Fully Differential Cross Sections for Heavy Particle Impact Ionization

M McGovern\(^1\), D. Assafrao\(^2\), J.R. Mohallem\(^2\), Colm T. Whelan\(^3\) and H.R.J. Walters\(^1\)

\(^1\) Department of Applied Mathematics and Theoretical Physics, Queen’s University, Belfast BT7 1NN, United Kingdom
\(^2\) Laboratório de Atomos e Moléculas Especiais, Departamento de Física, ICEx, Universidade Federal de Minas Gerais, P.O Box 702, 30123-970 Belo Horizonte, MG, Brazil
\(^3\) Department of Physics, Old Dominion University, Norfolk, VA 23529-0116, USA

E-mail: mmcgovern06@qub.ac.uk

Abstract. We describe a procedure for extracting fully differential ionization cross sections from an impact parameter coupled pseudostate treatment of the collision. Some examples from antiproton impact ionization of atomic Hydrogen are given.

1. Introduction
In a recent paper [1] we showed how fully differential cross sections for ionization by heavy projectiles could be extracted from an impact parameter coupled pseudostate treatment of the collision. Here we briefly describe the approach and give some sample results to illustrate the power of the method. We use atomic units (au) throughout.

2. Method
The method consists of two stages. The first is the extraction of the differential motion of the heavy projectile from the straight line impact parameter treatment. The second is the extraction of the differential ejection of the ionized electron from the pseudostates.

2.1. The Impact Parameter Method and Extraction of the Differential Motion of the Projectile
In the impact parameter approximation, the projectile is assumed to move with constant velocity \(v_0\) along a straight line at perpendicular distance \(b\) (the impact parameter) from the target nucleus. Its position relative to the target nucleus at time \(t\) can be described by \(R = v_0t + b\). Let \(\Psi\) be the electronic wave function of the atom at time \(t\). We introduce a set of eigenstates and pseudostates \(\psi_n\) which together diagonalise the atomic Hamiltonian \(H_A\): 

\[ \langle \psi_n | H_A | \psi_m \rangle = \epsilon_n \delta_{nm} \]

As described elsewhere [2, 3] pseudostates may be considered as "clumps" or "distributions" of eigenstates which give a discretized representation of the atomic continuum. We expand \(\Psi\) in the set \(\psi_n\) according to

\[ \Psi = \sum_n a_n(b,t)e^{-i\epsilon_n t}\psi_n \] (1)
Substitution of (1) into the time dependent Schrödinger equation and projection with the $\psi_n$ leads to the coupled equations

$$i\frac{da_n}{dt} = \sum_m e^{i(\varepsilon_n - \varepsilon_m)t} \langle \psi_n | V | \psi_m \rangle a_m$$

(2)

where $V$ is the interaction between the projectile and the atom. If the projectile is a bare ion of charge $Z_p$ this interaction takes the form

$$V = Z_p \left( Z_T \frac{1}{R} - \sum_{i=1}^{Z_T} \frac{1}{|R - r_i|} \right)$$

(3)

where the target nucleus has charge $Z_T$ and $r_i$ is the position of the $i$th electron relative to it. Note that we retain the interaction $Z_p Z_T / R$ between the projectile and target nucleus in (3). If the atom is initially in the state $\psi_0$ then we must solve (2) subject to the boundary conditions $a_n(-\infty, b) = \delta_{n0}$.

In a wave treatment of the collision the scattering amplitude for exciting the state $\psi_n$ would be (in the centre of mass coordinate system)

$$f = \langle e^{i k_n \cdot R} \psi_n | V | \psi_0^+ \rangle$$

(4)

where $k_n$ is the final momentum of the projectile and $\psi_0^+$ is the full scattering wave function starting from the state $\psi_0$. Let us consider making a perturbative treatment of (4).

In first order (the first Born Approximation (FBA)) we get

$$f^{B1} = \langle e^{i k_n \cdot R} \psi_n | V | e^{i k_0 \cdot R} \psi_0 \rangle$$

(5)

where $k_0$ is the incident momentum of the projectile and $\psi_0$ is the initial state of the atom. Let us take the z-direction to be along $k_0$ and write $R = b + Z \hat{k}_0$ where $\hat{a}$ denotes a unit vector and $b.\hat{k}_0 = 0$. Then we have

$$e^{i(k_0 - k_0) \cdot R} = e^{i q \cdot b} e^{i(k_0 - k_n) \cdot \hat{k}_0 Z}$$

(6)

where $q \equiv k_0 - k_f$ is the momentum transfer. Using the conservation of energy condition

$$k_n^2 = k_0^2 + 2\mu (\varepsilon_0 - \varepsilon_n),$$

(7)

where $\mu$ is the reduced mass, we can write

$$(k_0 - k_n) \cdot \hat{k}_0 = \frac{(\varepsilon_n - \varepsilon_0)}{v_0} + O \left( \frac{1}{\mu} \right)$$

