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LETTER TO THE EDITOR

Unitarisation of the eikonal–Born series method for electron– and positron–atom collisions

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Abstract. The eikonal–Born series approximation is unitarised by using a method due to Wallace. Application is made to electron and positron elastic scattering from atomic hydrogen and to the excitation of the 2s state of atomic hydrogen by electron and positron impact.

In recent years, a number of methods have been introduced in the study of electron– and positron–atom scattering which have the interesting feature of including an infinite number of channels. In contrast to a method like the close-coupling approximation (see, for example, Burke and Williams 1977 and Bransden and McDowell 1977) which treats a small number of channels exactly, methods such as the Glauber approximation (Glauber 1959), the eikonal–Born series (EBS) method (Byron and Joachain 1973, 1977a) and the second-order potential method (Bransden and Coleman 1972, see also Bransden and McDowell 1977) include all channels, but in an approximate way.

Careful studies of electron–atom scattering have shown that the Glauber approximation suffers from severe difficulties (see, for example, Byron and Joachain 1977a and Bransden and McDowell 1977). Nevertheless, the Glauber scattering amplitude, f_G, has one particularly attractive property, namely, unitarity. Unlike the EBS method, which includes only terms of perturbation theory complete through order k_i^{-2} (where k_i is the incident particle wavenumber), the Glauber method includes terms from all orders of perturbation theory in such a way as to ensure unitarity.

It was in recognition of the importance of unitarity that Byron and Joachain (1977b, 1981) transformed the EBS method for elastic scattering into an optical model approximation in which the lowest order terms of perturbation theory, calculated by using the EBS method, were converted into an optical potential which could then be treated in a unitary, partial-wave manner. This retained all the advantages of the EBS method at small and intermediate angles but included approximations to higher terms in perturbation theory which are important at large angles, where the effects of the singular Coulomb potential are most important.

However, for the case of inelastic scattering the situation is considerably more complicated, since the first Born amplitude, f_{B1}, falls off very rapidly with increasing angle, thereby causing large-angle scattering to be dominated by the second Born term.

This is to be contrasted with the case of elastic scattering where f_{B1} provides the leading approximation at all angles.

This problem was recognised by Byron and Latour (1976) in a study of the excitation of atomic hydrogen to the 2s state. They noticed that at large angles terms of higher order than are normally included in the EBS method, particularly the imaginary parts of these terms, could have a significant effect on the scattering amplitude. In order to meet this difficulty, Byron and Joachain (1975) suggested, in the context of an investigation of the excitation of helium to the 2^1S state, that one could modify the Glauber amplitude by writing

$$f_{EBS'} = f_G - \bar{f}_{G2} + \bar{f}_{B2} \tag{1}$$

so that

$$\mathrm{Re}\, f_{EBS'} = \mathrm{Re}\, f_G + \mathrm{Re}\, \bar{f}_{B2} \tag{2a}$$

$$\mathrm{Im}\, f_{EBS'} = \mathrm{Im}(f_G - \bar{f}_{G2}) + \mathrm{Im}\, \bar{f}_{B2}. \tag{2b}$$

Here $\bar{f}_{G2}$ is the second term in the Glauber series and $\bar{f}_{B2}$ is the second Born term calculated in the closure approximation but with the low-lying states inserted exactly (see, for example, Byron and Joachain 1977a). The amplitude $f_{EBS'}$, contains *all* the higher Glauber terms and yet, like the EBS amplitude, eliminates the serious deficiencies of $\bar{f}_{G2}$. However, even this method suffers from a lack of unitarity resulting mainly from the addition of $\mathrm{Re}\, \bar{f}_{B2}$ to the Glauber amplitude.

We now consider an approximation which should improve matters considerably. Applying the eikonal expansion derived by Wallace (1973) together with results we have obtained previously in potential scattering (Byron *et al* 1975, 1979) within the framework of the 'frozen target' model, we construct a many-body Wallace amplitude for the direct transition from a state $\psi_n(X)$ to a state $\psi_{n'}(X)$:

$$f_W = \frac{k_i}{2\pi i}\int \exp(i\boldsymbol{\Delta}\cdot\boldsymbol{b}_0)\left\langle \psi_{n'}\left|\exp\left[i\left(\frac{1}{k_i}\chi_0 + \frac{1}{k_i^3}\chi_1\right)\right]-1\right|\psi_n\right\rangle \mathrm{d}^2 b. \tag{3}$$

