ and in a direction making an angle of 45° with $\vec{v}$. In this collision the positron is deflected through an angle of 45° and also emerges with a speed $v/\sqrt{2}$. The electron then scatters elastically from the heavy proton, is deflected through an angle of 90°, and emerges from this second collision with a velocity roughly equal to that of the positron. Capture may then occur easily. (b) The positron strikes the electron and knocks the electron out of the atom with a speed $v/\sqrt{2}$ and in a direction making an angle of 45° with $\vec{v}$. The positron is deflected, through 45°, toward the proton from which it scatters elastically with a speed $v/\sqrt{2}$, is deflected through 90°, and emerges with a velocity roughly equal to that of the electron so that capture may again easily occur. Mechanisms (a) and (b) are represented by the second Born matrix elements of $V_{Te}G_0V_{Pe}$ and $V_{PT}G_0V_{Pe}$, respectively, where $G_0$ is the Green's function for three noninteracting particles. The two matrix elements interfere. To leading order in $e^2/\hbar v$ the interference is totally destructive or totally constructive according to whether the orbital-angular-momentum quantum number $l$ of the final state is even or odd. This can be understood as follows[17]: The two mechanisms differ only in the nature of the second collision. The (first Born) amplitude for the second collision has the same magnitude but a different sign in the two mechanisms. The position vector of the electron relative to the positron, immediately after the second collision, also has the same magnitude but different sign (i.e., it is inverted) in the two mechanisms. Hence the matrix elements of $V_{Te}G_0V_{Pe}$ and $V_{PT}G_0V_{Pe}$ differ only by $(-1)^{l+1}$ to leading order in $e^2/\hbar v$. The consequence of this is that capture occurs primarily to states of positronium having odd $l$ when $e^2/\hbar v \ll 1$. In fact, the asymptotic $v$ dependence of the cross section for Ps formation is $(e^2/\hbar v)^{12}$ if $l$ is even and $(e^2/\hbar v)^{11}$ if $l$ is odd.

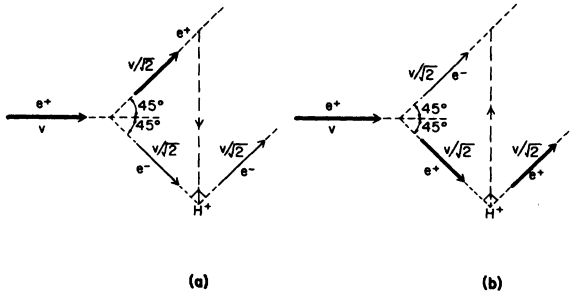


FIG. 3. Two mechanisms for positronium formation at high-impact speeds. The thick and thin lines, respectively, describe the paths of the positron and electron. The vertical dashed line is the position vector of the electron relative to the positron immediately after the second collision.

There is currently much interest in the process of charge transfer to the continuum since it is a primary source of ionization.[18] The quantity being measured is the singly differential cross section $d\sigma/dv_e$ for the electron to be ejected by a projectile ion with a lab speed $v_e$ (velocity $\vec{v}_e$) into a narrow forward cone whose axis is parallel to $\vec{v}$. When $v_e \approx v$, $d\sigma/dv_e$ exhibits a cusp, which is the signature of charge transfer to the continuum. Strong asymmetries in this cusp have been observed[19] for electron capture to the continuum by fast-moving *ions*. These asymmetries have been attributed[20] to the fact that the electron is captured by the ion into many different partial-wave components of the electron-projectile continuum, not just the $l=0$ component; this fact implies that the amplitude for capture to the continuum depends on the vector difference $\vec{v}_e - \vec{v}$, not on $|\vec{v}_e - \vec{v}|$, so that this amplitude is not invariant under the transformation $(\vec{v}_e - \vec{v}) \rightarrow -(\vec{v}_e - \vec{v})$ and hence $d\sigma/dv_e$ is asymmetric about $v_e = v$ even when $e^2/\hbar v \ll 1$. The situation is different for electron capture to the continuum by positrons. Since the electron is captured primarily to states of Ps with odd $l$, that is, states with the same (odd) parity, the net amplitude for electron capture to the continuum of Ps will be invariant under $(\vec{v}_e - \vec{v}) \rightarrow -(\vec{v}_e - \vec{v})$. Hence the cusp in $d\sigma/dv_e$ (where now the electrons are ejected into a narrow cone whose axis makes an

angle of 45° with $\vec{v}$) is symmetric about $v_e = v$ when $e^2/\hbar v \ll 1$. However, we may require $e^2/\hbar v$ to be so small for this result to be true that $d\sigma/dv_e$, and hence the cusp, are too small to be observed.