(8)

where $v_0 = k_0 / \mu$ is the incident velocity of the projectile (it is assumed that the target is initially at rest in the laboratory). Introducing $t = Z/v_0$, and neglecting terms of $O \left( \frac{1}{\mu} \right)$, we get
\[
\begin{align*}
\mathcal{B}_1 &= v_0 \int d^2 \mathbf{b} e^{i \mathbf{q} \cdot \mathbf{b}} \int_{-\infty}^{+\infty} e^{i(\varepsilon_n - \varepsilon_0) t} \langle \psi_n | V(t) | \psi_0 \rangle dt \\
&= f^{B1} \tag{9}
\end{align*}
\]

But, from (2), the first Born approximation in the impact parameter treatment gives

\[
\alpha_n^{B1} (\mathbf{b}, \infty) = \delta_{n0} - i \int_{-\infty}^{+\infty} e^{i(\varepsilon_n - \varepsilon_0) t} \langle \psi_n | V(t) | \psi_0 \rangle dt \tag{10}
\]

We therefore see that (9) has the form

\[
f^{B1} = iv_0 \int e^{i \mathbf{q} \cdot \mathbf{b}} (\alpha_n^{B1} (\mathbf{b}, \infty) - \delta_{n0}) d^2 \mathbf{b} \tag{11}
\]

Consider next the second Born approximation to (4). The second Born term is

\[
f^{B2} = \frac{\mu}{4\pi\varepsilon} \lim_{\varepsilon \to 0+} \sum_m \int d\mathbf{k} \langle e^{i\mathbf{k} \cdot \mathbf{R}} \psi_m | V | e^{i\mathbf{k} \cdot \mathbf{R}} \psi_m \rangle \langle \psi_m | e^{i\mathbf{k} \cdot \mathbf{b}} \psi_m \rangle \frac{\langle \psi_m | V | e^{i\mathbf{k} \cdot \mathbf{R}} \psi_0 \rangle}{k_m^2 - k^2 + i\varepsilon} \tag{12}
\]

Typically \(k_0, k_n\) and \(k_m\) will be of the order of 1000s of au but, see (7), will differ by a few au. Also, the matrix elements will be negligible beyond a few au about \(k_0\) and \(k_n\). Then we can approximate the propagator in (12) by

\[
k_m^2 = k^2 + i\varepsilon \approx 2k_0(k_m - k_z) + i\varepsilon \tag{13}
\]

where we write \(k = k_z \mathbf{k}_0 + \mathbf{k}_b\) with \(k_b \mathbf{k}_0 = 0\). Then writing

\[
e^{i \mathbf{k} \cdot (\mathbf{R} - \mathbf{R}')} = e^{i \mathbf{k}_z (Z - Z')} e^{i \mathbf{k}_b \cdot (\mathbf{b} - \mathbf{b}')} \tag{14}
\]

using

\[
\lim_{\varepsilon \to 0+} \int_{-\infty}^{+\infty} \frac{dk_z}{2k_0(k_m - k_z) + i\varepsilon} e^{i k_z (Z - Z')} = \begin{cases} -\frac{2i}{k_0} e^{i k_m (Z - Z')} & \text{if } Z > Z' \\ 0 & \text{if } Z < Z' \end{cases} \tag{15}
\]

and neglecting terms of \(O(1/\mu)\) we get

\[
f^{B2} = -iv_0 \sum_m \int d^2 \mathbf{b} e^{i \mathbf{q} \cdot \mathbf{b}} \left\{ \int_{-\infty}^{+\infty} dt e^{i(\varepsilon_n - \varepsilon_0) t} \langle \psi_n | V(t) | \psi_m \rangle \int_{-\infty}^{t} dt' e^{i(\varepsilon_n - \varepsilon_0) t'} \langle \psi_m | V(t') | \psi_0 \rangle \right\} \tag{16}
\]

But, solving the equations (2) to second order we get

\[
\alpha_n^{B2} (\mathbf{b}, \infty) = \sum_m \int_{-\infty}^{+\infty} dt e^{i(\varepsilon_n - \varepsilon_0) t} \langle \psi_n | V(t) | \psi_m \rangle \int_{-\infty}^{t} dt' e^{i(\varepsilon_n - \varepsilon_0) t'} \langle \psi_m | V(t') | \psi_0 \rangle \tag{17}
\]
Clearly, therefore, in the approximation (16)

\[ f^{B2} = iv_0 \int e^{i\mathbf{q} \cdot \mathbf{b}} \delta_n^{B2}(\mathbf{b}, \infty) d^2\mathbf{b} \]  

(18)

A similar treatment of higher Born terms gives the same relationship as (18). Summing over all Born terms we finally get the connection

\[ \langle e^{i\mathbf{k} \cdot \mathbf{R}} \psi_{\mathbf{k}} | \mathbf{V} | \psi_{\mathbf{0}}^+ \rangle \rightarrow iv_0 \int e^{i\mathbf{q} \cdot \mathbf{b}} (a_n(b, \infty) - \delta_n0) d^2\mathbf{b} \]  

(19)

which enables us to extract the differential motion of the projectile out of the straight line impact parameter treatment.

