Nearly normalized, distorted strong-potential Born state vector

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Whether an approximate scattering state vector retains the normalized nature of its exact counterpart reflects on the quality of the approximation made. It is shown that the distorted-wave strong-potential Born state vector, employed in asymmetric electron-capture theory, is normalized (in a near-the-energy-shell approximation) to within a few percent, even at intermediate energies where capture is most likely. There is thus little need to renormalize the state, in contrast to the analogous undistorted state vector [J. Phys. B **25**, 3823 (1992)], where a radical loss of normalization occurs.

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At intermediate projectile energies in asymmetric collisions, the strong-potential Born approximation to the exact electron-capture amplitude has been much studied in the past decade. The original form was built on the conceptual framework of virtual ionization of the target electron and showed promising agreement with experiment [1], but it suffered from an elastic-channel singularity (due to the long range of the Coulomb potential), which compromised the use of approximate evaluations [2]. A distorted-wave form of the theory maintained the conceptual basis while incorporating a short-range final-channel interaction that ensures a well behaved theory [3,4]. Calculations employing realistic atomic potentials have shown good agreement with experiment [5]. The normalization of the undistorted strong-potential Born scattering state was considered [6] and found to deviate appreciably from unity at intermediate energies [7], where capture is most likely (and the experimental data exist). A renormalization of the theory was introduced to improve agreement with the data, but it was not integrated into the overall scattering formalism. The normalization of the distorted strong-potential Born approximation is studied in the present article. A minimal need for renormalization of the distorted strong-potential Born (DSPB) theory is found and only when the impact velocity becomes small (below ~ 4 a.u.).

A numerical evaluation of the exact form of the DSPB normalization is not feasible with the incorporation of a realistic atomic target potential. The approximate treatment presented here relies on the small binding energy of the electron relative to its scattering energy to introduce the near-the-energy-shell representation of the scattering wave function and, further, on the neglect of factors that introduce errors of the order of m/M_P and m/M_T (with M_P, M_T, and m the projectile, target nuclear, and electronic masses, respectively). In the rest of this article, the definition of the normalization for the general scattering state is given and then the normalization for the distorted strong-potential Born scattering state is derived in the near-shell approximation. The normalization constant is numerically evaluated, as is the constant for the undistorted theory. Atomic units are used.

In a one-electron model, an asymmetric three-body collision is treated where a projectile ion P with small nuclear charge Z_P is incident on a target consisting of an electron e and a target ion T with large nuclear charge Z_T. Electron capture is assumed to occur. Either the target or projectile may contain passive electrons; thus the interactions between each pair of particles have the modified Coulomb form. The potentials reduce asymptotically to pure Coulomb forms: $V_{Te}(r_T) \sim -Z_T^\infty/r_T$ as $r_T \to \infty$ and $V_{PT}(R) \sim Z_P^\infty Z_T^\infty/R$ as $R \to \infty$, where the asymptotic charges are Z_P^∞ and Z_T^∞. The coordinates of the electron relative to the projectile and target ions are denoted by $\mathbf{r}_P$ and $\mathbf{r}_T$, respectively, the projectile coordinates relative to the target ion by $\mathbf{R}$, the projectile-electron system coordinates relative to the target ion by $\mathbf{R}_P$, and the projectile coordinates relative the target by $\mathbf{R}_T$.

For this three-body problem with relative motion of wave vector $\mathbf{K}$ and internal state f, the exact final, incoming-wave scattering state $\Psi^-_{\mathbf{K},f}$ satisfies the normalization condition

$$\langle \Psi^-_{\mathbf{K}',f} \,|\, \Psi^-_{\mathbf{K},f} \rangle = \delta(\mathbf{K}' - \mathbf{K}), \tag{1}$$

assuming that the final internal motion is asymptotically bound and the corresponding state normalized [8,9]. Generally, the loss of normalization of an approximate scattering state can affect the transition amplitude; thus the retention of normalization is desirable.