We have calculated the asymptotic contribution from the sum of the first- and second-order Born terms to the cross section for the reaction

$$e^+ + \mathrm{H}(1s) - \mathrm{Ps}(1s) + p\,,$$

where H(1$s$) is any member of the H(1$s$) isoelectronic sequence. We find the asymptotic form of the cross section to be

$$\sigma \sim cZ^5(e^2/\hbar v)^{12}(\pi a_0^2)\,, \tag{5.1}$$

where $Z$ is the atomic number of the target and

$$c = f(y_0) - f(y_1)$$
$$= 1.02 \times 10^5$$

with

$$f(y) = 8\left(\frac{1}{5y^5} - \frac{2}{y^4} + \frac{8}{3y^3} + \frac{16}{y^2} + \frac{16}{y}\right),$$

$$y_0 = \tfrac{1}{2}(3 - 2\sqrt{2})\,,$$

$$y_1 = \tfrac{1}{2}(3 + 2\sqrt{2})\,.$$

The first and second Born terms involving $V_{\mathrm{PT}}$ do not cancel, of course.

At an impact energy of 200 eV the right-hand side of Eq. (5.1) is about $1.0 \times 10^{-2}$ $(\pi a_0^2)$, which is considerably larger than the MGS result shown in Table III. However, the asymptotic form of the cross section given by Eq. (5.1) is probably inaccurate at 200 eV. To gain a crude idea of when the asymptotic formula is valid, we have evaluated the Brinkman-Kramers cross section (computed from the matrix element $\langle \psi_f | V_{\mathrm{Pe}} | \psi_i \rangle$) both exactly and asymptotically. At 200 eV the asymptotic estimate is too large by a factor of about 3.5. At 2000 eV the discrepancy is about 15%.

There have been no measurements of the cross section for positronium formation at high impact speeds. Such measurements would be extremely difficult since the positronium would be destroyed by collisions very quickly after its formation. However, it is possible (but highly speculative) that one could study positronium formation indirectly by studying charge transfer to the continuum. In charge transfer to the continuum, the positron leaves its mark long after its death. This mark, the cusp in $d\sigma/dv_e$, contains a wealth of information about positronium formation.

## ACKNOWLEDGMENTS

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## APPENDIX A: EFFECT OF $V_{\mathrm{PT}}$ WHEN $m \ll M_{\mathrm{T}}$, AND $M_{\mathrm{P}}$

If $m/M_{\mathrm{T}}$, and $m/M_{\mathrm{P}} \ll 1$, the impact-parameter approximation is valid so that P and T can be treated as classical particles that move with constant relative velocity $\vec{v}$, and we have $\vec{R} = \vec{b} + \vec{v}t$ where $\vec{b}$ is the impact parameter and $t$ is the time.[1] Let $A(\vec{b})$ and $A'(\vec{b})$ be the amplitudes for the transition $i \to f$ when $\lambda V_{\mathrm{PT}}$ is included and excluded, respectively, from the electron Hamiltonian. (We have introduced an arbitrary "strength parameter" $\lambda$.) Wick[21] pointed out that

$$A(\vec{b}) = A'(\vec{b})e^{i\xi}\,, \tag{A1}$$

where

$$\xi = -\frac{\lambda}{\hbar}\int_{-\infty}^{\infty} V_{\mathrm{PT}}(R)dt$$
$$= -\frac{\lambda}{\hbar v}\int_{-\infty}^{\infty} V_{\mathrm{PT}}(R)du\,, \tag{A2}$$

where $u = vt$. (Note that $\xi$ decreases as $1/v$ as $v$ increases.) Since $A(\vec{b})$ and $A'(\vec{b})$ differ only by a phase factor, the cross section integrated over $\vec{b}$ is the same whether or not $V_{\mathrm{PT}}$ is included in the electron Hamiltonian.

