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Equivalence of the first-order target-continuum distorted-wave and a simplified form of the second-order Faddeev-Watson approximations

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Abstract : The first order target-continuum distorted wave (TCDW1) approximation has been shown to be equivalent to a simplified form of the second order Faddeev Watson (FW2) approximation when the projectile-target interaction is weak. The TCDW1 is then compared with a peaking approximation to the FW1 and FW2 total and differential cross sections for the formation of positronium by the impact of positrons on helium.

Keywords : Charge transfer, ion atom Scattering, Faddeev Watson approach

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1. Introduction

In the high energy ion-atom rearrangement collisions, many theoretical approaches are shown to be interconnected after some further approximations are made. Dube[1] established such connections among the strong potential Born (SPB) approximation [2], the impulse approximation [3] (IA),the peaked impulse approximation[4] (PIA) and the continuum distorted wave (CDW) approximation [5]. Starting from the SPB approximation Briggs *et al* [6] were able to derive several simplifications such as IA,continuum intermediate state (CIS) approximation [7] and eikonal approximation [8]. Recently, Datta *et al* [9] established a connection between the first order boundary corrected Born [10] (B1B) and the Coulomb-Born [11] (CB) approximations. All these efforts were made in order to bridge the gap among the well-known theoretical methods for ion-atom collisions. In the present investigation, we shall show the equivalence of the first order target continuum distorted wave (TCDW1)

approximation [12], [13] and a simplified form of the second order Faddeev-Watson (FW2) approximation [14], [15] in which the projectile-target-nucleus and projectile-electron interactions are considered weak and taken only upto first order in the respective T-matrices. The interaction between the target-nucleus and the bound electron is considered to be the strongest and taken all orders into the corresponding T-matrix through the two-body Green's functions. We first establish the equivalence of the two methods mathematically and then for a numerical check we apply these methods to positronium formation from atomic helium.

2. Equivalence of TCDW1 and FW2 approaches

We consider the charge transfer process

$$1 + (2,3) \rightarrow (1,2) + 3 \tag{1}$$

with arbitrary masses m_i and charges z_i The reduced masses are defined by

$$\mu_{ij} = \frac{m_i m_j}{m_i + m_j}, \qquad \mu_i = \frac{m_i(m_j + m_k)}{m_i + m_j + m_k},$$

with the usual cyclic permutation of [1,2,3] and the mass ratios are given by

$$\alpha = \frac{m_3}{m_2 + m_3}, \qquad \beta = \frac{m_1}{m_1 + m_2}.$$

We use the Jacobi space-coordinate $\boldsymbol{r}_i$, $\boldsymbol{r}_{jk}$ with conjugate momenta $\boldsymbol{q}_i$, $\boldsymbol{q}_{jk}$ in which $\boldsymbol{r}_i$ is the position coordinate of i relative to the centre of mass of j and k and $\boldsymbol{r}_{jk}$ is the position vector of j relative to k. These notations are similar to that used by Macek and Shakeshaft [16] for charge transfer processes. We denote by $|I>$ the initial target bound state, which corresponds to energy ε_i and by $|P>$ the final projectile bound state with energy ε_f If the initial relative momentum is $\boldsymbol{Q}_i = \hbar \boldsymbol{k}_i = \mu_1 \boldsymbol{v}_i$ and the final relative momentum is $\boldsymbol{Q}_f = \hbar \boldsymbol{k}_f = \mu_3 \boldsymbol{v}_f$ Then the energy conservation gives

$$\frac{Q_i^2}{2\mu_1} + \varepsilon_i = \frac{Q_f^2}{2\mu_3} + \varepsilon_f = E$$

The FW2 transition operator for the process (1) is

$$T_{1W2} = T_2 + V_3 + T_1 G_0^+ T_2 + T_1 G_0^+ T_3 + T_2 G_0^+ T_3. \tag{2}$$

Here V_i denotes the interaction of the particle j and k with i spectating T_i is the corresponding transition operator which is given in terms of the two-body Green's operator $G_i^+(E)$ by the Lippmann-Schwinger equation

$$T_i = V_i + V_i G_i^{(+)}(E)\, V_i \tag{3}$$

We shall now show how eq (2) gives rise naturally to the first order target continuum distorted wave approximation [12]. We consider the case where the interactions for the pairs

