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Strong potential wave functions with elastic channel distortion

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The strong-potential Born (SPB) approximation is analyzed in a channel-distorted-wave approach. Channel-distorted SPB wave functions are reduced to a conventional form in which the standard off-energy-shell factor g has been replaced by a modified factor γ, which represents a suitable average of g over the momentum distribution of the distorted-channel function. The modified factor is evaluated in a physically realistic model for the distortion potential, and it is found that γ is well represented by a slowly varying phase factor. The channel-distorted SPB approximation is accordingly identical to the impulse approximation if the phase variation of γ can be ignored. This is generally the case in applications to radiative electron capture and to a good approximation for ordinary capture at not too small velocities.

The strong-potential Born (SPB) approximation was originally introduced[1,2] to provide a consistent first-order theory of electron capture in asymmetric ion-atom collisions. It is obtained when the exact Green's operator, as it appears in T-matrix elements or in scattering states, is approximated by the corresponding strong potential Green's operator. Considering the motion of one electron in the field of two nuclear charges Z_P and Z_T with $Z_P \gg Z_T$, and assuming that the electron initially is bound to the target nucleus, the SPB approximation for the initial scattering state is given by[3]

$$|\Psi_i^{+(\mathrm{SPB})}\rangle = (1+G_P^+ V_P)\,|\Phi_i\rangle\,, \tag{1}$$

where G_P^+ is the projectile Green's operator

$$G_P^+ = (E - H_0 - V_P + i\eta)^{-1}\,, \tag{2}$$

and

$$\Phi_i(\mathbf{r}_T,\mathbf{R}_T) = \varphi_i(\mathbf{r}_T)\phi_{\mathbf{K}_i}(\mathbf{R}_T)\,. \tag{3}$$

Here, φ_i represents the initial bound-state wave function of the electron, while $\phi_{\mathbf{K}_i}$ is a plane wave with vector $\mathbf{K}_i$ to represent the relative motion of the projectile with respect to the center-of-mass of the electron-target system. We use the definition of Macek and Shakeshaft[4] for the Jacobi coordinates $(\mathbf{r}_T,\mathbf{R}_T)$ and the complementary pair $(\mathbf{r}_P,\mathbf{R}_P)$. The interaction potential of the electron with the projectile is denoted by V_P.

It is to be emphasized that SPB wave functions represent the development of a bound-electron state as it propagates in the field of the other collision partner.[3,5] The factor $G_P V_P\,|\Phi_i\rangle$, which describes this propagation, is well defined since $|\Phi_i\rangle$ is not an eigenstate of G_P. In contrast, other approximate wave functions for which $|\Phi_i\rangle$ is an eigenstate of the Green's operator require careful limiting procedures for their proper definition.[6-8] These procedures are now well understood and of no further concern here since we employ only the well-defined Eq. (1) in this work.

For later convenience, we note that Eq. (1) may be expressed in the alternative form

$$|\Psi_i^{+(\mathrm{SPB})}\rangle = G_P^+ V_T\,|\Phi_i\rangle\,, \tag{4}$$

where V_T represents the potential of the electron with respect to the target nucleus. A formal demonstration of this equivalence rests on the fact that $i\eta G_P\,|\Phi_i\rangle$ is identically zero, as demonstrated by Faddeev.[9]

The SPB scattering states given by Eq. (1), and corresponding states developed from final states on the projectile have provided the basis for a more general distorted-wave theory for rearrangement collisions.[8] In practical applications, the SPB functions have been used primarily in physical situations where they can be evaluated in a peaking approximation, leading to a near-shell approximation for the electron motion in the projectile field. Equation (1) may then be expressed as

$$\Psi_i^{+(\mathrm{SPB})}(\mathbf{r}_P,\mathbf{R}_P) = \int d^3k\,\tilde{\varphi}_i(\mathbf{k})\,g^+(q,\varepsilon)\,\psi_{\mathbf{q}}^+(\mathbf{r}_P)\,\phi_{\mathbf{Q}}(\mathbf{R}_P)\,. \tag{5}$$

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

$$\mathbf{q} = \mathbf{k} - \mathbf{v}, \quad \mathbf{Q} = \alpha\mathbf{K}_i + \mathbf{k}\,, \tag{6}$$

where $\mathbf{v} = \mathbf{K}_i/\mu_i$ is the incident velocity vector and $\alpha = M_T/(M_T+1)$. (Atomic units are used throughout this paper.) The function $\psi_{\mathbf{q}}^+(\mathbf{r}_P)$ is an ordinary Coulomb wave in the projectile field, and it is multiplied in Eq. (5) by the off-energy-shell factor $g^+(q,\varepsilon)$ given by

$$g^+(q,\varepsilon) = \Gamma(1+i\nu)\exp(\pi\nu/2)\left[\left(\tfrac{1}{2}q^2-\varepsilon\right)/2q^2\right]^{-i\nu}, \tag{7}$$

where $\nu = Z_P/q$ is the Sommerfeld parameter. Finally, the energy parameter ε is given by

$$\varepsilon - \tfrac{1}{2}q^2 = \varepsilon_i - \tfrac{1}{2}k^2\,, \tag{8}$$

where ε_i is the binding energy of the initial state. Equation (5) is also obtained when the peaking approximation is made in the alternative form of the SPB given by Eq. (4).

