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Evaluation of the single ionisation transition amplitude using the CDW-EIS model within the framework of the impact-parameter method

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Abstract. The continuum distorted-wave model with an eikonal initial state for ionisation is discussed within the framework of the impact-parameter method. Particular attention is paid to the *surface* term, which describes the transition by a distorting potential, and which has been omitted in all of the previous calculations performed using the model. However, this term is included in the transition amplitude in a recent application of the model based upon a quantum-mechanical treatment. The present study, in which the *surface* term is evaluated within the impact-parameter method, shows that this term does not contribute to the transition amplitude. In describing the electron-ejection mechanism for a $p^{\pm}$–H collision, the cross-sections evaluated using the impact-parameter model show numerical agreement with those determined in the quantum-mechanical version. This agreement indicates that the contribution of the *surface* term calculated in the wave treatment is negligible over the region in which the impact-parameter model is valid.

PACS. 34.50.Fa Electronic excitation and ionization of atoms (including beam-foil excitation and ionization)

1 Introduction

Distorted-wave models provide a very useful tool for treating energetic atomic collision processes. Amongst the models, the continuum distorted-wave approximation (CDW) enjoys great success when the collision of a heavy ion with an atomic target is considered [1–3]. The model was proposed by Cheshire [4] and applied to electron capture and ionisation by Gayet [5] and Belkić [6], respectively. Subsequently, and mostly because of the incorrect normalisation of the CDW wave function, variants of the model were proposed that depend on the actual forms of distortion [1]. The lack of normalisation was most apparent in the domain of low and intermediate impact energy, resulting in overestimated values of the cross-sections. To correct the failure of normalisation, Crothers and McCann introduced the continuum distorted-wave model with an eikonal initial state (CDW-EIS), wherein the CDW distortion of the initial channel is replaced by its eikonal form [7]. The model proved to be very successful, especially in treating the process of ionisation, as demonstrated in numerous examples [3]. One of the main features of the theory is that in both the CDW and CDW-EIS models, the ejected electron is considered as moving in a two-centre potential due to the projectile and target nuclei [8]. The application of the model has also received particular attention because the amplitude for hydrogenic systems can be given in analytical form.

Although all of the aforementioned derivations and applications of the CDW-EIS approximation are based upon the semiclassical impact-parameter (IP) method [9], its quantum- (wave-) mechanical formulation has been developed recently [10–12]. The IP approximation, through describing the projectile as moving in a straight-line trajectory, provides a significant simplification of the treatment at high impact energies [9], while a quantum-mechanical version is appropriate for light particles at small impact energies (less than 50 eV). Of course, one can expect that in the region where the IP picture is valid, both the IP and the quantum-mechanical formulations of the model will provide identical results.

In distorted-wave model, the post form of the wave-mechanical transition amplitude can be determined from

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the equation [10]

$$T_{if} = \langle \chi_f^- | (H - \mathcal{E})^\dagger | \Psi_i^+ \rangle + \langle \chi_f^- | (H - \mathcal{E}) - (H - \mathcal{E})^\dagger | \psi_i \rangle, \tag{1}$$

where χ_f^- is the distorted final state with incoming boundary conditions, H is the total Hamiltonian of the system, $\mathcal{E}$ is the total energy, Ψ_i^+ is the scattering state resulting from the unperturbed initial state ψ_i, and † signifies complex conjugates (operating to the left). Noting that the kinetic energy operator is not Hermitian when it appears between scattering states satisfying different boundary conditions [13], the transition amplitude can be expressed as

$$T_{if} = \langle \chi_f^- | W_f^\dagger | \Psi_i^+ \rangle + \langle \chi_f^- | V_i - W_f^\dagger | \psi_i \rangle, \tag{2}$$

with $(H - \mathcal{E})\psi_i = V_i \psi_i$ and $(H - \mathcal{E})\chi_f^- = W_f \chi_f^-$. The last term in (1) and (2) describes the transition amplitude due to the distorting potential, and as in [14], we will hereafter refer to it as the *surface* term. Different conditions can be considered when selecting the distorting potential, which will involve different contribution of the *surface* term in (1) and (2) [9].