We can expand the phase factor in Eq. (A1) in powers of $\lambda$, which is equivalent to expanding in powers of $\xi$. Since $\lambda$ is arbitrary and since $A'(\vec{b})$ is independent of $\lambda$, it follows that in the Born expansion of $A(\vec{b})$ all those Born terms involving $\lambda V_{\mathrm{PT}}$ linearly must sum to $i\xi A'(\vec{b})$. Let $A_{\lambda n}$ be the sum of those $n$th-order terms involving $\lambda V_{\mathrm{PT}}$ linearly in the Born expansion of $A(\vec{b})$, and let $A_n'$ be the sum of all $n$th-order terms in the Born expansion of $A'(\vec{b})$. We have

$$(A_{\lambda 1} + A_{\lambda 2} + A_{\lambda 3} + \cdots) = i\xi(A_1' + A_2' + A_3' + \cdots)\,. \tag{A3}$$

For direct excitation processes it can be shown that

$$A_{\lambda 1} = 0\,, \quad A_{\lambda n} = i\xi A_{n-1}'\,, \quad n > 1\,.$$

For capture processes $A_{\lambda 1} \neq 0$. However, without loss in generality we can choose $\phi_i$ and $\phi_f$ so that $A_{\lambda 1}$ has the same phase as $A_1'$. In fact, we can assume that $A_{\lambda 1}$ and $A_1'$ are both real. It follows from Eq. (A3) that

$$A_{\lambda 1} + \mathrm{Re}(A_{\lambda 2} + A_{\lambda 3} + \cdots) = -\xi\,\mathrm{Im}(A_2' + A_3' + \cdots)\,, \tag{A4a}$$

$$\mathrm{Im}(A_{\lambda 2} + A_{\lambda 3} + \cdots) = \xi A_1' + \xi\,\mathrm{Re}(A_2' + A_3' + \cdots)\,. \tag{A4b}$$

Since $\xi A_2'$ is of third order in the potentials (note $\xi$ is of first order) we see from Eq. (A4a) that $A_{\lambda 1}$ is canceled through at least second order by higher terms in the Born expansion of $A(\vec{b})$. Therefore,

it is not meaningful to retain $A_{\lambda 1}$ in the Born expansion of $A(\vec{b})$ unless higher terms are kept.

We now suppose that $v \gg e^2/\hbar$. The Born terms $A_{\lambda 1}$, $A_{\lambda 2}$, and $A_1'$ are appreciable only for $b \equiv |\vec{b}| \lesssim \hbar/mv$. (For $b \gg \hbar/mv$ these terms are exponentially small.[22]) If $b \lesssim \hbar/mv$ the terms $A_{\lambda 3}$, $A_{\lambda 4}, \ldots$, and $A_2', A_3', \ldots$ are much smaller (by one or more powers of $e^2/\hbar v$) than $A_{\lambda 1}$ and $A_{\lambda 2}$, provided, as is the case here, that the potentials $V_{PT}$, $V_{Pe}$, and $V_{Te}$ are of the same kind.[22] Noting that $\xi$ decreases as $1/v$ with increasing $v$ it follows from Eq. (A4a) that $A_{\lambda 1}$ and $\mathrm{Re}A_{\lambda 2}$ cancel through at least one power of $e^2/\hbar v$ if $b \lesssim \hbar/mv$. In fact, since from Eq. (A4b) we see that $\mathrm{Im}A_{\lambda 2}$ is smaller than $A_1'$ by one power of $e^2/\hbar v$ for $b \lesssim \hbar/mv$, and since $A_{\lambda 1}$ and $A_1'$ are of the same order in this range, we can say that $A_{\lambda 1}$ and $A_{\lambda 2}$ cancel through at least one power of $e^2/\hbar v$.