The asymptotic conditions in ion-atom collisions are

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often governed by long-range Coulomb forces. A suitable relation between cross sections and T-matrix elements, therefore, mainly relies on the distorted-wave formulation of scattering theory. This implies that the SPB wave function must be regarded as the limit of a function employing an elastically distorted-wave function rather than a plane wave to describe the relative motion in the initial channel.[8] The corresponding distortion potential is formally arbitrary except for an asymptotic Coulomb condition. Physically, however, it is important to choose the distortion in such a way that it describes the elastic scattering in the considered channel with good accuracy since elastic scattering by long-range forces is poorly represented by perturbation methods. It is, in principle, possible to model virtual transitions and polarization effects in the determination of the distortion potential. For practical convenience, however, U_i is assumed to be given as the following static single-channel potential or as simpler approximations thereof:

$$U_i(\mathbf{R}_T)=\int d^3r_T\,|\varphi_i(\mathbf{r}_T)|^2 V_P(\mathbf{r}_P)\,, \tag{9}$$

where $\mathbf{r}_P=-\mathbf{R}_T+\alpha\mathbf{r}_T$ may be used.

Corresponding to the elastically distorted initial state

$$\Phi_i^+(\mathbf{r}_T,\mathbf{R}_T)=\varphi_i(\mathbf{r}_T)\phi_{\mathbf{K}_i}^+(\mathbf{R}_T)=\varphi_i(\mathbf{r}_T)\phi_{\mathbf{K}_i}(\mathbf{R}_T)D_{\mathbf{K}_i}^+(\mathbf{R}_T)\,, \tag{10}$$

modified SPB functions may be defined according to standard distorted-wave theory as

$$|\Psi_i^{+(\mathrm{DSPB})}\rangle=[1+G_P^+(V_P-U_i)]\,|\Phi_i^+\rangle\,, \tag{11}$$

or similar to Eq. (4), as

$$|\Psi_i^{+(\mathrm{DSPB})}\rangle=G_P^+V_T\,|\Phi_i^+\rangle\,. \tag{12}$$

It is the purpose of this Rapid Communication to evaluate the distorted SPB functions in a peaking approximation similar to that applied in the derivation of Eq. (5). The result turns out to be equivalent to Eq. (5) except that the off-shell factor g^+ is replaced by a modified factor γ^+. We derive an explicit expression for this factor in terms of a one-dimensional integral involving the elastically distorted-channel function. The modified off-shell factor is evaluated in a simple, but representative, case.

Introducing the Fourier transform of the distorted-wave function, $\phi_{\mathbf{K}_i}^+(\mathbf{R}_T)$ and of the function $W_i(\mathbf{r}_T)$ defined as

$$W_i(\mathbf{r}_T)=V_T(\mathbf{r}_T)\varphi_i(\mathbf{r}_T)\,, \tag{13}$$

the elastically distorted SPB wave defined by Eq. (11) may be expressed exactly in the following form:

$$\Psi_i^{+(\mathrm{DSPB})}(\mathbf{r}_P,\mathbf{R}_P)=\int d^3k\int d^3K\,\tilde{W}_i(\mathbf{k})\tilde{\phi}_{\mathbf{K}_i}^+(\mathbf{K})(\varepsilon_\Delta-\tfrac{1}{2}q^2)^{-1}\psi_{\mathbf{q},\varepsilon_\Delta}^+(\mathbf{r}_P)\phi_{\mathbf{Q}+\Delta}(\mathbf{R}_P)\,. \tag{14}$$