For heavy-particle collision, and invoking the IP picture, the above form of the transition amplitude can be written as [6,9]

$$T_{if} = v \int_{-\infty}^{+\infty} \mathrm{d}t \int \mathrm{d}\boldsymbol{b} \mathrm{e}^{\mathrm{i}\boldsymbol{q}_\perp \boldsymbol{b} - \mathrm{i}\Delta\mathcal{E}\mathrm{t}} \times \{ \langle \chi_f^- | W_f^\dagger | \Psi_i^+ \rangle + \langle \chi_f^- | V_i - W_f^\dagger | \psi_i \rangle \}, \tag{3}$$

where $\boldsymbol{b}$ is the impact parameter, $\boldsymbol{v}$ is the projectile velocity, $\Delta\mathcal{E}$ is the difference of atomic energies between the initial and final states, and $\boldsymbol{q}_\perp$ denotes the component of momentum transfer perpendicular to projectile motion. Note that, although the same symbols are used here for wave functions, those used in (3) correspond to the ones defined in (1) but exclude the part corresponding to the heavy-particle motion. Thus, in (3), $\langle \ | \ | \ \rangle$ denotes an integration over only the electronic coordinates.

If one considers the numerous applications of the CDW-EIS model for ionisation, it can be observed that in the calculations based on the IP model, the *surface* term is always omitted [8]. The excellent reproduction of the experimental results indicates implicitly that it is unnecessary to include this term in the calculations [3]. At the same time, the recent quantum-mechanical version of the theory [10–12,16] is based upon the evaluation of the full transition amplitude (2). It has been claimed that the *surface* term cannot be excluded from the evaluation [16], and it has also been reported that neither term in (1) or (2) has a strong physical meaning individually [12]. This seems to be a contradiction, in that the inclusion of the *surface* term is unimportant in the IP treatment [3] while it is required in the quantum-mechanical one [12,16], since (as noted above) the quantal and IP treatments are equivalent at high impact energies, when heavy-particle collision is considered. A solution of this contradiction can be achieved by performing a separate evaluation of the *surface* term. The contribution of this term has already been addressed in the literature, although one can still encounter contradictory conclusions. In [6], the *surface* term is omitted from the analysis by referring to the asymptotic orthogonality of the distorted waves, while in [14,15] (without evaluation), finite and vanishing values are attributed to this term, respectively.

Therefore, one might pose the following questions: is it really necessary to include the *surface* term in the CDW-EIS model for ionisation? And does its contribution equal zero and hence was correctly omitted in previous calculations? The aim of the present article is to calculate exactly the contribution of the *surface* term in the CDW-EIS treatment of ionisation within the IP picture, in order to answer these questions. Atomic units are used, except where stated otherwise.

2 Theory of the surface term

Consider a general ionisation process, wherein a bare ion with nuclear charge Z_P collides with a hydrogen-like ion of nuclear charge Z_T. In the IP model, the relative motion can be described by a classical straight-line trajectory characterised by a velocity $\boldsymbol{v}$ and an impact parameter $\boldsymbol{b}$, while the electronic motion in the field of the two heavy particles is treated quantum-mechanically. Locating the target nucleus at the origin of the coordinate system with the z-axis oriented along the constant-velocity vector $\boldsymbol{v}$, the position vector $\boldsymbol{R}(t)$ of the projectile varies with time as $\boldsymbol{R}(t) = \boldsymbol{b} + \boldsymbol{v}t$. In this predetermined straight-line trajectory, both $\boldsymbol{b}$ and $\boldsymbol{v}$ remain constant during the collision.

This reduces the problem to the solving of the time-dependent electronic Schrödinger equation

$$\left(h(\boldsymbol{x}, t) - i \left(\frac{\partial}{\partial t} \right)_x \right) \Psi(\boldsymbol{x}, t) = 0, \tag{4}$$

where the semiclassical Hamiltonian is given by

$$h = -\frac{1}{2}\nabla_x^2 - \frac{Z_T}{x} - \frac{Z_P}{s} + \frac{Z_P Z_T}{R}, \tag{5}$$

with $\boldsymbol{x}$ ($\boldsymbol{s}$) being the electronic coordinate relative to the target (projectile) nucleus. In (4), t and $\boldsymbol{x}$ are considered to be independent variables. Other coordinates, such as $\boldsymbol{s}$ or $\boldsymbol{r} = (\boldsymbol{x} + \boldsymbol{s})/2$, can also be chosen instead of $\boldsymbol{x}$ [7]. However, the transition amplitude is independent of the choice of coordinates, and the present choice has been made so that the wave functions are free of translation factors.