Within a distorted-wave framework, the strong-potential Born approximation to this exact state is defined using the Green operator for the strong target potential and the effective short-range final-state interaction [3], viz.,

$$|\, \Psi^-_{\mathbf{K},f} \rangle \approx [1 + G_T^- (V_{Te} - U_f)] |\, \Phi^-_{\mathbf{K},f} \rangle, \tag{2}$$

where the strong-potential Born designation here and below is not explicitly noted in order to keep the notation manageable. In Eq. (2), U_f is the final-channel distortion potential and $G_T^-(E) = (E - H_0 - V_T - i\eta)^{-1}$ is the target Green operator with H_0 the free Hamiltonian for

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the heavy-particle and electronic motion and $\eta \to 0+$. The total system energy is given by $E = (1/2\nu_f)K^2 + \varepsilon_f$, where ε_f is the final bound-state energy. The velocity is defined in terms of the final-state wave vector as $\mathbf{v} = \mathbf{K}/\nu_f$, where the relative reduced mass and associated mass ratio are $\nu_f = M_T(m+M_P)/(m+M_P+M_T)$ and $\beta = M_P/(m+M_P)$.

The final asymptotic scattering state is given by

$$\langle \mathbf{R}_P, \mathbf{r}_P \,|\, \Phi^-_{\mathbf{K},f} \rangle \equiv \phi_f(\mathbf{r}_P)\,\phi_{\mathbf{K}}(\mathbf{R}_P)\,D^-_{\mathbf{K}}(\mathbf{R}_P) \qquad (3)$$

with a plane-wave function normalized as $\phi_{\mathbf{K}}(\mathbf{R}_P) \equiv (2\pi)^{-3/2}\; e^{i\mathbf{K}\cdot\mathbf{R}_P}$. The distorted part of the heavy-particle motion in Eq. (3) is given by

$$D^-_{\mathbf{K}}(\mathbf{R}) \equiv (vR + \mathbf{v}\cdot\mathbf{R})^{i\tilde{\nu}_T^\infty} \times \exp\left(\frac{i}{v}\int_Y^\infty dY'\,[U_f(R) + Z_T^\infty/R]\right), \qquad (4)$$

with $Y = \mathbf{R}\cdot\hat{\mathbf{v}}$ and $\tilde{\nu}_T^\infty = Z_T^\infty/v$ [10]. The distorting potential, though arbitrary in principle, is defined here by assuming that only the final electronic charge cloud need be considered for the purpose of screening the target nucleus, that is, it is defined by folding the final-channel interaction with the final bound-state wave function

$$U_f(\mathbf{R}_P) = \int d\mathbf{r}_P\; |\phi_f(\mathbf{r}_P)|^2\; V_{Te}(\beta\mathbf{r}_P + \mathbf{R}_P). \qquad (5)$$

The state in Eq. (2) is used, specifically, in the amplitude $\langle \Psi^-_{\mathbf{K},f}\,|V_{Pe} - U_i|\Phi^+_{\mathbf{K}_i,i}\rangle$, where $V_{Pe}(r_P) = -Z_P/r_P$, U_i is the initial-channel distortion potential and $|\Phi^+_{\mathbf{K}_i,i}\rangle$ is defined analogously to $|\,\Phi^-_{\mathbf{K},f}\,\rangle$. The initial wave vector is $\mathbf{K}_i$.

Taulbjerg, Barrachina, and Macek have reduced the distorted strong-potential Born scattering state in coordinate representation to the form [4]

$$\Psi^-_{\mathbf{K},f}(\mathbf{r}_T,\mathbf{R}_T) \equiv (2\pi)^{-3/2}\int d\mathbf{k}\,\tilde{\phi}_f(\mathbf{k})\int d\mathbf{S}\,\tilde{D}^-_{\mathbf{K}}(\mathbf{S}) \times \frac{\Delta\varepsilon}{\Delta\varepsilon - \mathbf{v}\cdot\mathbf{S}}\,\psi^-_{\mathbf{q},\varepsilon_{\mathbf{S}}}(\mathbf{r}_T)\,\phi_{\mathbf{Q}+\mathbf{S}}(\mathbf{R}_T), \qquad (6)$$

where $\mathbf{q} = \mathbf{k} + \mathbf{v}$ and $\mathbf{Q} = \beta\mathbf{K} - \mathbf{k}$. The off-the-energy-shell scattering wave function for the intermediate electronic state (in the strong potential) is $\psi^-_{\varepsilon,\mathbf{q}}(\mathbf{r}_T)$ with off-shell energy $\varepsilon_{\mathbf{S}} = \frac{1}{2}v^2 + \mathbf{v}\cdot(\mathbf{k}-\mathbf{S}) + \varepsilon_f$. The energy defect is defined as $\Delta\varepsilon = \varepsilon_f - \frac{1}{2}k^2$.

