Considerations in the Use of Born Closure Schemes for positron-Atom Collisions

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Abstract.

In this letter a commonly used procedure to ensure partial-wave convergence in the differential cross section is examined. Although the closure scheme in which the first Born approximation is used to represent contributions from weakly scattered partial waves is found to work well, the additional approximation of using the long-range form of the positron-atom interaction potential for all space can be problematic at intermediate scattering energies. An example involving elastic positron-Ar scattering is presented.

New theoretical interest in calculating low- and intermediate-energy differential cross sections (DCS) for positron collisions with noble gas atoms has been sparked by recent relative [Smith *et al* 1990] and absolute [Dou *et al* 1992a, 1992b] DCS measurements. However, the DCS converges slowly with regard to the number of partial waves that must be included, even at relatively low scattering energies. This means that one must either approximate convergence by explicitly including a very large number of partial waves in the calculation [Ali and Fraser 1977, McEachran *et al* 1979, De Fazio *et al* 1994], or one must make use of a closure scheme [Thompson 1966, Wadhera and Nahar 1987, Lino *et al* 1994] which implicitly includes contributions from all partial waves. The purpose of this letter is to point out a "defect" in most methods currently being used to ensure convergence in the DCS that, while negligible at low energies, can lead to significant errors at intermediate energies and to suggest an efficient alternative. The nature of the approximations being used in most current strategies are less appropriate for positron collisions than for electron collisions and will be problematic for more polarizable systems.

Within the context of a single-center expansion of the scattering equations the truncated (in l) expression for the single-channel, elastic scattering amplitude for collision energy $E = k^2/2$ and angle θ is given by

$$f_t(k,\theta) = \frac{1}{2ik}\sum_{l=0}^{l_{max}}(2l+1)\,[e^{2i\delta_l(k)}-1]\,P_l(\cos\theta), \tag{1}$$

where δ_l is the phase shift for the l^{th} partial wave and P_l is the l^{th} Legendre function. The standard procedure is to solve for the phase shifts from $l=0$ to l_{max}, compute f_t, and then obtain the DCS for energy E and angle θ from

$$\sigma_k(\theta) = |f_t(k,\theta)|^2\,. \tag{2}$$

Unfortunately, f_t and the DCS obtained from it are only approximately converged since, in principle, l_{max} in equation (1) should be infinity. In practice, of course, a finite (though possibly large) value of l_{max} is used to achieve a given level of convergence with the particular value depending on the system, the scattering energy, and the scattering quantity of interest [Zigman 1995]. However, it has been pointed out [van Wyngaarden and Walters 1986, Nesbet and Geltman 1986] that to achieve convergence in the forward direction, the partial wave sum for the DCS must be extended to infinity. An elegant and practical way around this difficulty is to use a closure scheme for the scattering amplitude that includes contributions from all partial waves. Since the centrifugal barrier term in the effective potential prevents higher partial waves from penetrating too deeply into the near-target region where the positron-atom interaction potential would induce strong distortions, the high-angular-momentum partial waves are only weakly scattered. Thus, a weak scattering method such as the first Born approximation (FBA) can be used to include contributions from $l_{max}+1$ to ∞ in the scattering amplitude. The scattering amplitude obtained from such a Born closure scheme has the form [Wadhera and Nahar 1987]

$$\begin{aligned} f(k,\theta) &= f^B(k,\theta) \; - \; f_t^B(k,\theta) \; + \; f_t(k,\theta) \\ &= \Delta f^B(k,\theta) \; + \; f_t(k,\theta) \qquad (3) \end{aligned}$$

where the scattering amplitude in the FBA, f^B, contains contributions from *all* partial waves and the truncated FBA amplitude,

$$f_t^B(k,\theta) \;=\; \sum_{l=0}^{l_{max}} f_l^B(k)\, P_l(\cos\theta), \qquad (4)$$

contains contributions only up to l_{max}. Although the FBA is a poor approximation for the strongly scattered low-angular-momentum partial waves, the closure scheme removes the contribution from these lower partial waves by subtracting f_t^B from f^B and replaces it with the correct result f_t obtained from solving the full scattering equations numerically.