Let us consider an ionisation process wherein the electron is ejected with momentum $\boldsymbol{k}$ and energy $\varepsilon_k = k^2/2$ from an initial target state $\phi_i(\boldsymbol{x})$ of energy ε_i. The exact outgoing (Ψ_i^+) and incoming ($\Psi_{\boldsymbol{k}}^-$) solutions of (4), specified by the initial $\phi_i(\boldsymbol{x})$ and final $\phi_{\boldsymbol{k}}^-(\boldsymbol{x})$ states respectively, obey the following boundary conditions:

$$\lim_{t \to -\infty} \Psi_i^+(\boldsymbol{x}, t) = \exp(-i\varepsilon_i t) \phi_i(\boldsymbol{x}) E_{\boldsymbol{v}}^*(\boldsymbol{s}, \eta_i) E_{-\boldsymbol{v}}(\boldsymbol{R}, \eta_N),$$

$$\lim_{t,s,x \to \infty} \Psi_{\boldsymbol{k}}^-(\boldsymbol{x}, t) = \exp(-i\varepsilon_k t) \phi_{\boldsymbol{k}}^-(\boldsymbol{x}) E_{\boldsymbol{p}}(\boldsymbol{s}, \eta_P) E_{\boldsymbol{v}}^*(\boldsymbol{R}, \eta_N), \tag{6}$$

with

$$\begin{aligned}\phi_{\boldsymbol{k}}^{-}(\boldsymbol{x}) &= \exp(i\boldsymbol{k}\cdot\boldsymbol{x})D_{\boldsymbol{k}}(\boldsymbol{x},\eta_T),\\ D_{\boldsymbol{u}}(\boldsymbol{r},\eta) &= e^{\pi\eta/2}\Gamma(1+i\eta)_1F_1(-i\eta,1,-i(ur+\boldsymbol{u}\cdot\boldsymbol{r})),\\ E_{\boldsymbol{u}}(\boldsymbol{r},\eta) &= (ur+\boldsymbol{u}\cdot\boldsymbol{r})^{i\eta},\ \eta_i = Z_P/v,\ \eta_N = Z_PZ_T/v,\\ \eta_P &= Z_P/p,\ \eta_T = Z_T/k,\ \boldsymbol{p}=\boldsymbol{k}-\boldsymbol{v}. \end{aligned} \tag{7}$$

The wave function $\Psi_{\boldsymbol{k}}^{-}$ in (6) describes the final state, where asymptotically all particles are at infinite separation [6,7].

In distorted-wave models, it is usual to propose approximate solutions ξ_i^{+} and $\xi_{\boldsymbol{k}}^{-}$ of the Schrödinger equation (4) that satisfy the correct boundary conditions

$$\begin{aligned}\xi_i^{+}(\boldsymbol{x},t) &= \Psi_i^{+}(\boldsymbol{x},t)\ \text{ for } t\to-\infty,\\ \xi_{\boldsymbol{k}}^{-}(\boldsymbol{x},t) &= \Psi_{\boldsymbol{k}}^{-}(\boldsymbol{x},t)\ \text{ for } t\to+\infty. \end{aligned} \tag{8}$$

The transition amplitude at a given impact parameter $\boldsymbol{b}$ is given by the overlap integral

$$A_{i\boldsymbol{k}}^{-}(\boldsymbol{b}) = \lim_{t\to-\infty}\langle\Psi_{\boldsymbol{k}}^{-}(t)|\Psi_i^{+}(t)\rangle = \lim_{t\to-\infty}\langle\Psi_{\boldsymbol{k}}^{-}(t)|\xi_i^{+}(t)\rangle \tag{9}$$

in the *prior* form, and similarly by

$$A_{i\boldsymbol{k}}^{+}(\boldsymbol{b}) = \lim_{t\to+\infty}\langle\Psi_{\boldsymbol{k}}^{-}(t)|\Psi_i^{+}(t)\rangle = \lim_{t\to+\infty}\langle\xi_{\boldsymbol{k}}^{-}(t)|\Psi_i^{+}(t)\rangle \tag{10}$$