Considering that the relevant interaction region is centered around the target nucleus $r_T \lesssim Z_T$ and using previous work on modified Coulomb potentials [11,12], which extends the result of Chen and Chen [13] on pure Coulomb scattering, the off-shell wave function can be approximated to order $(Z_P/v)^2$ by a target continuum eigenstate $\psi^-_{\mathbf{q}}(\mathbf{r}_T)$ multiplied by an off-shell factor

$$\psi^-_{\varepsilon,\mathbf{q}}(\mathbf{r}_T) \approx g^-(q,\varepsilon)\,\psi^-_{\mathbf{q}}(\mathbf{r}_T) \qquad (7)$$

for $\frac{1}{2}q^2 - \varepsilon \ll \varepsilon$ with $\varepsilon \equiv \frac{1}{2}v^2 + \mathbf{v}\cdot\mathbf{k} + \varepsilon_f$. The Coulomb off-shell factor is defined as

$$g^-(q,\varepsilon) = e^{\pi\nu^\infty/2}\,\Gamma(1 + i\nu^\infty)\;\left[\left(q^2 - 2\varepsilon\right)/8\varepsilon\right]^{i\nu^\infty}, \qquad (8)$$

where $\nu^\infty \equiv Z^\infty/(2\varepsilon + i\eta)^{1/2}$ and $\Gamma(x)$ is the Gamma function.

Using the near-the-energy-shell approximation of Eq. (7) in Eq. (6) and noting that since the distortion part of the heavy-particle motion is sharply peaked about $\mathbf{S} = \mathbf{0}$ the factor $e^{i\mathbf{S}\cdot\mathbf{R}_T}$ in the $\mathbf{S}$ integrand of Eq. (6) can be neglected, the scattering wave function can be written in the form [4]

$$\Psi^-_{\mathbf{K},f}(\mathbf{r}_T,\mathbf{R}_T) \approx (2\pi)^{-3/2}\int d\mathbf{k}\,\tilde{\phi}_f(\mathbf{k})\,\gamma^-(q,\varepsilon) \times \psi^-_{\mathbf{q}}(\mathbf{r}_T)\,\phi_{\mathbf{Q}}(\mathbf{R}_T). \qquad (9)$$

A new, integrated off-shell factor appears in this expression, deriving from an interplay of the pure Coulomb off-shell factor and the distorted motion of the projectile, which has the form

$$\gamma^-(q,\varepsilon) = (2\pi)^{-3/2}\,(2q^2)^{-i\nu_T^\infty}\,e^{\pi\nu_T^\infty}\,\Gamma(1 - i\nu_T^\infty)\,\Delta\varepsilon \times \int d\mathbf{S}\,\tilde{D}^-_{\mathbf{K}}(\mathbf{S})\,(\Delta\varepsilon - \mathbf{v}\cdot\mathbf{S})^{-1-i\nu_T}. \qquad (10)$$

Equation (9) represents an electronic "wave packet" as seen from the *target* frame that, during the capture process, scatters off the target ion. The momentum distribution of the packet, centered on $\mathbf{v}$ (the outgoing projectile's velocity), is determined by the final bound state $\tilde{\phi}_f(\mathbf{k})$. This distribution is modified in both magnitude and phase by the off-shell factor. The question is then whether this affects the scattering-state normalization.

The normalization condition entails an integration over both heavy-particle and electronic coordinates

$$\langle\,\Psi^-_{\mathbf{K}',f}\,|\,\Psi^-_{\mathbf{K},f}\,\rangle = \int d\mathbf{r}_T\,d\mathbf{R}_T\;\Psi^-_{\mathbf{K}',f}(\mathbf{r}_T,\mathbf{R}_T)^* \times \Psi^-_{\mathbf{K},f}(\mathbf{r}_T,\mathbf{R}_T). \qquad (11)$$