Writing the total positron-atom interaction potential $V_{sp}(\mathbf{r})$ as

$$V_{sp}(\mathbf{r}) = V_{st}(\mathbf{r}) + V_{pol}(\mathbf{r}), \tag{5}$$

where $V_{st}(\mathbf{r})$ is the static field, $V_{pol}(\mathbf{r})$ represents the induced polarization potential, and defining $\mathbf{q} \equiv \mathbf{k}_i - \mathbf{k}_f$ with $|\mathbf{k}_i| = |\mathbf{k}_f| = k$ for elastic collisions, we have [Mott and Massey 1965]

$$f^B(k,\theta) = -\frac{1}{2\pi}\int V_{sp}(\mathbf{r})\, e^{i\mathbf{q}\cdot\mathbf{r}}\, d\mathbf{r}. \tag{6}$$

By making use of the spherical symmetry of V_{sp} as well as the known long-range dependence of this potential on the induced dipole polarizability α,

$$V_{sp}(r) \sim V_{LR}(r) = -\frac{\alpha}{2r^4} \qquad \text{for} \quad (r \geq r_m), \tag{7}$$

we can rewrite equation (6) as

$$f^B(k,\theta) = -\frac{2}{q}\int_0^{r_m} r\, \sin(qr) V_{sp}(r) dr + \frac{\alpha}{2}\left\{\frac{\sin(qr_m)}{qr_m^2} + \frac{\cos(qr_m)}{r_m} + q\,\mathrm{si}(qr_m)\right\}, \tag{8}$$

where $\mathrm{si}(z) = \mathrm{Si}(z) - \pi/2$ and $\mathrm{Si}(z)$ is the Sine integral [Abramowitz and Stegun 1965]. The matching radius r_m defines the distance at which the positron-atom interaction potential assumes the asymptotic form shown in equation (7); for the positron-Ar scattering calculations reported here a value of $r_m = 15\ a_o$ was used. Once f^B is obtained for a set of quadrature angles, the Legendre expansion coefficients for equation (4) may be obtained from projection

$$f_l^B(k) = \left(\frac{2l+1}{2}\right)\int_0^{\pi} \sin(\theta)\, f^B(k,\theta)\, P_l(\cos\theta)\, d\theta, \tag{9}$$

or, independently from [Thompson 1966]

$$f_l^B(k) = -2\,(2l+1)\int_0^{\infty} [r\, j_l(kr)]^2\, V_{sp}(r)\, dr, \tag{10}$$

where $j_l(kr)$ is a spherical Bessel function.

Thus far the procedure we have discussed involves replacing f_t in equation (2) with the Born closure amplitude of equation (3), and providing that the FBA accurately represents contributions for $l > l_{max}$, there are no other approximations. Although closure schemes involving the FBA have been widely used for a variety of systems and processes [Collins and Norcross 1978, Norcross and Padial 1982, Rescigno and Schneider 1992], most of the positron-atom schemes incorporate the *additional approximation* that V_{sp} is replaced by the long-range form V_{LR} of equation (7) for $0 \leq r \leq \infty$. This is done for the following (sound) reasons. First, since the Born closure includes contributions from the higher-order partial waves—which at low scattering energies are largely excluded from the near-target region by the centrifugal barrier—the long-range potential is primarily responsible for the scattering. Second, this leads to a closed form for the long-range, Born-closure correction [Thompson 1966, Wadhera and Nahar 1987]

$$\begin{aligned}
\Delta f^{B_{LR}}(k,\theta) &= f^{B_{LR}}(k,\theta) - f_t^{B_{LR}}(k,\theta) \\
&= -\pi k \alpha \left\{ \frac{\sin(\theta/2)}{2} + \sum_{l=0}^{l_{max}} \frac{P_l(\cos\theta)}{(2l-1)(2l+3)} \right\}.
\end{aligned} \tag{11}$$

Here, the appropriate value of l_{max} is determined by the additional constraint that no partial wave $l > l_{max}$ penetrate into the region where V_{sp} is substantially different from V_{LR}. We will show that the value of l_{max} needed to satisfy this additional assumption is significantly larger for intermediate collision energies than the value needed to satisfy the FBA alone.