Here $\boldsymbol{\Delta} = \boldsymbol{k}_i - \boldsymbol{k}_f$ is the momentum transfer, and we are working in a cylindrical coordinate system. The projectile coordinate is $\boldsymbol{r}_0 = \boldsymbol{b}_0 + z_0\hat{\boldsymbol{n}}$, $\hat{\boldsymbol{n}}$ being the direction perpendicular to $\boldsymbol{\Delta}$. The quantity χ_0 is the familiar Glauber phase, while the Wallace correction, χ_1, is given by (Wallace 1973) as

$$\chi_1 = \tfrac{1}{2}\int_{-\infty}^{\infty} (\boldsymbol{\nabla}\chi_+)\cdot(\boldsymbol{\nabla}\chi_-)\,\mathrm{d}z_0 \tag{4}$$

where

$$\chi_+ = -\int_{-\infty}^{z_0} V_d(\boldsymbol{b}_0, z_0', X)\,\mathrm{d}z_0' \qquad \chi_- = -\int_{z_0}^{\infty} V_d(\boldsymbol{b}_0, z_0', X)\,\mathrm{d}z_0' \tag{5}$$

and V_d is the direct interaction between the projectile and the target.

As an illustration, we apply the above method to the case of an atomic hydrogen target. Then

$$V_d = Q\left(\frac{1}{r_0} - \frac{1}{r_{01}}\right) \tag{6}$$

where $\boldsymbol{r}_1$ is the coordinate of the target electron, $r_{01} = |\boldsymbol{r}_0 - \boldsymbol{r}_1|$ and Q is the charge of the

projectile (+1 for positrons, −1 for electrons). The Glauber phase then reads

$$\chi_0 = -Q \ln(\beta^2/b^2) \tag{7}$$

where $\boldsymbol{\beta} = \boldsymbol{b}_0 - \boldsymbol{b}_1$, while the Wallace correction is given by

$$\chi_1 = \frac{\pi}{(b_0\beta)^{1/2}}\left\{P_{-1/2}\left(\frac{b_0^2+\beta^2+z_1^2}{2b_0\beta}\right) - \hat{\boldsymbol{b}}_0 \cdot \hat{\boldsymbol{\beta}}\left[P_{1/2}\left(\frac{b_0^2+\beta^2+z_1^2}{2b_0\beta}\right) - P_{1/2}\left(\frac{b_0^2+\beta^2}{2b_0\beta}\right)\right]\right\} - \frac{\hat{\boldsymbol{b}}_0 \cdot \hat{\boldsymbol{\beta}}}{b_0\beta} f(b_0, \beta, 0). \tag{8}$$

Here $P_{1/2}$ and $P_{-1/2}$ are the usual Legendre functions, and

$$f(b_0, \beta, z_1) = \int_{-\infty}^{\infty} \left(1 - \frac{z_0(z_0 - z_1)}{r_0|\boldsymbol{r}_0 - \boldsymbol{r}_1|}\right) \mathrm{d}z_0. \tag{9}$$

When $z_1 = 0$, one finds

$$f(b_0, \beta, 0) = \begin{cases} \pi b_0 \, {}_2F_1(-\frac{1}{2}, \frac{1}{2}; 1; (b_0^2 - \beta^2)/b_0^2) & \text{for } b_0 \geqslant \beta \\ \pi\beta \, {}_2F_1(-\frac{1}{2}, \frac{1}{2}; 1; (\beta^2 - b_0^2)/\beta^2) & \text{for } \beta \geqslant b_0. \end{cases} \tag{10}$$

With χ_0 and χ_1 available in closed form, the five-dimensional integral implied by equation (3) must be performed. The integral on ϕ_0 can clearly be done analytically once the symmetry of $\psi_{n'}$ and ψ_n is specified. The remaining four-dimensional integral may be performed numerically. An excellent check on the numerical procedures may be obtained by realising that since the 'frozen target' model is derived from a simplified many-body Green's function in which closure has been applied and the average excitation energy set equal to zero, the expression

$$\mathrm{Re}\, \bar{f}_{\mathrm{W}2} = \frac{1}{2\pi k_i^2} \int \exp(\mathrm{i}\boldsymbol{\Delta} \cdot \boldsymbol{b}_0) \langle \psi_{n'} | \chi_1 | \psi_n \rangle \, \mathrm{d}^2 b_0 \tag{11}$$

must be equal to the real part of the second Born term calculated in the closure approximation and with all energy differences set equal to zero. Numerical results from equation (11) were checked by comparing them with the exact expressions obtained by Byron and Joachain (1973) for elastic scattering and Byron and Latour (1976) for 1s − 2s excitation.