Here Δ is a measure of the spread in momentum of the distorted-channel function

$$\Delta=\mathbf{K}-\mathbf{K}_i\,, \tag{15}$$

and ε_Δ is given by a relation similar to Eq. (8)

$$\varepsilon_\Delta-\tfrac{1}{2}q^2=\varepsilon_i-\tfrac{1}{2}k^2+\mathbf{v}\cdot\Delta\,, \tag{16}$$

where terms of order $(1/\mu_i)$ have been neglected. The electron wave function $\psi_{\mathbf{q},\varepsilon_\Delta}^+(\mathbf{r}_P)$ is the off-energy shell according to Eq. (16). For regions of coordinate space such that $r_P\,|\,(2\varepsilon_\Delta)^{1/2}-q\,|\ll 1$, the near-shell approximation[2]

$$\psi_{\mathbf{q},\varepsilon_\Delta}^+(\mathbf{r}_P)\simeq g^+(q,\varepsilon_\Delta)\psi_{\mathbf{q}}^+(\mathbf{r}_P) \tag{17}$$

is valid, and we obtain

$$\Psi_i^{+(\mathrm{DSPB})}(\mathbf{r}_P,\mathbf{R}_P)=\int d^3k\,\tilde{\varphi}_i(\mathbf{k})\gamma^+(q,\varepsilon)\psi_{\mathbf{q}}^+(\mathbf{r}_P)\phi_{\mathbf{Q}}(\mathbf{R}_P)\,, \tag{18}$$

where

$$\gamma^+(q,\varepsilon)=\int d^3K\,\tilde{\phi}_{\mathbf{K}_i}^+(\mathbf{K})\frac{\varepsilon-\frac{1}{2}q^2}{\varepsilon_\Delta-\frac{1}{2}q^2}g^+(q,\varepsilon_\Delta)\,. \tag{19}$$

In this derivation we have used the identity

$$(\varepsilon_i-\tfrac{1}{2}k^2)\tilde{\varphi}_i(\mathbf{k})=\tilde{W}_i(\mathbf{k})\,, \tag{20}$$

i.e., the momentum-space representation of the Schrödinger equation for the initial state. Further, we have neglected a factor $\exp(i\Delta\cdot\mathbf{R}_P)$. It is easy to see that this is valid if $\mathbf{R}_P$ is restricted to the same region around the origin as required for the validity of the near-shell approximation given in Eq. (17).

The channel distorted form of the SPB wave function (18) is equivalent to the original form of the SPB function given in Eq. (5) except for the fact that the off-shell factor g^+ has been replaced by a suitable average over the momentum distribution $\tilde{\phi}^+(K)$ in the elastic channel. To evaluate this modified off-shell factor γ^+, we insert Eq. (7) into Eq. (19) to obtain

$$\gamma^+(q,\varepsilon)=(2q^2)^{iv}\exp(\pi v/2)\Gamma(1+iv)(\tfrac{1}{2}q^2-\varepsilon)\times\int d^3K\,\tilde{\phi}_{\mathbf{K}_i}^+(\mathbf{K})(\tfrac{1}{2}q^2-\varepsilon-\mathbf{v}\cdot\Delta)^{-1-iv}\,. \tag{21}$$

Using the representation[10]

$$A^{-b}=i^b\frac{1}{\Gamma(b)}\int_0^\infty x^{b-1}\exp(-ixA)dx\,, \tag{22}$$

with $A=(\frac{1}{2}q^2-\varepsilon-\mathbf{v}\cdot\Delta)$ in Eq. (21), the K integral is expressed in terms of the distortion factor $D_{\mathbf{K}_i}^+(\mathbf{R})=\phi_{\mathbf{K}_i}^+(\mathbf{R})/\phi_{\mathbf{K}_i}(\mathbf{R})$ in coordinate space, and we find

$$\gamma^+(q,\varepsilon)=(2q^2)^{iv}(\tfrac{1}{2}q^2-\varepsilon)\times\int_0^\infty dx\,x^{iv}\exp[-ix(\tfrac{1}{2}q^2-\varepsilon)]D_{\mathbf{K}_i}^+(-x\mathbf{v})\,. \tag{23}$$

This is the main result of the present work. A detailed evaluation of γ^+ for a realistic channel distortion is a cen-

tral task for theory; however, in this Rapid Communication it suffices to discuss its qualitative features.

First, note that when $D^+_{\mathbf{K}_i}=1$ everywhere, corresponding to no distortion, the original off-shell factor g is obtained. Altnernatively, if a pure Coulomb potential is used so that the distortion factor is just a confluent hypergeometric function, Eq. (23) may be evaluated analytically, and we find that $\gamma^+(q,\varepsilon)=1$ to a good approximation. In this way, we recover the impulse approximation,[11] which has previously been obtained by the *ad hoc* omission of g^+ in Eq. (5). Note that the impulse approximation is obtained even though the Coulomb form at large distances of all two-body potentials is retained. The essential feature is that the difference V_P-U_i when operating on $|\Phi_i^+\rangle$ vanishes faster than R_T^{-1} for finite values of $\mathbf{r}_T$. Then our factor $\gamma^+(q,\varepsilon)$ generally extracts a residual influence of off-shell propagation characteristic of intermediate states of an effective short-range potential in the electronic coordinate $\mathbf{r}_P$.