A good method for determining l_{max} is to compare (for a given collision energy) the phase shifts $\delta_l^{B_{LR}}$ obtained from the FBA using V_{LR} with the phase shifts obtained from the FBA and full scattering methods when the actual interaction potential V_{sp} is used, δ_l^B and δ_l, respectively. The respective Born phase shifts are given by [Mott and Massey

1965]

$$\tan(\delta_l^B) = -2k \int_0^\infty [r\, j_l(kr)]^2\, V_{sp}(r)\, dr, \tag{12}$$

and by [O'Malley *et al* 1962]

$$\tan(\delta_l^{B_{LR}}) = \frac{\pi \alpha k^2}{(2l-1)(2l+1)(2l+3)} \qquad \text{for} \quad l \geq 1. \tag{13}$$

Results for positron-Ar elastic collisions calculated in the Distributed Positron Model (DPM) [Gibson 1990, 1992] are presented in table 1 for scattering energies of 5 and 200 eV. In this method, a modified adiabatic approach that approximates (nonadiabatic) short-range correlation effects is used to calculate the polarization component of the positron-atom interaction potential. The total interaction potential is then obtained by adding a near-Hartree-Fock static field to the polarization potential. As currently implemented, the DPM does not account for energy-dependent, inelastic, or rearrangement effects. Details of the DPM calculation for positron-Ar and positron-Ne scattering will be presented elsewhere [Gibson *et al* 1995]. It is clear from the values in table 1 that for 5 eV the FBA using the full interaction potential provides excellent agreement (5% or better) with the actual scattering phase shifts for $l \geq 3$ and that the long-range FBA phase shifts are also in reasonable agreement (no worse than 23%) for this range. The situation at 200 eV is significantly different. The results for 200 eV show that the full-potential FBA phase shifts δ_l^B are (aside from $l = 6$, where the phase shift is passing through 0) still in good agreement (better than 20%) with δ_l for $l \geq 1$. However, the long-range-potential FBA phase shifts $\delta_l^{B_{LR}}$ not only disagree with δ_l in magnitude for $l < 10$, but are opposite in sign for $l < 7$. Similar results are observed for a collision energy of 100 eV (not shown). Thus, if V_{LR} is used for all r, then a value of $l_{max} > 10$ for collision energies on the order of 200 eV must be used in equation (11) *and* in equation (1), whereas $l_{max} = 4$ is sufficient if V_{sp} is used instead.

Table 1: Elastic e^{+}-Ar scattering phase shifts at 5 and 200 eV

	5 eV			200 eV		
l	$\delta_l(k)$	$\delta_l^B(k)$	$\delta_l^{B_{LR}}(k)$	$\delta_l(k)$	$\delta_l^B(k)$	$\delta_l^{B_{LR}}(k)$
0	-0.2917	-1.2853	——	0.8071	-1.3815	——
1	0.2339	0.1759	0.6980	-1.3605	-1.1327	1.5410
2	0.1457	0.1314	0.1193	-0.7762	-0.8193	1.3651
3	0.0517	0.0493	0.0399	-0.4190	-0.4919	1.0116
4	0.0207	0.0204	0.0182	-0.2014	-0.2395	0.6282
5	0.0103	0.0102	0.0098	-0.0730	-0.0864	0.3728
6	0.0060	0.0060	0.0059	-0.0014	-0.0048	0.2305
7	0.0038	0.0038	0.0038	0.0354	0.0350	0.1507
8	0.0026	0.0026	0.0026	0.0516	0.0518	0.1035
9	0.0019	0.0019	0.0019	0.0560	0.0561	0.0741
10	0.0014	0.0014	0.0014	0.0541	0.0540	0.0548

The reason that a much larger value of l_{max} is required for $\Delta f^{B_{LR}}$ is due entirely to the physics of the centrifugal barrier. At intermediate collision energies, more partial waves penetrate the intermediate- and near-target regions where V_{sp} is quite different from V_{LR}—for example, near the target the actual potential is strongly repulsive, while the long-range form is everywhere attractive. Thus, only those higher partial waves that fail to sample the inner region of the potential will be accurately represented in a closure scheme that uses $\Delta f^{B_{LR}}$. This is illustrated in figure 1 where, for $l = 4$ and $l = 5$ at 200 eV scattering energy, the effective potentials and scattering solutions for V_{sp} and V_{LR} are shown. A comparison of the effective potential curves and the classical turning points shows that the Ricatti functions have substantial amplitude over the region where the effective potentials bifurcate. It can also be seen that the FBA scattering solution j_4^R is quite close to the actual solution u_4 and that for $l = 5$ the two solutions are barely distinguishable on the graph. However, the actual scattering solutions for V_{LR} are distinctly different, which demonstrates