in the *post* form, where the relations (8) have been used, and $\langle\,\rangle$ denotes integration over $\boldsymbol{x}$. Here, we restrict our analysis to the *prior* form, while the equivalent *post* form can be analysed in a similar way. The transition amplitude in (9) can be transformed into

$$\begin{aligned}A_{i\boldsymbol{k}}^{-}(\boldsymbol{b}) &= -\int_{-\infty}^{\infty}dt\frac{d}{dt}\langle\Psi_{\boldsymbol{k}}^{-}(t)|\xi_i^{+}(t)\rangle + \lim_{t\to+\infty}\langle\Psi_{\boldsymbol{k}}^{-}(t)|\xi_i^{+}(t)\rangle\\ &= a_{i\boldsymbol{k}}^{-}(\boldsymbol{b}) + s_{i\boldsymbol{k}}^{-}(\boldsymbol{b}), \end{aligned} \tag{11}$$

where the first term

$$a_{i\boldsymbol{k}}^{-}(\boldsymbol{b}) = -i\int_{-\infty}^{\infty}dt\,\langle\Psi_{\boldsymbol{k}}^{-}(t)|\ [h-i(\partial/\partial t)_x]\xi_i^{+}(t)\rangle \tag{12}$$

is the main term for ionisation. If we denote by w_i the distorting potential in the initial channel ($h_i^w = h - w_i$, $(h_i^w - i\partial/\partial t)\xi_i^{+}(t) = 0$), and $\psi_{\boldsymbol{k}}^{-}$ is equivalent to $\Psi_{\boldsymbol{k}}^{-}$ at $t\to+\infty$ ($(h_f + v_f - i\partial/\partial t)\psi_{\boldsymbol{k}}^{-} = v_f\psi_{\boldsymbol{k}}^{-}$ with $h = h_f + v_f$), the second term of (11) can be expressed as

$$\begin{aligned}s_{i\boldsymbol{k}}^{-}(\boldsymbol{b}) &= \lim_{t\to+\infty}\langle\Psi_{\boldsymbol{k}}^{-}(t)|\xi_i^{+}(t)\rangle = \lim_{t\to+\infty}\langle\psi_{\boldsymbol{k}}^{-}(t)|\xi_i^{+}(t)\rangle\\ &= \int_{-\infty}^{\infty}\mathrm{d}t\frac{\mathrm{d}}{\mathrm{d}t}\langle\psi_{\boldsymbol{k}}^{-}(t)|\xi_i^{+}(t)\rangle\\ &= -i\int_{-\infty}^{\infty}\mathrm{d}t\langle\psi_{\boldsymbol{k}}^{-}(t)|h_i^w\xi_i^{+}(t)\rangle - \langle h_f\psi_{\boldsymbol{k}}^{-}(t)|\xi_i^{+}(t)\rangle\\ &= -i\int_{-\infty}^{\infty}\mathrm{d}t\langle\psi_{\boldsymbol{k}}^{-}(t)|v_f - w_i|\xi_i^{+}(t)\rangle, \end{aligned} \tag{13}$$

which is the prior-form counterpart of the second term of (3) (the already-noted *surface* term).

The CDW-EIS model adopts the eikonal wave function $\xi^{EIS}(\boldsymbol{x},t)$ for the initial distorted wave $\xi_i^{+}(\boldsymbol{x},t)$ and approximates the incoming wave function $\Psi_{\boldsymbol{k}}^{-}$ as the CDW wave function $\xi_{\boldsymbol{k}}^{CDW}(\boldsymbol{x},t)$ in (13). These are written as

$$\xi_i^{EIS} = e^{-i\varepsilon_i t}\phi_i(\boldsymbol{x})E_{\boldsymbol{v}}^{*}(\boldsymbol{s},\eta_i)E_{-\boldsymbol{v}}(\boldsymbol{R},\eta_N) \tag{14}$$

and

$$\xi_{\boldsymbol{k}}^{CDW} = e^{-i\varepsilon_k t}\phi_{\boldsymbol{k}}^{-}(\boldsymbol{x})D_{\boldsymbol{p}}(\boldsymbol{s},\eta_P)E_{\boldsymbol{v}}^{*}(\boldsymbol{R},\eta_N). \tag{15}$$