Inserting Eq. (9) for the scattering state into Eq. (11), one has

$$\langle\,\Psi^-_{\mathbf{K}',f}\,|\,\Psi^-_{\mathbf{K},f}\,\rangle \approx (2\pi)^{-3}\int d\mathbf{k}'\,d\mathbf{k}\;\tilde{\phi}_f(\mathbf{k}')^*\,\tilde{\phi}_f(\mathbf{k})\,\gamma^-(q',\varepsilon')^* \times \gamma^-(q,\varepsilon)\,\langle\psi^-_{\mathbf{q}'}\,|\,\psi^-_{\mathbf{q}}\rangle\,\langle\phi_{\mathbf{Q}'}\,|\,\phi_{\mathbf{Q}}\rangle. \qquad (12)$$

Using normalization of the electronic continuum eigenstates and plane-wave states to three-dimensional δ functions and performing the $\mathbf{k}'$ integration gives

$$\langle\,\Psi^-_{\mathbf{K}',f}\,|\,\Psi^-_{\mathbf{K},f}\,\rangle = N_f(v)^2\,\delta(\mathbf{K}' - \mathbf{K}), \qquad (13)$$

where

$$N_f(v) \equiv \left(\int d\mathbf{k}\,\left|\tilde{\phi}_f(\mathbf{k})\right|^2\,\left|\gamma^-(q,\varepsilon)\right|^2\right)^{1/2}. \qquad (14)$$

The dependences of the normalization constant $N_f(v)$ on the final bound-state wave function and on the velocity are noted. Because the bound-state wave function is normalized, the normalization of the distorted strong-potential Born scattering state rests on whether the modulus of the off-shell factor, when integrated over all momentum values, deviates from unity. This condition on the scattering state is only a global one, consistent with the normalization procedure itself. The loss of normalization at the near-shell level of approximation is due entirely to the norm of the off-shell factor.

To evaluate the normalization constant $N_f(v)$, an integral representation [14] and the change of variables $u = vx/\Delta\varepsilon$ and $W = R/u$ [5] are used in Eq. (10), giving the form [4]

$$\gamma^-(q,\varepsilon) = -\frac{i}{v}\left(2q^2/v\right)^{-i\nu_T^\infty}(2v)^{i\tilde{\nu}_T^\infty} \times \int_0^\infty du\, u^{i(\nu_T^\infty-\tilde{\nu}_T^\infty)} e^{-iu\Delta\varepsilon/v} \times \exp\left(\frac{i}{v}\int_1^\infty dW\,[uU_f(uW)+Z_T^\infty/W]\right).$$

Use of the hydrogenic momentum wave function $\tilde{\phi}_{1s}(\mathbf{k}) = (2^3Z^5)^{1/2}/\pi(k^2+Z^2)^2$ then leads to

$$N_f(v)^2 = \frac{2^3 Z_P^5}{\pi^2 v^2}\int d\mathbf{k}\,(k^2+Z_P^2)^{-2}\left|\left(2q^2/v\right)^{-i\nu_T^\infty}(2v)^{i\tilde{\nu}_T^\infty}\right|^2 \times\left|\int_0^\infty du\, u^{i(\nu_T^\infty-\tilde{\nu}_T^\infty)}e^{-iu\Delta\varepsilon/v}\exp\left(\frac{i}{v}\int_1^\infty dW[uU_f(uW)+Z_T^\infty/W]\right)\right|^2. \quad (15)$$

This form is useful because the W integration can be done using the exponential integral $E_1(z) = \int_1^\infty dz\; e^{-zt}/t$, leaving a two-dimensional numerical integration [15]. Note that $\nu_T^\infty \neq \tilde{\nu}_T^\infty$, due to the $\mathbf{k}\cdot\mathbf{v}$ term in the former. The atomic potential used is

$$V_{Te}(r_T) = -\frac{1}{r}\left(\frac{Z_T - Z_T^\infty}{H(e^{r/d}-1)+1} + Z_T^\infty\right),$$

where the screening d and scaling H parameters are optimized for each atom [16]. This potential is used in Eq. (5) to obtain U_f, which appears in Eq. (4) for $D^-_{\mathbf{K},f}$ [5].