1,2 (*i.e.* V_3) and 1,3 (*i.e.* V_2) are weak, but that between the particle 2 and the target nucleus 3 (*i.e.* V_1) is strong. This would be the case for smaller deflection angles. Using eq. (3) we can then replace T_2 and T_3 by V_2 and V_3 respectively and retaining T_1 we have from eq. (2)

$$T_{\mathrm{FW2}} \approx \left(1 + T_1 G_0^+\right)\left(V_2 + V_3\right) + V_2 G_0^+ V_3. \tag{4}$$

Taking the matrix element of (4) between the initial $|i>$ and final $|f>$ states of the entire system and introducing an off-shell state vector

$$\left\langle \psi_f^{(-)} \right| = \langle f | \left(1 + T_1 G_0^{(+)}\right) = \langle f | \left(1 + V_1 G_1^{(+)}\right), \tag{5}$$

we have

$$\langle f | T_{\mathrm{IW2}} | i \rangle \approx \left\langle \psi_f^{(-)} \right| \left(V_2 + V_3\right) | i \rangle + \langle f | V_2 G_0^{(+)} V_3 | i \rangle. \tag{6}$$

The first term on the right hand side of eq. (6) is similar in structure to the TCDW1 approximation with an undistorted initial state and the internuclear potential V_2 ignored. To see the relationship between the TCDW1 and FW2 approximations more clearly, we have from eq. (5)

$$\left| \psi_f^{(-)} \right\rangle = \left(1 + G_1^{(-)} V_1\right) \left| f \right\rangle$$

and the corresponding position-space wavefunction is

$$\left\langle \boldsymbol{r}_1, \boldsymbol{r}_{23} \right| \left. \psi_f^{(-)} \right\rangle = e^{i\beta \boldsymbol{r}_1 \cdot \boldsymbol{k}_f} \int d\boldsymbol{q}\, e^{i(\alpha \boldsymbol{r}_{23} \cdot \boldsymbol{q}/\hbar)} \langle \boldsymbol{r}_{12} | \boldsymbol{q} \rangle \langle \boldsymbol{q} | \boldsymbol{P} \rangle \times \psi^{(-)}_{\boldsymbol{P}_1, E_1}(\boldsymbol{r}_{23}). \tag{7}$$

Here

$$\psi^{(-)}_{P_1, E_1}(\boldsymbol{r}_{23}) = \langle \boldsymbol{r}_{23} | \left(1 + \bar{G}_1^{(-)} \bar{V}_1\right) | \boldsymbol{P}_1 \rangle \tag{8}$$

is the off-shell Coulomb wavefunction, with incoming wave boundary condition at energy E_1, given by

$$E_1 = E - \frac{q_1^2}{2\mu_1}, \qquad \boldsymbol{q}_1 = \boldsymbol{q} + \beta \mu_3 \boldsymbol{v}_f$$

and the momentum $\boldsymbol{P}_1$ is given by

$$\boldsymbol{P}_1 = \hbar \boldsymbol{k}_f = \mu_{23} \boldsymbol{v}_f - \alpha \boldsymbol{q}.$$

The bars on the operators in eq. (8) denotes that they refer to their own centre-of-mass frames.

If the main contribution to the integral in (7) is assumed to come from the region of localization $\boldsymbol{q} = \boldsymbol{o}$ of the final bound state wavefunction $\langle \boldsymbol{q} | \boldsymbol{P} \rangle$ then

$$\boldsymbol{P}_1 \sim \mu_{23} \boldsymbol{v}_f \quad \text{and} \quad E_1 = \frac{P_1^2}{2\mu_{23}} \simeq \epsilon_f .$$

Thus for $E \gg |\epsilon_f|$, $\psi^{(+)}_{\boldsymbol{P}_1 f_1}(\boldsymbol{r}_{23})$ is near its energy shell. The on-shell limit of the off shell Coulomb wave function is not defined in the strict mathematical sense [2]. However, by taking account of the long range Coulomb distortion in its definition (8) [cf. references 17,18] we can obtain

$$\lim_{P_1 \to \sqrt{2\mu_{23}E_1}} \psi^{(+)}_{\boldsymbol{P}_1 f_1}(\boldsymbol{r}_{23}) = (2\pi)^{-3/2} \exp(-\pi\gamma/2)\, \Gamma(1-i\gamma)\, e^{i\boldsymbol{k}_f \cdot \boldsymbol{r}_{23}} \times {}_1F_1(i\gamma, 1; -ik_f r_{23} - i\boldsymbol{k}_f \cdot \boldsymbol{r}_{23}),$$