At this point, we note that since the excitation energies in both the initial and final channels have been set equal to zero, the long-range dynamic polarisation effects will be missing from f_{W}, and $\mathrm{Im}\, \bar{f}_{\mathrm{W}2} (= \mathrm{Im}\, \bar{f}_{\mathrm{G}2})$ will diverge at $\Delta = 0$. We therefore construct a modified amplitude $f_{\mathrm{W}'}$, with the 'exact' second Born term inserted, namely,

$$f_{\mathrm{W}'} = f_{\mathrm{W}} - \bar{f}_{\mathrm{W}2} + \bar{f}_{\mathrm{B}2}. \tag{12}$$

Given the above remarks, $f_{\mathrm{W}'}$ and f_{W} will differ negligibly at large angles, since when Δ is large off-shell elastic scattering (for which the correct excitation energy is zero) will dominate, but at small angles, where higher terms of perturbation theory are rather unimportant, one will have the benefit of a careful evaluation of $\bar{f}_{\mathrm{B}2}$. Thus, the amplitude $f_{\mathrm{W}'}$ will be very nearly unitary at all angles and should provide an accurate approximation to the direct scattering amplitude.

In order to compare the results of equation (12) with electron scattering experiments, we need an approximation to the exchange amplitude, g. Then the differential

cross section can be obtained from the expression

$$\frac{d\sigma}{d\Omega}=\frac{k_f}{k_i}\left(\frac{1}{4}|f+g|^2+\frac{3}{4}|f-g|^2\right). \tag{13}$$

Unfortunately, our knowledge of the exchange amplitude for electron–atom scattering remains in a very unsatisfactory state up to the present time. Given the kinematical approximations made in obtaining the many-body Glauber wavefunction and the importance of very high continuum states in second and higher terms of the Born series for the exchange amplitude, it seems unlikely that Glauber exchange amplitudes (Madan 1975, see also Byron and Joachain 1977a) will be reliable.

On the other hand, since we are treating the direct amplitude in a particularly careful way, it seems reasonable to evaluate g by using a better approximation than the Ochkur amplitude, g_{Och}. We have therefore elected to obtain the exchange amplitude, g, from an approximate second-order treatment in which we write

$$g \simeq g_{B1}^{01}+\tilde{g}_{B2}. \tag{14}$$

Here

$$g_{B1}^{01}=-\frac{1}{2\pi}\langle \exp(i\boldsymbol{k}_f\cdot\boldsymbol{r}_1)\psi_{n'}(\boldsymbol{r}_0)|r_{01}^{-1}|\exp(i\boldsymbol{k}_i\cdot\boldsymbol{r}_0)\psi_{1s}(\boldsymbol{r}_1)\rangle \tag{15}$$

is the piece of the first Born exchange amplitude arising from the electron–electron interaction. It is easy to prove that the electron–nucleus term ($-r_0^{-1}$) is cancelled by higher-order terms of the Born series for g. The term $\tilde{g}_{B2}$ in equation (14) is given by

$$\begin{aligned}\tilde{g}_{B2}=\frac{1}{8\pi^4}\int d\boldsymbol{q} &<\exp(i\boldsymbol{k}_f\cdot\boldsymbol{r}_1)\psi_{n'}(\boldsymbol{r}_0)|r_{01}^{-1}|\exp(i\boldsymbol{q}\cdot\boldsymbol{r}_0)\psi_{1s}(\boldsymbol{r}_1)\rangle(q^2-k_i^2-i\varepsilon)^{-1}\\ &\times\langle\exp(i\boldsymbol{q}\cdot\boldsymbol{r}_0)\psi_{1s}(\boldsymbol{r}_1)|r_{01}^{-1}-r_0^{-1}|\exp(i\boldsymbol{k}_i\cdot\boldsymbol{r}_0)\psi_{1s}(\boldsymbol{r}_1)\rangle\\ &+\frac{1}{8\pi^4}\int d\boldsymbol{q}\langle\exp(i\boldsymbol{k}_f\cdot\boldsymbol{r}_1)\psi_{n'}(\boldsymbol{r}_0)|r_{01}^{-1}-r_1^{-1}|\exp(i\boldsymbol{q}\cdot\boldsymbol{r}_1)\psi_{n'}(\boldsymbol{r}_0)\rangle\\ &\times(q^2-k_f^2-i\varepsilon)^{-1}\langle\exp(i\boldsymbol{q}\cdot\boldsymbol{r}_1)\psi_{n'}(\boldsymbol{r}_0)|r_{01}^{-1}|\exp(i\boldsymbol{k}_i\cdot\boldsymbol{r}_0)\psi_{1s}(\boldsymbol{r}_1)\rangle.\end{aligned} \tag{16}$$