For reference purposes, in the undistorted strong-potential Born approximation [7], where $D^-_{\mathbf{K}}$ is omitted from Eq. (3) and U_f is omitted from Eq. (2), the normalization constant is obtained by replacing γ^- by g^- to give, again in the near-shell approximation,

$$N_f(v) \approx \left(\int d\mathbf{k}\,\left|\tilde{\phi}_f(\mathbf{k})\right|^2\,\left|g^-(q,\varepsilon)\right|^2\right)^{1/2}. \quad (16)$$

Noting Eq. (8), it is seen that the rapidly varying parts of g^- are canceled by $(g^-)^*$. Thus, since $|\tilde{\phi}_f(\mathbf{k})|^2$ is *highly* localized about $\mathbf{k} = \mathbf{0}$, an accurate approximation to Eq. (16) can be made as follows:

$$N_f(v) \approx \left|g^-(q,\varepsilon)\right|_{\mathbf{k}=\mathbf{0}}\left(\int d\mathbf{k}\,|\tilde{\phi}_f(\mathbf{k})|^2\right)^{1/2} = \left[2\pi\nu_T^\infty/(1-e^{-2\pi\nu_T^\infty})\right]^{1/2}, \quad (17)$$

where $\nu_T^\infty = Z_T^\infty/(v^2 - 2\varepsilon_f)^{1/2}$. For high velocities, $N_f \approx 1 + \pi\nu_T^\infty/2$, showing that the normalization approaches unity. For lower velocities, however, the correction can become significant and the scattering state needs to be corrected (renormalized).

The normalization constants for the distorted strong-potential Born approximate scattering state Eq. (15) and the similar constant for the undistorted state Eq. (17), as functions of impact velocity, are plotted in Fig. 1. Equation (15) is evaluated using an adaptive eight-panel quadrature scheme [15] with great care taken in performing the barely convergent u integration. The calculated values are obtained to four digit accuracy. Potential parameters used in the calculations are listed in Ref. [5]. Results are presented for protons on carbon, neon, and argon over a range of intermediate velocities spanning the available experimental data. It is seen that the deviation from unity of the normalization for the distorted theory is generally a few percent. For argon, the deviation from unity is at most a few tenths of a percent. For neon, the deviation varies from slightly under 2% up to about 5%. (The lowest velocity for which data exist is $v/v_T = 0.5$ a.u.) For carbon, where the largest deviation (up to 7.5%) exists, the smallest velocity shown is 2 a.u., very low in absolute terms for a perturbative theory. (The lowest velocity for which data exist occurs at $v/v_T = 0.61$ a.u., where the error is 7%.) Even the largest velocity is only about 6.5 a.u. The constants for

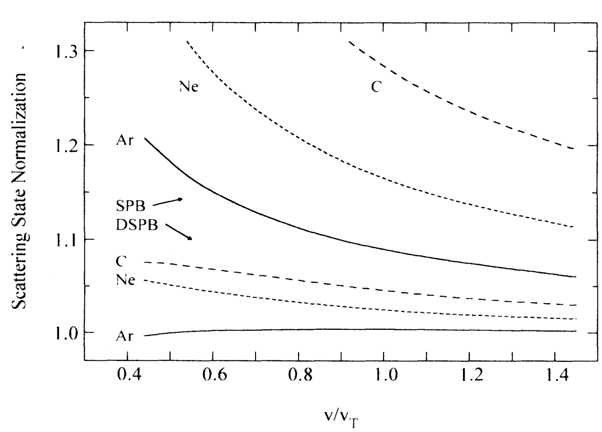

FIG. 1. Normalization constants for the distorted (DSPB, lower curves) and undistorted (SPB, upper curves) strong-potential Born scattering states are shown versus projectile velocity scaled by the characteristic orbital velocity of the target K shell.

the distorted theory all approach unity as the velocity increases. By contrast, the deviations from unity for the undistorted theory are very large and they remain larger than for the distorted theory at larger velocities, even in the argon case. Thus one can conclude that the distorted strong-potential Born electron-capture cross sections, differential or integrated, need to be corrected minimally for loss of normalization in the scattering state and then only for very low velocities in the less asymmetric systems.

In summary, an explicit form for the normalization constant of the distorted strong-potential Born approximation to the final scattering state has been derived. Using a realistic atomic potential, calculations of the constant versus projectile velocity for protons on carbon, neon, and argon show that the scattering state, in a near-shell approximation, experiences only a slight loss of normalization. The largest error is seen in the carbon case, which is attributable to the small velocities encountered. Only for carbon would the correction of the wave function (i.e., its renormalization) be noticeable on a plot.

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$$\Gamma(1+i\nu)(iA)^{-1-i\nu} = \int_0^\infty dx\, x^{i\nu}\, e^{-ixA}.$$

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