where $\gamma = Z_2 Z_3 / v_f$ so that eq (7) becomes

$$\langle \boldsymbol{r}_1, \boldsymbol{r}_{23} | \psi^{(+)}_f \rangle = \langle \boldsymbol{r}_{12} | p \rangle (2\pi\hbar)^{-3/2} \exp(-\pi\gamma/2)\, \Gamma(1-i\gamma) \times e^{i\boldsymbol{k}_f \cdot \boldsymbol{r}_{23}} {}_1F_1(i\gamma, 1; -ik_f r_{23} - i\boldsymbol{k}_f \cdot \boldsymbol{r}_{23}) \qquad (9)$$

Here we again note that a similar technique of approximating the off shell wavefunction by its on-shell limit, has been used before by Briggs *et al* [6] but starting from the strong potential Born approximation rather than the Faddeev–Watson approach. Another important assumption in our approach is the replacement of T_i by V_i, $(i = 2,3)$ in eq (2) by using eq. (3). We also note that eq. (9) reduces to the position representation of $|f\rangle$ when $\gamma = 0$ *i.e.* when distortion is neglected.

In the case of electron capture by heavy particles, $Z_2 = -1$, $Z_3 = Z_P$, and using the more physically meaningful co-ordinates of Macek and Shakeshaft [16] we have

$$\langle \boldsymbol{r}_{12} | \boldsymbol{p} \rangle = \langle -\boldsymbol{r}_p | \boldsymbol{p} \rangle = \phi(\boldsymbol{r}_p), \boldsymbol{r}_{23} = \boldsymbol{r}_f ,$$
$$\boldsymbol{r}_3 = -\boldsymbol{R}_p \quad \text{and} \quad \gamma = -Z_f / v_f = -v_f .$$

We now see that, apart from the momentum-space normalizing factor $(2\pi\hbar)^{-3/2}$ eq (9) is precisely the final state distorted wave used in the TCDW approximation (c.f. eq (3) in ref [12]). We therefore, conclude that a simplified form of the FW2 approximation is equivalent to the TCDW1 approximation if the second term in the right-hand side of eq (6) is neglected. This term, $\langle f | V_2 G_0 V_3 | i \rangle$, is usually neglected in ion-atom collision due to the presence of the nucleus-nucleus interaction V_2. In the TCDW1 approximation this term does not appear, nor in fact, does it appear in the TCDW2 approximation since higher order terms in the latter are accounted for by a Green's operator with a connected Kernel (c.f. ref [12] and references therein).

Returning to eq (2) again, an alternative approach is to effect a peaking approximation directly to the T-matrices. The second order terms in (2) have been shown [19] to be well behaved if regular Coulomb T matrices, which are analogous to the regularized off-shell

Coulomb wavefunctions, are used. The peaking approximation then results in a factoring out of Rutherford scattering amplitude which for certain terms can be interpreted as corresponding to classical Thomas double scattering mechanisms. We shall refer to this approach as the second order Faddeev–Watson peaking approximation (FWPA2). A similar peaking approximation applied to the first two terms in eq. (2) yields FWPA1. Thus for electron capture by heavy particles, the term $T_1 G_0^{(+)} T_3$ dominates at higher angles and accounts quite well for the observed Thomas peak [19,20]. For capture by positrons two terms are important, *viz.* $T_1 G_0^{(+)} T_3$ and $T_2 G_0^{(+)} T_3$ which can interfere constructively for odd parity positronium states or destructively for even parity states [21–23], although no experimental evidence is yet available to test these predictions.

3. Numerical results

Because the FWPA2 does not take account of the effect of distant collisions, such as target distortion, it might not be expected to be reliable for total cross sections. In contrast the TCDW approximation treats the target distortion explicitly and the resulting total cross-section are in good agreement with experiment for electron capture by heavy particles [12,24] and by positrons [25] as shown in Figure 1 in this calculation. By contrast, in the latter case, the FWPA2 fails badly at these energies, although for capture by high energy protons, of the