This represents the second term in the Born series for g in which only 'elastic' intermediate states ψ_{1s} and $\psi_{n'}$, corresponding to initial and final state interactions, have been included. In the rearrangement matrix elements of equation (16), the electron–nucleus term has been omitted since it takes part in the cancellation discussed above. We have shown that these 'elastic' intermediate states dominate over g_{B1}^{01} in the large-angle region. Thus, the amplitude g of equation (14) contains the leading contribution to the exchange amplitude at all angles.

In figures 1 and 2 we show the differential cross sections for elastic scattering and 1s–2s excitation in atomic hydrogen by electron and positron impact, at an incident energy of 100 eV. We see from figure 1 that the results of the present calculation are in excellent agreement with the experimental data of Williams (1975) and of Lloyd *et al* (1974) as renormalised by van Wingerden *et al* (1977), although recently Kingston and Walters (1980) have suggested that the experimental results may be systematically too large. Also displayed in figure 1 are the results of our recent third-order optical model (Byron and Joachain 1981) calculation (for incident electrons) which are seen to be in good agreement with the present calculation. It is satisfying to see that these two very different ways of unitarising the EBS method should give such similar results at this

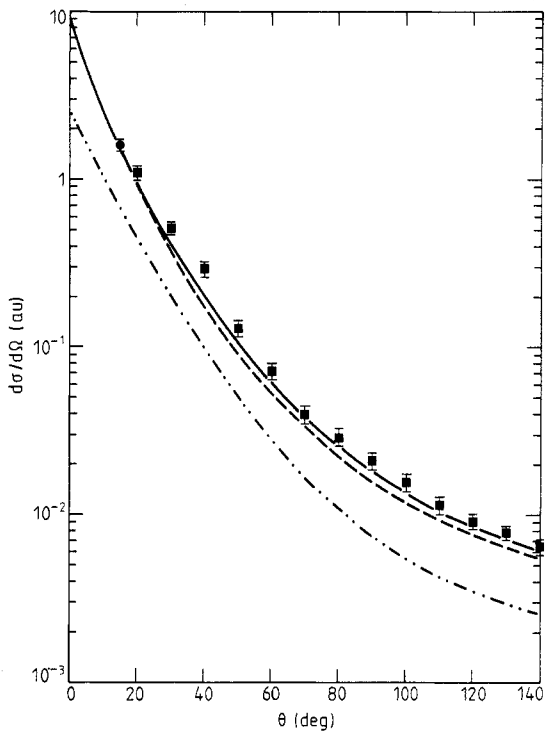

Figure 1. The elastic scattering of electrons and positrons by atomic hydrogen at 100 eV. ———, the results of the present calculation for electron impact; – – –, optical model results of Byron and Joachain (1981) for electron impact; —··—, the results of the present calculation for positron scattering. Also shown are the experimental results for electron scattering: ■, the results of Williams (1975); ●, the results of Lloyd *et al* (1974) as normalised by van Wingerden *et al* (1977). At angles greater than 15° the difference between the two sets of experimental data is small, and we have elected to show only those of Williams (1975).

rather low incident energy; this agreement encourages one to apply the present method to inelastic processes where the optical potential method is not available. Our third-order optical model results for positron elastic scattering are also very close to the present positron results shown in figure 1.

In figure 2 we compare the results of the present method with the first Born approximation and the EBS and EBS′ calculations performed for 1s–2s excitation. In all calculations, we have used the second-order expression of equation (14) to obtain the exchange amplitude. At small angles, the agreement between the three higher-order approximations is excellent, but at larger angles the EBS results diverge significantly from those obtained from the EBS′ method and from the present results, which shows the importance of higher-order terms of perturbation theory in this angular region. As the energy is increased these differences, of course, decrease, albeit rather slowly. As expected, the first Born differential cross section differs significantly from the other results, particularly at large angles. It is worth noting that the modified Glauber approximation of Gien (1979), in which equation (1) is used but with $\bar{f}_{B2}$ given simply by the closure approximation, gives a differential cross section which at small angles lies considerably above the EBS, EBS′ and present results. This is due to the fact that the