The form of ξ_i^{EIS} is identical to that of $\Psi_i^{+}(t\to-\infty)$ in (6). The CDW wave function satisfies the boundary condition in (8) and describes the electron as moving in the combined field of the projectile and target nuclei in the final state. The main term in (12) is expressed as

$$\begin{aligned}a_{i\boldsymbol{k}}^{-}(\boldsymbol{b}) &= -i\int_{-\infty}^{\infty}\mathrm{d}tM(t),\\ M(t) &= \langle\xi_{\boldsymbol{k}}^{CDW}|[h-(\partial/\partial t)_x]\xi_i^{EIS}\rangle\\ &= -\frac{1}{2}(vb)^{2i\eta_N}e^{i(\varepsilon_k-\varepsilon_i)t}\,\langle\phi_{\boldsymbol{k}}D_{\boldsymbol{p}}(\boldsymbol{s},\eta_P)|\Xi_i\rangle\,,\\ \Xi_i &= \phi_i\left(\nabla_x^2E_{\boldsymbol{v}}(\boldsymbol{s},\eta_i)\right) + 2\left(\nabla_x\phi_i\right)\left(\nabla_xE_{\boldsymbol{v}}(\boldsymbol{s},\eta_i)\right), \end{aligned} \tag{16}$$

where we have used the fact that $E_{\boldsymbol{v}}(\boldsymbol{R},\eta_N)E_{-\boldsymbol{v}}(\boldsymbol{R},\eta_N) = (vb)^{2i\eta_N}$.

In the asymptotic $t\to+\infty$ limit with $\boldsymbol{R}\simeq-\boldsymbol{s}$, $\xi_i^{EIS}(t)$ has the form

$$\lim_{t\to+\infty}\xi_i^{EIS} = \exp(i[\delta_i(t)-\varepsilon_it])\ \phi_i(\boldsymbol{x})\ \left[\frac{|\boldsymbol{b}-\boldsymbol{x}_b|}{b}\right]^{-2i\eta_i} \tag{17}$$

while the CDW function can be expressed as

$$\lim_{t\to+\infty}\xi_{\boldsymbol{k}}^{CDW} = \exp(i[\delta_f(t)-i\varepsilon_kt])\ \phi_{\boldsymbol{k}}^{-}(\boldsymbol{x}). \tag{18}$$

In the above equations, it is assumed that $|\boldsymbol{x}|\ll R$, as the electron is initially localised around the target, $\boldsymbol{x}_b$ is the component of $\boldsymbol{x}$ perpendicular to $\boldsymbol{v}$, and δ_i and δ_f are real functions having logarithmic time-dependence for large t. Finally, the surface term can be cast as

$$s_{i\boldsymbol{k}}^{-} = \lim_{t\to+\infty}\langle\xi_{\boldsymbol{k}}^{CDW}|\xi_i^{EIS}\rangle = T_G\lim_{t\to+\infty}e^{i\Delta(t)} \tag{19}$$

with $T_G = \langle\phi_{\boldsymbol{k}}^{-}(\boldsymbol{x})|\ \left[\frac{|\boldsymbol{b}-\boldsymbol{x}_b|}{b}\right]^{-2i\eta_i}|\phi_i(\boldsymbol{x})\rangle$ and $\Delta(t) = (\varepsilon_k-\varepsilon_i)t+\delta_i-\delta_f$. T_G is a term that appears in the Glauber approximation [18,19], and has a well-defined value. However, the limit of $\exp(i\Delta(t))$ in (19) as $t\to+\infty$ is undefined. Formally, this oscillation arises due to the fact that the theory employs initial and final states with definite energies [9,20]. Clearly, this oscillation must be dampened out if one wishes to obtain a definite value for the transition amplitude.