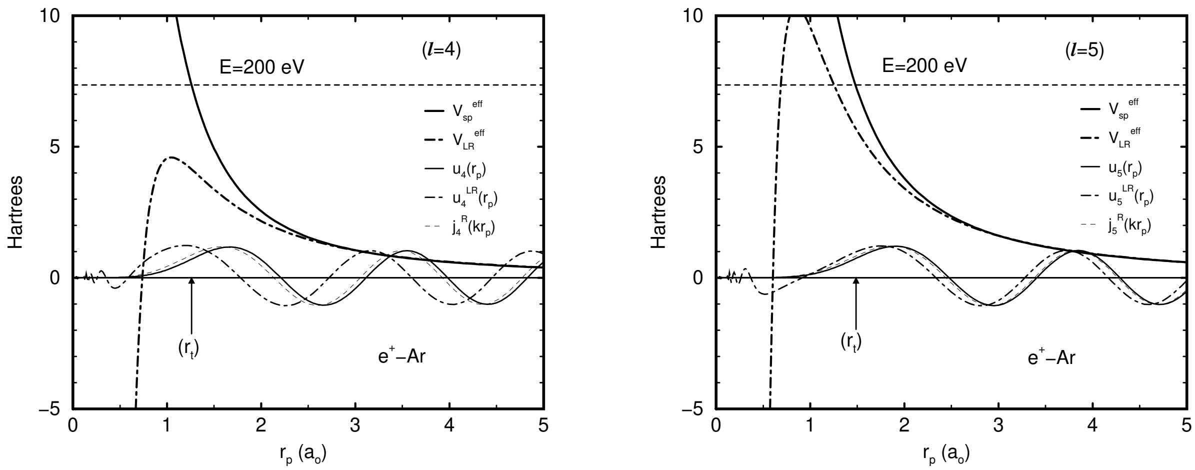

Figure 1: Effective potentials for $l=4$ and $l=5$ at 200 eV: thick solid curve (V_{sp}^{eff}); thick chain-dashed curve (V_{LR}^{eff}). Also shown are the scattering energy (thick dashed curve) and the classical turning radius (r_t) for V_{sp}^{eff}. The scattering solutions for V_{sp} are shown as the thin solid lines (u_4 and u_5), while the solutions for V_{LR} are shown as the thin chain-dashed curves (u_4^{LR} and u_5^{LR}). For comparison the zero-potential, Ricatti-Bessel functions are plotted as the thin dashed lines (j_4^R and j_5^R).

that the centrifugal barrier term is insufficient to keep these partial waves from sampling at least some of the region where the two potentials deviate. Due to the difference in sign of the short-range effective potentials, these discrepancies are more pronounced for positron collisions than for electron collisions. Such a dichotomy has been observed by McEachran and Stauffer (1986) who report using $l_{max}=6$ for electron and $l_{max}=13$ for positron collisions with He, Ne, and Ar up to 250 eV.

As shown in the figure and table above, the appropriate value of l_{max} when V_{LR} is used is significantly larger than is required for just the validity of the FBA. Although calculating Δf^B requires more numerical work than does $\Delta f^{B_{LR}}$, this effort is more than offset at higher collision energies by not having to include additional partial waves in the computation of f_t. For efficiency we utilize a Born r-closure procedure [Morrison *et al*

1984] for computing f_l^B (see equation (10)) that makes use of the closed form expressions available for $f_l^{B_{LR}}$ [Nesbet and Geltman 1986], *viz*

$$\begin{aligned} f_l^B(k) &= \Delta f_l^B + f_l^{B_{LR}} \\ &= -2(2l+1)\int_0^{r_m} [r\, j_l(kr)]^2\, \left(V_{sp}(r) - V_{LR}(r)\right)\, dr \\ &\quad + \frac{\pi\alpha k}{(2l-1)(2l+3)} \quad \text{for } (l \geq 1). \end{aligned} \tag{14}$$

For $l = 0$ we use

$$\begin{aligned} f_0^B(k) &= -2\left\{\frac{1}{k^2}\int_0^{r_m} \sin^2(kr)\, V_{sp}(r)\, dr \; - \; \frac{\alpha}{12k^2 r_m^3}\Big(1 + [2(kr_m)^2 - 1]\, \cos(2kr_m) \right. \\ &\quad \left. + \; kr_m \sin(2kr_m) \; + \; 4(kr_m)^3\, \mathrm{si}(2kr_m)\Big)\right\}. \end{aligned} \tag{15}$$

This formulation allows us to restrict the numerical integration to a finite region while still including contributions from all space in the scattering amplitude.