2.2. Extracting the Differential Motion of the Ejected Electron

The required ionization amplitude is

\[ f_{ion} = \langle e^{i\mathbf{k} \cdot \mathbf{R}} \psi_{\mathbf{k}}^- | \mathbf{V} | \psi_{\mathbf{0}}^+ \rangle \]  

(20)

where \( \psi_{\mathbf{k}}^- \) is the ionized state of the atom corresponding to an ejected electron with momentum \( \mathbf{k} \). Assuming that the pseudostates \( \psi_n \) approximate a complete set, (20) may be written

\[ f_{ion} = \sum_n \langle \psi_{\mathbf{k}}^- | \psi_n \rangle \langle e^{i\mathbf{k} \cdot \mathbf{R}} \psi_{\mathbf{k}}^- | \mathbf{V} | \psi_{\mathbf{0}}^+ \rangle \]  

(21)

Then, using (19), we obtain the key result which is the basis of our method:

\[ f_{ion} = iv_0 \sum_n (\psi_{\mathbf{k}}^- | \psi_n \rangle \int e^{i\mathbf{q} \cdot \mathbf{b}} (a_n(b, \infty) - \delta_n0) d^2\mathbf{b} \]  

(22)

As discussed in [1], (22) may be reduced to a more manageable form. Also, there is an energy shell subtlety about the approximation. The upshot is that the pseudostate set \( \psi_n \) must be constructed so that there is one state of each angular momentum symmetry with the same energy as the ionized state \( \psi_{\mathbf{k}}^- \). Only these pseudostates actually contribute to the sum in (22). The reader is referred to [1] for a more detailed discussion.

3. Some Results

To illustrate the power of the method we show some results for antiproton ionization of H(1s). The calculations have been made using the 165 state set described in [1] which was specifically constructed for an ejected electron energy of 5 eV. All cross sections are referred to the laboratory frame of reference, see [1].

First, a test of the method at the first Born level. In figure 1 we show the triple differential cross section (TDCS) for ionization in coplanar geometry at 500 keV. For atomic Hydrogen there is an exact analytic expression for the first Born TDCS, see equation (77) of [1]. This exact cross section is shown in figure 1. Sitting essentially on top of it is the first Born cross section calculated from (22) but with \( a_n \) replaced by \( a_n^{B1} \) of (10). This level of agreement provides very strong support for our method. Also shown in figure 1 is the full coupled 165 state
Figure 1. Coplanar TDCS for an impact energy of 500 keV, ejected electron energy 5 eV and $q = 0.25 \text{au}$. Solid red curve, exact FBA; dashed blue curve, impact parameter pseudostate FBA; solid black curve labelled 165, full coupled pseudostate calculation.

Figure 2. TDCS in three dimensions for an ejected electron of 5 eV: (a) impact energy 500 keV, $q = 0.25 \text{ au}$; (b) impact energy 2 keV, $q = 2.5 \text{ au}$. Wire cage, FBA; solid surface, full coupled pseudostate calculation. The antiproton is incident along the z-direction.

approximation. Compared with first Born it shows a reduced binary peak and an enhanced recoil peak, both rotated away from the outgoing antiproton. This pattern is exactly the same as we see in $(e, 2e)$ [4, 5] and exactly what we would expect at such a high impact energy.

Figure 2(a) shows the same TDCS but in full three dimensions. Figure 2(b) shows the TDCS but now at the very low impact energy of 2 keV. Here the first Born approximation continues to predict “forward” electron ejection but the full coupled 165 state calculation shows that the electron ejection is “backwards”. This is a result of the post collisional interaction between the slow outgoing antiproton and the ionized electron.

An important aspect of the approximation, relevant to on-going questions concerning the importance of projectile-nucleus scattering in differential ionization studies [6], is that it includes a proper representation of this interaction, i.e., the $Z_p Z_T / R$ term in (3). Whereas this term is irrelevant to total cross section studies (it can be transformed away as an overall phase factor) it cannot be ignored in differential ionization. To illustrate its importance in low energy antiproton ionization we show in figure 3 the double differential cross section $d^2\sigma / dE dq$ in the energy of the ejected electron and the magnitude $q$ of the momentum transfer to the projectile. The impact energy is 2 keV. Figure 3(a) shows this cross section for an ejected electron with energy 5 eV. In the FBA this cross section falls rapidly with increasing $q$. This is because the FBA only
permits the antiproton to interact with the target electron, the nuclear term is cancelled out by the orthogonality of the initial and final atom states, see (3) and (5). The light electron is unable to provide large momentum transfers to the projectile and consequently the FBA “dies” rapidly with increasing $q$. By contrast, the 165 coupled pseudostate approximation initially falls like the FBA with increasing $q$ but then quickly reaches a sharp minimum and then rises to a pronounced maximum. This behaviour is the result of the nuclear interaction taking over at larger $q$.

Figure 3(b) shows $d^2\sigma/dEdq$ as a function of both $q$ and the ejected electron energy. In this picture the growing dominance of the nuclear interaction results in a “crease” in the cross section surface.

4. Conclusions
The formalism described in this paper advances the capability of calculating to a high degree of accuracy any aspect of differential ionization by a heavy projectile.

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