The damping procedure, although not emphasised, is already required in the evaluation of the main term (16),

since $M(t)$ does not vanish but rather has a time-dependence similar to $\exp(i\Delta)$ for large t (note, the term $\langle\phi_{\boldsymbol{k}} D_{\boldsymbol{p}}(\boldsymbol{s},\eta_P)|\Xi_i\rangle$ in (16) has a finite value at $t\to\infty$; see Eqs. (17)–(19)). In order to dampen $M(t)$ at large t, we replace ξ_i^{EIS} by $\tilde{\xi}_i^{EIS}=\xi_i^{EIS}Y(t)$ in (14), and take $Y(t)$ as $Y=1$ for $t<0$ and $Y=\exp(-\alpha t)$ for $t\geq 0$, with an infinitesimal positive parameter α that goes to zero after the time integration (similar methods are commonly used in treating, for example, indefinite integrals; see pp. 270 and 311 of [9]). However, the extra term appearing in (16), which includes $\frac{\mathrm{d}}{\mathrm{d}t}Y(t)$, does not contribute after letting $\alpha\to 0+$. It is to be noted that the initial distorted wave ξ_i^+ in (13) can be chosen arbitrarily, as long as it fulfils the boundary condition (8).

The replacement $\xi_i^{EIS}\to\tilde{\xi}_i^{EIS}$, required in (16), should also be implemented in the evaluation of the *surface* term (19):

$$s_{i\boldsymbol{k}}^{-} = \lim_{t\to+\infty}\left\langle \xi_{\boldsymbol{k}}^{CDW}|\tilde{\xi}_i^{EIS}\right\rangle = T_G \lim_{t\to+\infty} e^{-\alpha t+i[(\varepsilon_k-\varepsilon_i)t+\delta_i(t)-\delta_f(t)]}, \qquad (20)$$

and we have $s_{i\boldsymbol{k}}^{-}=0$ without ambiguity, since the last term goes to zero when $t\to\infty$. That is, the *surface* term in the CDW-EIS model does not contribute to the scattering amplitude within the framework of the impact-parameter description. This explains the success of the CDW-EIS model, as demonstrated by the interpretation of several kinds of ion-atom collision process when only the main term (16) was considered [3]. It should also be noted that, as mentioned above, the *post* form of the transition amplitude can be evaluated in a similar way, and it is also concluded that the *surface* term is zero. This has the important consequence that for a three-body treatment, there is no *post-prior* discrepancy, as was studied recently by considering the amplitudes as omitting the surface terms [21].

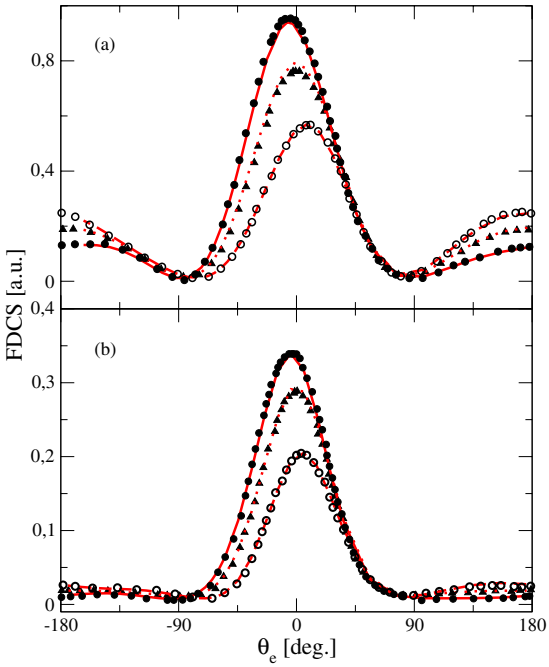

Fig. 1. Scattering-plane fully differential cross-sections (FDCS) in the centre-of-mass frame (c.m.) for ionisation of H by proton and antiproton impact with 212 keV impact energy, under the CDW-EIS and first Born approximations. The energy of ejected electron is 5 eV, while θ_e denotes the polar angle of the ejected electron relative to the momentum transfer vector. The present results are shown by: a solid line for CDW-EIS with proton impact; a dashed line for CDW-EIS with antiproton impact; and a dotted line for the first Born approximation. The results from [12] are shown by: full circles for CDW-EIS with proton impact; open circles for CDW-EIS with antiproton impact; and full triangles for the Born-approximation results. The c.m. scattering angle of the projectile is: (a) 3.23×10^{-3} deg. and (b) 8.86×10^{-3} deg.