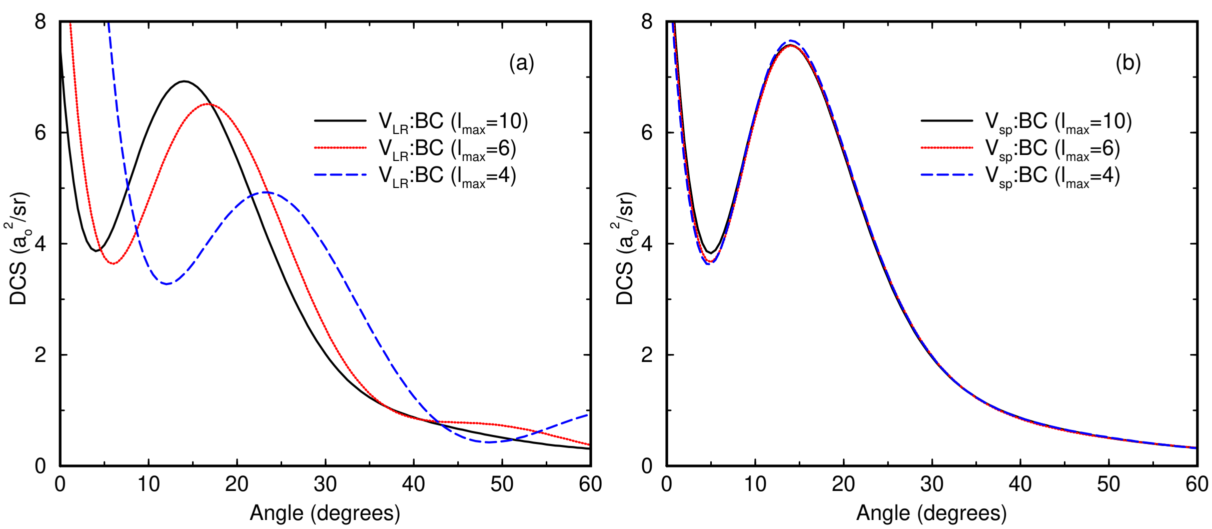

Figure 2: e^+−Ar elastic DCS at 200 eV using (a) V_{LR} and (b) V_{sp}: Solid ($l_{max} = 10$); Dot ($l_{max} = 6$) ; Dash ($l_{max} = 4$).

Finally, we demonstrate the effect of an inappropriate choice of l_{max} on the elastic DCS calculated using Born closure at 200 eV. In figure 2(a) we show the results obtained using

$\Delta f^{B_{LR}}$. Although each DCS shown contains contributions from *all* partial waves, there remains a strong dependence on the value of l_{max}. The corresponding DCS when the full interaction potential is used to compute Δf^{B} are shown in figure 2(b). It is exquisitely clear that the Born closure results obtained using the actual interaction potential do *not* show a strong dependence on l_{max} and that, in fact, a value of $l_{max} = 4$ is sufficient. It should be pointed out that the discrepancies seen in figure 2(a) will diminish with scattering energy and are solely a consequence of selecting too small a value of l_{max}, rather than some inherent flaw in the formulation of $\Delta f^{B_{LR}}$. Even if an actual closure scheme is not used, but higher-order partial-wave contributions are included via equation (13), too small a choice of l_{max} will result in similar shortcomings.

In summary, we have shown that although closure schemes based on the FBA remain an excellent way to ensure partial-wave convergence in the elastic DCS, considerable care must be exercised if additional approximations such as replacing the interaction potential by its asymptotic form V_{LR} for all space are used. For intermediate scattering energies, such an approximation will (at best) require that many more partial waves be included in the full scattering calculation, especially for positron collisions with highly-polarizable systems where the region that V_{LR} deviates from V_{sp} extends further from the target. For positron-atom collisions at intermediate energies we find that a closure scheme using the full interaction potential is efficient, reliable, and offers a clear means of determining an appropriate value for l_{max}.

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