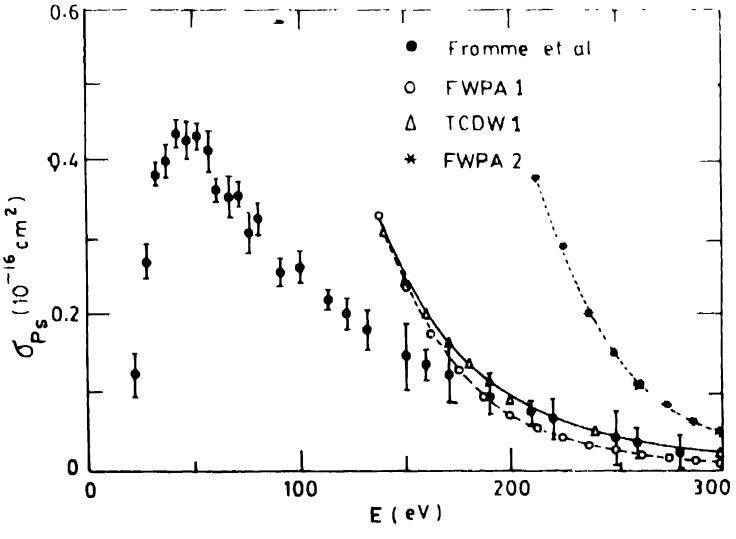

Figure 1. Total cross sections for positronium formation in e^+ + He scattering as a function of incident e^+ energy Solid circles , measurement of Fromme *et al* [26], open circle , FWPA1 [23], open triangles , TCDW1 [25] and stars , FWPA2 results [23] Solid, dashed and dotted lines are drawn through TCDW1, FWPA1 and FWPA2 results respectively to guide the eye All theoretical results are for 1S – 1S capture

order of several MeV, the total cross sections are not bad [19]. From Figure 1 we also note that the TCDW1 and FWPA1 total cross sections are in good agreement with the

measurement of Fromme et al [26] at the higher energies. This is interesting since the FWPA1 does not account of the target distortion but includes the positron-target-core interaction explicitly via T_2 while TCDW1 accounts for target distortion but excludes positron-target-core interaction V_2 in (6). In Figure 2, we present differential cross sections in both the approximations at 250 eV. In the forward angles the TCDW1 (excluding $e^+ - He^+$ interaction)

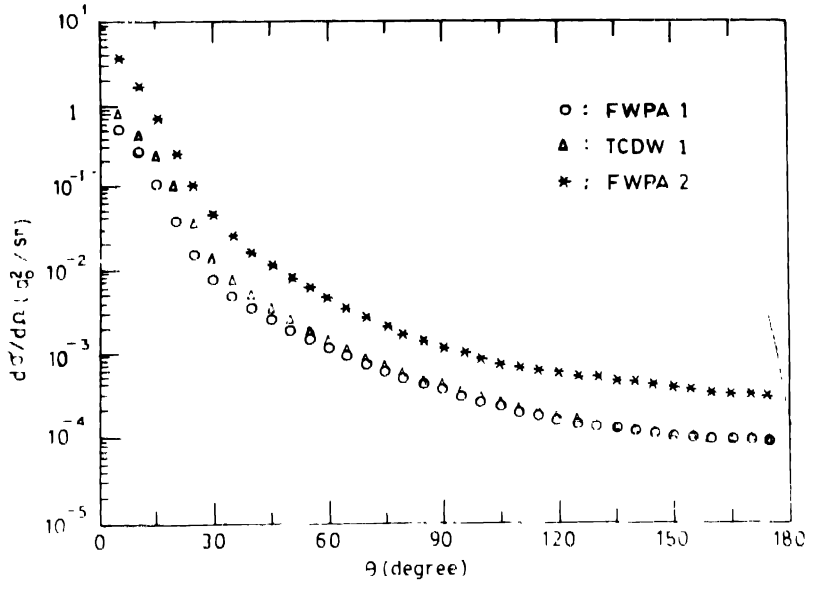

Figure 2. 1S - 1S differential cross sections for the same system at 250 eV. The symbols represent the results in the same theories as described in Figure 1

results are a factor of two large compared to FWPA1 (including $e^+ - He^+$ interaction) results while in the backward direction they nearly match with each other. At this energy FWPA2 results are too large throughout the entire angular range.

4. Summary

We have established a relationship between the TCDW1 and the FW2 approximations when the projectile–target interaction is ignored. We also demonstrate that the TCDW1 (excluding $e^+ - He^+$ interaction) total cross sections gives energy dependence similar to the FWPA1 (including $e^+ - He^+$ interaction) total cross sections.

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