3 Numerical results and discussion

In the previous section, we have shown theoretically that within the IP method the *surface* term is zero. In the following, we compare CDW-EIS results for the ionisation of hydrogen by fast proton and antiproton impact obtained within the IP and wave treatments. We consider the fully differential cross-section (FDCS), which has been studied by Jones and Madison within the quantal treatment [12]. In the IP picture, the FDCS can be expressed as

$$\frac{\mathrm{d}^5\sigma}{\mathrm{d}\varepsilon_k \mathrm{d}\Omega_e \mathrm{d}\Omega_P} = \left|\frac{\mu v}{2\pi}\int \mathrm{d}\boldsymbol{b}\, e^{i\boldsymbol{q}_\perp\boldsymbol{b}} a_{i\boldsymbol{k}}^{-}(\boldsymbol{b})\right|^2 \qquad (21)$$

using the main term (16), where $\Omega_e(\theta_e,\phi_e)$ and $\Omega_P(\theta_P,\phi_Q)$ denote the solid angle of the ejected electron and the scattered projectile, respectively, and $\boldsymbol{q}_\perp$ is the transverse component of momentum transfer. The magnitude $|\boldsymbol{q}_\perp|$ can be written as $2\mu v\sin(\theta_P/2)$, with μ the reduced mass between projectile and target nuclei. Figures 1 and 2 show the present results obtained within the framework of the IP method in comparison with those evaluated by Jones and Madison using the quantum-mechanical treatment [12]. The FDCS were calculated for 212 and 32.9 keV proton and antiproton impacts on H at different projectile scattering angles. In both cases, the electron energy is fixed at 5 eV and the FDCS is plotted as a function of the ejected electron emission angle. The results from the two CDW-EIS calculations are in full agreement for all values of the electron momentum and projectile scattering angle considered. These results are not completely unexpected, since the wave and IP treatments are equivalent up to order $1/\mu$ at such high velocities. However, it should be emphasised that the calculation by Jones and Madison, in which both terms in (2) are evaluated, includes the *surface* term [12]. Its actual value was not determined separately, since the method of calculation employed does not allow for this. Therefore, we can expect from our theoretical and numerical analysis that the *surface* term in the quantum-mechanical treatment is negligibly small. A formal proof, similar to that presented here within the IP

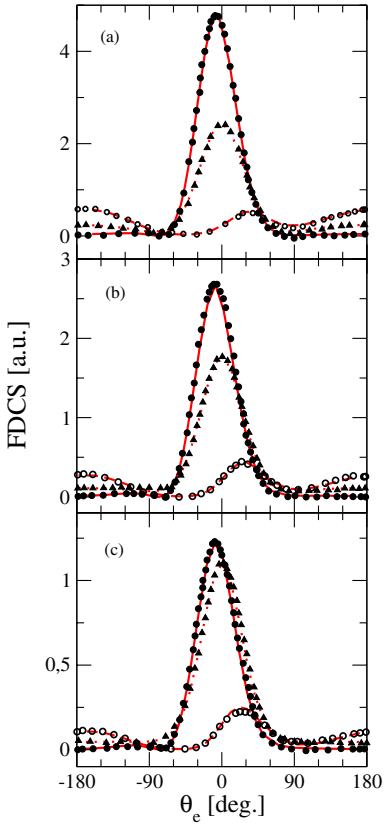

Fig. 2. Same as in (1), for a c.m. impact energy of 32.9 keV and scattering angles of the projectile of: (a) 9.69×10^{-3} deg., (b) 17.9×10^{-3} deg., and (c) 26.7×10^{-3} deg.

method, would be most welcome in order to establish the exact contribution from the *surface* term in the quantal version of the CDW-EIS model.

4 Conclusions

In summary, we have studied the CDW-EIS transition amplitude for ionisation derived within the impact-parameter method. This amplitude is a sum of the main and *surface* terms. It was found that the *surface* term, characteristic of the distorting waves, does not contribute to the transition amplitude. This explains the success of previous studies [3] wherein the *surface* term was excluded from the transition amplitude (although without formal justification). Moreover, in studying the fully differential electron-ejection cross-sections in proton/antiproton collisions with H, numerical agreement has been obtained between our present results within the IP treatment and CDW-EIS calculations using the quantal treatment, wherein the *surface* term was included. These results appear to indicate that the *surface* term calculated in the quantal treatment is negligibly small in the region where the IP model is valid.

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