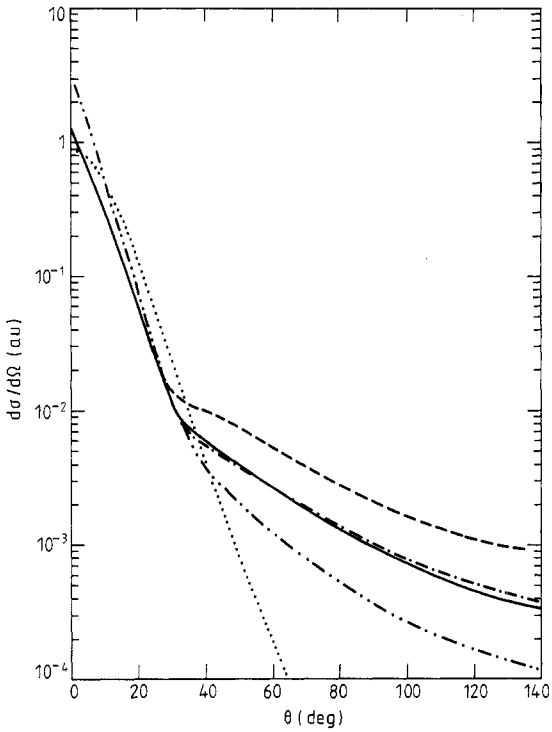

Figure 2. The excitation of atomic hydrogen to the 2s state by electron and positron impact. ———, the present calculation; – – –, the EBS results; —·—, the EBS' results, all for electron impact. —··—, the present calculation for positron impact. ····, the first Born approximation for both electron and positron impact. The incident energy is 100 eV.

intermediate p states which give rise to the long-range, off-diagonal polarisation effects must be treated with great care in the small-angle region (Byron and Latour 1976). It should be noted that the pure EBS differential cross sections shown in figure 2 differ significantly from the EBS cross sections of Byron and Latour (1976) since these authors included in a rather *ad hoc* way selected higher-order corrections to $d\sigma/d\Omega$. These corrections are unsatisfactory in that they are not in the form of an approximation to the scattering amplitude, but as far as the differential cross section is concerned they do lead to values in fair agreement with the present results and the EBS' results. Also shown in figure 2 is the positron impact differential cross section obtained from the present method. It is seen to be larger at small angles and much smaller at large angles than the corresponding electron impact results.

Finally, we show in table 1 our integrated cross sections at 100 and 200 eV obtained from the present theory for elastic scattering and 1s–2s excitation of atomic hydrogen. For elastic scattering, our electron impact results are in close agreement with the experimental data of Williams (1975), the experimental values obtained by Lloyd *et al* (1974) being larger, particularly at 200 eV. For 1s–2s excitation our values for electron impact are in good agreement with the data of Kauppila *et al* (1970) when cascade contributions are removed by using the approximation of Hummer and Seaton (1961),

$$\sigma_{\text{cascade}} = 0.23\sigma_{1s3p} \tag{17}$$

Table 1. Integrated elastic and inelastic cross sections (in units of πa_0^2) for electron and positron scattering by atomic hydrogen.

Energy (eV)	Elastic				Inelastic (1s–2s)		
	Experiment		Theory		Experiment[c]	Theory	
	e^-		e^-	e^+	e^-	e^-	e^+
100	0.56[a]	0.58[b]	0.514	0.228	0.038(4)	0.0386	0.0614
200	0.21[a]	0.25[b]	0.203	0.131	0.029(3)	0.0245	0.0299

[a] Williams (1975) quoted in van Wingerden *et al* (1977).
[b] Lloyd *et al* (1974) renormalised by van Wingerden *et al* (1977).
[c] Kauppila *et al* (1970) with cascade contributions subtracted. The numbers in parentheses give the uncertainty in the last significant figure.

where σ_{1s3p} is the integrated cross section for excitation to the 3p state. Equation (17) was derived in the context of the first Born approximation, so we have used the Born result for σ_{1s3p} in correcting the data of Kauppila *et al* (1970) for cascade effects. Since equation (17) is only an approximate result the experimental values for 1s–2s excitation shown in table 1 contain uncertainties beyond the statistical one indicated in parentheses. It is interesting to note in table 1 that the positron results differ substantially from the electron results, being significantly smaller for elastic scattering and larger for 1s–2s excitation. A similar effect was found recently in the case of positron collisions with helium at intermediate energies (Willis *et al* 1981).

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