Neglecting corrections of order $m/M_T$ and $m/M_P$ the scattering amplitude $T(\vec{K})$ in the full wave treatment is[1]

$$T(\vec{K}) = \hbar v \int d^2b\, e^{i\vec{K}\cdot\vec{b}} A(\vec{b}). \tag{A5}$$

Let $T_{\lambda n}$ be the sum of those $n$th-order Born terms involving $\lambda V_{PT}$ linearly in the Born expansion of $T(\vec{K})$. To obtain $T_{\lambda 1} + T_{\lambda 2}$ we simply replace $A(\vec{b})$ by $A_{\lambda 1} + A_{\lambda 2}$ in Eq. (A5). If we make this replacement then for $e^2/\hbar v \ll 1$ the main contribution to the integral over $\vec{b}$ comes from the region $b \lesssim \hbar/mv$. But we have seen that in this range of $b$ the terms $A_{\lambda 1}$ and $A_{\lambda 2}$ cancel through at least one power of $e^2/\hbar v$. Hence $T_{\lambda 1}$ and $T_{\lambda 2}$ cancel through the same order, which is the result that Drisko and Dettmann and Leibfried[2] obtained by explicitly evaluating $T_{\lambda 1}$ and $T_{\lambda 2}$ in the small $e^2/\hbar v$ limit.

## APPENDIX B: EXPRESSIONS FOR AMPLITUDES AS INTEGRALS OVER MOMENTUM SPACE

In this Appendix we express $T_1$, $T_2^+$, and $T_2^-$, where these amplitudes are defined by Eqs. (3.9)–(3.11), as integrals over momentum space. We have

$$T_1 = N_1 + N_2 + N_3, \tag{B1}$$

$$N_1 = (2\pi)^{3/2} \int d^3p\, \tilde{\phi}_f^*(\vec{K} - \vec{p}) \tilde{V}_{PT}(p) \tilde{\phi}_i(-\vec{J} - \vec{p}), \tag{B2a}$$

$$N_2 = -(2\pi)^3 [(\tfrac{1}{2}/\mu_P) K^2 - \epsilon_f] \tilde{\phi}_f^*(\vec{K}) \tilde{\phi}_i(-\vec{J}), \tag{B2b}$$

$$N_3 = -(2\pi)^{3/2} \int d^3p\, \tilde{\phi}_f^*(\vec{p} + \vec{K}) \tilde{U}_i(p) \tilde{\phi}_i(\alpha\vec{p} - \vec{J}). \tag{B2c}$$

$N_2$ is the Brinkman-Kramers amplitude, which can be expressed in closed form. We also have

$$T_2^+ = L_1 + L_2 + L_3, \tag{B3}$$

where

$$L_1 = \int d^3p \int d^3q\, \tilde{\phi}_f^*(\beta\vec{K}_f - \vec{p} - \vec{q}) \tilde{V}_{PT}(p) \tilde{g}_i^+(\vec{q}) \tilde{\phi}_i(\vec{K}_f - \vec{p} - \alpha\vec{q}), \tag{B4a}$$

$$L_2 = -(2\pi)^{3/2} \int d^3p [(\tfrac{1}{2}/\mu_P)(\beta\vec{K}_f - \vec{p})^2 - \epsilon_f] \tilde{\phi}_f^*(\beta\vec{K}_f - \vec{p}) \tilde{g}_i^+(\vec{p}) \tilde{\phi}_i(\vec{K}_f - \alpha\vec{p}), \tag{B4b}$$

$$L_3 = -\int d^3p \int d^3q\, \tilde{\phi}_f^*(\beta\vec{K}_f - \vec{p} - \vec{q}) \tilde{U}_i(p) \tilde{g}_i^+(\vec{q}) \tilde{\phi}_i(\vec{K}_f - \alpha\vec{p} - \alpha\vec{q}), \tag{B4c}$$

and

$$T_2^- = M_1 + M_2 + M_3, \tag{B5}$$

where

$$M_1 = \int d^3p \int d^3q\, \tilde{g}_f^{-*}(\vec{p}) \tilde{\phi}_f^*(\beta\vec{p} + \vec{q} - \vec{K}_i) \tilde{V}_{PT}(q) \tilde{\phi}_i(\vec{p} + \vec{q} - \alpha\vec{K}_i), \tag{B6a}$$

$$M_2 = -(2\pi)^{3/2} \int d^3p [(\tfrac{1}{2}/\mu_P)(\beta\vec{p} - \vec{K}_i)^2 - \epsilon_f] \tilde{g}_f^{-*}(\vec{p}) \tilde{\phi}_f^*(\beta\vec{p} - \vec{K}_i) \tilde{\phi}_i(\vec{p} - \alpha\vec{K}_i), \tag{B6b}$$

$$M_3 = -\int d^3p \int d^3q\, \tilde{g}_f^{-*}(\vec{p}) \tilde{\phi}_f^*(\beta\vec{p} + \vec{q} - \vec{K}_i) \tilde{U}_i(q) \tilde{\phi}_i(\vec{p} + \alpha\vec{q} - \alpha\vec{K}_i). \tag{B6c}$$