It is readily seen that the channel potential given by Eq. (9) approaches a constant at small distances. The divergent Coulomb potential is accordingly not a reasonable approximation to the distortion potential in this region of space. To evaluate γ^+ for arbitrary distortion potentials, it may be noted that very large wave numbers are involved in the internuclear motion (K_i is typically of order 10^4) and that it is the distortion in the backward direction that enters in Eq. (23). This implies that the distortion $D^+_{\mathbf{K}_i}(-x\mathbf{v})$ to an excellent approximation may be represented by the Eikonal form

$$D^+_{\mathbf{K}_i}(\mathbf{R})=i(vR-\mathbf{v}\cdot\mathbf{R})^{-i\nu_P}\exp\left[-\frac{i}{v}\int_{-\infty}^{Y}\left[U_i(R)+\frac{Z_P}{R}\right]dY\right], \tag{24}$$

where Y is the coordinate of $\mathbf{R}$ along the incident momentum vector $\mathbf{K}_i=\mu_i\mathbf{v}$. The Sommerfeld parameter ν_P is given by $\nu_P=Z_P/v$. The overall phase of the right-hand side of Eq. (24) was chosen for later convenience. Inserting Eq. (24) in Eq. (23) and replacing q by v in all slowly varying functions in anticipation of a peaking approximation in the integration over the momentum distribution of the initial electron state in Eq. (18), we find

$$\gamma^+(q,\varepsilon)=i\int_0^\infty dx\,e^{-ix}\exp\left[-\frac{i}{v}\int_{xv/(q^2/2-\varepsilon)}^{\infty}\left[U_i(R)+\frac{Z_P}{R}\right]dR\right]. \tag{25}$$

This expression is readily evaluated for a channel potential which is constant inside and Coulombic outside a certain radius R_0. The result is given by the following expression:

$$\gamma^+(q,\varepsilon)=e^{-ix_0}\nu_P/(\nu_P+x_0)+x_0/(x_0+\nu_P)\exp(i\nu_P)\times{}_1F_1(i\nu_P,1+i\nu_P,-i(x_0+\nu_P)), \tag{26}$$

where the positive quantity x_0 is given by

$$x_0=R_0(\tfrac{1}{2}q^2-\varepsilon)/v. \tag{27}$$

The limit $R_0=0$ in Eq. (25) recovers the impulse approximation and the limit $R_0\to\infty$ recovers the original off-shell factor. Equation (26) interpolates between these two limits. In most applications, we expect that $x\ll\nu_P$ so Eq. (28) simply reduces to

$$\gamma^+(q,\varepsilon)=\exp(-ix_0). \tag{28}$$

For qualitative purposes, it is realistic to assume that R_0 is of order $1/Z_T$, while $\frac{1}{2}q^2-\varepsilon$ is of order Z_T^2 according to Eq. (8). The condition $x_0\ll\nu_P$ is, accordingly, expected to be satisfied if $Z_P\gg Z_T$, as assumed from the outset in this paper. Equation (28) is, therefore, acceptable as a first approximation for asymmetric collisions. At low velocities, neither ν_P nor x_0 is necessarily small compared to unity. Retention of the phase factor in Eq. (28) is, therefore, important, particularly to correctly evaluate contributions from high-momentum components of the initial electron state.

In summary, we have shown that the incorporation of the channel distortion significantly alters the magnitude and phase of the SPB wave function in the physically important region of small separations. This change is expressed in terms of a modified factor γ^+ to replace the off-shell factor g^+. The new factor is of nearly unit magnitude and has a moderate phase variation. This should be contrasted with the large magnitude and rapid phase variation of the original off-shell factor.

It should be noticed that the pronounced compensation between channel distortion and off-energy-shell motion shows that approximations retaining one effect but not the other are incomplete. This conclusion also applies to first-order theories discussed recently in the literature.[12]

In applications to normal capture, it was shown in Ref. 1 that the large magnitude and the rapid phase of the undistorted g^+ factor tend to compensate when the average over the momentum distribution of the initial electron state is performed. The original SPB capture cross section is, as a matter of fact, smaller than that of the impulse approximation at lower velocities. The retention of the phase factor of γ^+ in Eq. (28) will produce a similar effect.

The situation is different in applications to radiative electron capture (REC). Here the off-shell factor appears in its unaveraged form as a factor multiplying the relevant matrix element.[13,14] The inclusion of the channel distortion, therefore, reduces the SPB cross section by the factor $|\gamma^+/g^+|^2$, i.e., typically an order of magnitude. Further, since the phase of the off-shell factor is immaterial for REC, we may conclude that the channel-distorted SPB approximation is fundamentally identical to the impulse approximation for radiative electron capture. This is essential because it is known that the impulse approximation is in good accord[14] with available experimental data.

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