## APPENDIX C: EVALUATION OF INTEGRALS

For $i$ and $f$ ground states (and $Z_P = Z_T = 1$) we have to evaluate the following three types of basic integrals:

$$I_1 = \int d^3p \, \frac{1}{[(\vec{p}-\vec{A})^2+a^2][(\vec{p}-\vec{B})^2+b^2](p^2+z^2)}, \tag{C1}$$

$$I_2 = \int d^3p \, \frac{1}{(\vec{p}-\vec{A})^2+a^2} \, \frac{1}{(\vec{p}-\vec{B})^2+b^2} \, \frac{1}{(\vec{p}-\vec{C})^2+c^2} \, \frac{1}{p^2-C^2-i\eta}, \tag{C2}$$

$$I_3 = \int d^3p \int d^3q \, \frac{1}{(\vec{p}+\vec{q}-\vec{A})^2+a^2} \, \frac{1}{(\vec{p}+\vec{q}-\vec{B})^2+b^2} \, \frac{1}{p^2+c^2} \, \frac{1}{(\vec{q}-\vec{D})^2+d^2} \, \frac{1}{q^2-D^2-i\eta}. \tag{C3}$$

Higher powers of any of the factors in the denominators can be obtained by differentiation. In the above equations $\eta$ is positive and infinitesimal, $a$, $b$, $c$, $d$, and the components of $\vec{A}$, $\vec{B}$, $\vec{C}$, and $\vec{D}$, are real, $z$ may be complex, and $C = |\vec{C}|$, $D = |\vec{D}|$. The integrals $N_1$ and $N_3$ of Eqs. (B2a) and (B2c) are of the type of $I_1$. If we write $d^3p = p^2 dp \, d\Omega$ in Eq. (C1), the integral over $d\Omega$ can be done simply with the use of the Feynman identity

$$\frac{1}{\alpha\beta} = \int_0^1 dx \, \frac{1}{[\alpha x + \beta(1-x)]^2}; \tag{C4}$$

the integration over $p$ can then be done simply by contour integration if $z$ is real. For $z$ real, we have

$$I_1 = \pi^2 \int_0^1 dx \, \frac{1}{E[F^2+(E+z)^2]} \tag{C5}$$

where

$$E^2 = x(1-x)(\vec{A}-\vec{B})^2 + xa^2 + (1-x)b^2, \tag{C6a}$$

$$\vec{F} = x\vec{A} + (1-x)\vec{B}, \tag{C6b}$$

where $E$ and $z$ are the positive square roots of $E^2$ and $z^2$, respectively, and where $F = |\vec{F}|$. Now the integral $I_1$ exists for all values of $z^2$ except those on the negative real axis. In fact, $I_1$ is an analytic function of $z^2$ in the complex $z^2$ plane cut along the negative real axis. Since the right-hand side of Eq. (C5) is also an analytic function of $z^2$ in this cut plane, we have by analytic continuation that Eq. (C5) is valid for all $z^2$ in the cut plane, provided that $z$ is that branch of the square root of $z^2$ which is positive when $z^2$ is real and positive. For example, if $z^2 = -(C^2+i\eta)$, we insert $z = -iC$ in Eq. (C5). The one-dimensional integral of Eq. (C5) can, in fact, be evaluated in closed form.[23] We chose to evaluate this integral and its derivatives numerically, since the algebra is much less cumbersome and numerical integration using Simpson's rule is rapid.

By a repeated use of the Feynman identity and use of Eq. (C5) we have

$$I_2 = \pi^2 \int_0^1 dx \int_0^1 dy \, \frac{y}{S^2T^2}\left(\frac{T}{2S} + S - iC\right), \tag{C7}$$

where $E$ and $\vec{F}$ are defined in Eqs. (C6) and where

$$S^2 = y(1-y)(\vec{F}-\vec{C})^2 + yE^2 + (1-y)c^2, \tag{C8a}$$

$$T = -C^2 - 2iCS + y(E^2+F^2) + (1-y)(c^2+C^2), \tag{C8b}$$

with $C$ and $S$ the positive square roots of $C^2$ and $S^2$, respectively. The integrals $L_2$ and $M_2$ of Eqs. (B4b) and (B6b) are of the type of $I_2$.

The integral $L_3$ of Eq. (B4c) is of the type of $I_3$ but the integrals $L_1$, $M_1$, and $M_3$ of Eqs. (B4a), (B6a), and (B6c), as they stand, are not of this type. This would be of this type if $\vec{p}$ and $\vec{q}$ always occurred in the combination $\vec{p}+\vec{q}$ in the arguments of $\vec{\phi}_i$ and $\vec{\phi}_f$. To a good approximation $\vec{p}$ and $\vec{q}$ do occur in the required combination. For example, consider $L_1$ of Eq. (B4a). The main contribution to the integral over $\vec{q}$ in Eq. (B4a) comes from the region $|\vec{q}-\vec{K}_i| \lesssim K, J$. Thus, provided $(1-\alpha)J \ll 1/a_T$, which is true in the angular range of interest, we can approximate the argument $\vec{K}_f - \vec{p} - \alpha\vec{q}$ of $\vec{\phi}_i$ by $-\vec{J}+\vec{K}_i-\vec{p}-\vec{q}$, so that $\vec{p}$ and $\vec{q}$ occur in the required combination. Similarly, provided that $(1-\beta)K \ll 1/a_P$, we can approximate the argument $\beta\vec{p}+\vec{q}-\vec{K}_i$ of $\vec{\phi}_f$ in Eqs. (B6a) and (B6c) by $\vec{p}+\vec{q}+\vec{K}-\vec{K}_f$. We also approximate the argument $\vec{p}+\alpha\vec{q}-\alpha\vec{K}$ of $\vec{\phi}_i$ in Eq. (B6c) by $\vec{p}+\vec{q}-\vec{J}-\vec{K}_f$ for $(1-\alpha)J \ll 1/a_T$. Note, however, that for positron impact the inequality $(1-\beta)K \ll 1/a_P$ is certainly not satisfied for all angles of interest since $\beta = \frac{1}{2}$. Fortunately, in this case the integrals $M_1$, $M_2$, and $M_3$ are zero since the distortion potential $U_f$ vanishes.

By a repeated use of the Feynman identity, and by use of Eq. (C5), we have

$$I_3 = \pi^4 \int_0^1 dx \int_0^1 dy \, \frac{1}{ES} \, \frac{1}{[T^2+(S-iD)^2]}, \tag{C9}$$

where $E$ and $\vec{F}$ are defined in Eqs. (C6) and where now

$$S^2 = y(1-y)(\vec{F}-\vec{D})^2 + y(E+c)^2 + (1-y)d^2, \tag{C10a}$$

$$\vec{T} = y\vec{F} + (1-y)\vec{D}, \tag{C10b}$$

with $c$ and $S$ the positive square roots of $c^2$ and $S^2$

and with $T = |\vec{T}|$.

The integrals $I_2$ and $I_3$ can be reduced to one-dimensional integrals, but we chose to evaluate the two-dimensional integrals and their derivatives, numerically since the algebra is then less cumbersome.


[1]See, e.g., L. Wilets and S. J. Wallace, Phys. Rev. 169, 84 (1968).

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[8]See Ref. 3 and references therein or any standard book on scattering theory, e.g., J. R. Taylor, *Scattering Theory* (Wiley, New York, 1972). Note that if $U_i$ (or $U_f$) is sufficiently attractive, Eq. (3.2a) [or (3.2b)] will, for specific eigenvalues, possess solutions corresponding to all three particles bound, and if one of these eigenvalues coincides with the energy $E$ of interest—in which case the three-body bound state is embedded in the continuum—Eq. (3.3b) [or (3.3a)] breaks down. Even if $E$ does not coincide with one of these eigenvalues, the distorted-wave Born approximation will be a poor approximation unless $E$ lies well above the eigenvalues. There is no difficulty in the present calculation since $U_i$ and $U_f$ are repulsive.

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