Coincidence Studies with Antiprotons

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Abstract. We present a short overview of a new method for calculating fully differential cross sections that is able to describe any aspect of coincidence measurements involving heavy projectiles. The method is based upon impact parameter close coupling with pseudostates. Examples from antiproton impact ionization are shown.

1. Introduction
In [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. In this paper we give a brief summary of the theory, with some new extensions [2], and illustrate it by some applications to antiproton ionization of atomic hydrogen. Throughout we use atomic units (au) in which $\hbar = m_e = e = 1$.

2. Theory
We consider antiprotons incident with velocity $\mathbf{u}_0$ upon a neutral target atom which is stationary in the laboratory. In the relative coordinate system the amplitude for single ionization of the target is

$$f_{\text{ion}} = -\frac{1}{2\pi}\langle e^{i\mathbf{k}_f \cdot \mathbf{R}} \psi_{\kappa}^- | V | \Psi_0^+ \rangle$$

where $\mathbf{k}_f$ is the final relative momentum of the scattered antiproton, $\kappa$ is the momentum of the ionized electron, $\psi_{\kappa}^-$ is the ionized state of the atom, $V$ is the interaction between the antiproton and the atom, and $\Psi_0^+$ is the full scattering wave function for the system. Let $\psi_n$ be a set of eigenstates and pseudostates that diagonalise the atomic Hamiltonian $H_A$:

$$\langle \psi_n | H_A | \psi_m \rangle = \varepsilon_n \delta_{nm}$$

If the $\psi_n$ approximate a complete set then we may write
Conservation of energy requires that $k_f^2 + 2\mu \varepsilon^+ + \mu \kappa^2 = k_0^2 + 2\mu \varepsilon_0$ where $k_0 = \mu v_0$ is the relative momentum of the incident antiproton, $\mu$ is the reduced mass of the system, $\varepsilon^+$ is the energy of the residual ion, and $\varepsilon_0$ is the energy of the initial atomic state $\psi_0$. Unless deliberately engineered $k_f^2 + 2\mu \varepsilon_n$ will not be equal to $k_0^2 + 2\mu \varepsilon_0$ and so the amplitude $f_{n0} \equiv \langle e^{ik_f \cdot \mathbf{R}} | \psi_n | V | \psi_0^+ \rangle$ will normally be off-energy-shell. However, in [1] the pseudostates were chosen so that one state from each angular momentum symmetry had exactly the right energy for conservation, i.e., $\varepsilon_n = \varepsilon^+ + \frac{\kappa^2}{2}$. With this choice it also transpired that $\langle \psi_n^- | \psi_n \rangle$ was effectively zero for all states $\psi_n$ with $\varepsilon_n \neq \varepsilon^+ + \frac{\kappa^2}{2}$ so that, in effect, (3) became an expression involving only on-energy-shell amplitudes $f_{n0}$.

Now, except at very low energies, a wave treatment of the collision, as implied by (1), is not practical. The natural choice then is the impact parameter method where the antiproton is assumed to move along a straight line path with constant velocity $v_0$. One then studies the electronic wave function, $\Psi$, of the atom as a function of time $t$. Expanding $\Psi$ in the basis $\psi_n$ according to

$$
\Psi = \sum_n a_n(b, t)e^{-i\varepsilon_n t}\psi_n,
$$

substituting into the time dependent Schrödinger equation, and projecting with the $\psi_n$ leads to the coupled equations

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

These equations must be solved subject to the boundary conditions $a_n(b, -\infty) = \delta_{n0}$. In [1] it is then shown that, to a very good approximation,

$$
f_{n0} = iv_0 \int e^{i\mathbf{q} \cdot \mathbf{b}} [a_n(b, \infty) - \delta_{n0}] d^2 \mathbf{b}
$$

where $\mathbf{q} \equiv k_0 - k_f$ is the momentum transfer and where $f_{n0}$ is on-energy-shell. Combining (3) and (6) we arrive at the final approximation that is used:

$$
f_{ion} = -\frac{iv_0}{2\pi} \sum_n \langle \psi_n^- | \psi_n \rangle \int e^{i\mathbf{q} \cdot \mathbf{b}} [a_n(b, \infty) - \delta_{n0}] d^2 \mathbf{b}
$$

Exploiting symmetries, (7) can be reduced to a more manageable practical form, see [1].

Given (7) we can now calculate the most fully differential cross section, the triple differential cross section (TDCS). This is given by

$$
\frac{d^3 \sigma}{dE d\Omega_e d\Omega_p} = \frac{v_f}{v_0} m_p^2 |f_{ion}|^2
$$
where \( v_f = k_f/\mu \) and \( m_p \) is the mass of the projectile. This is the cross section for an electron being ejected with energy in the range \( E \) to \( E + dE \) and into the solid angle \( d\Omega_e \) while the antiproton is scattered into the solid angle \( d\Omega_p \). It is very important to specify the frame of reference in which the measurements are to be made. Formula (8) applies to the laboratory frame of reference. In the relative coordinate frame of reference (the natural frame for theoretical calculations) the \( m_p^2 \) in (8) must be replaced by \( \mu^2 \) (for Gold ions incident on He this is a factor of 2525 difference!). In all of the results reported here we assume that we are in the laboratory frame. From (8) double differential, single differential, and total cross sections can be calculated by integration.

As described above, the approximation (7) assumes that the pseudostate set \( \psi_n \) has been constructed so that one state from each angular momentum symmetry has exactly the energy \( \varepsilon^+ + \kappa/2 \). This means that for each ejected electron energy a new set of pseudostates must be constructed and the equations (5) solved. This is highly inconvenient if one needs to average cross sections over experimental energy resolutions or wants to calculate cross sections such as \( d\sigma/d\Omega_e \), \( d\sigma/d\theta \) or \( d\sigma/dE \) for comparison with experiment. It is therefore important to see if (7) can be easily extended to a range of ejected energies while using a single set of pseudostates. What if we simply take (7) at face value and forget about the on-energy-shell requirement? Recent new work [2] suggests that this is reasonable provided that we do not move too far away from the particular ejected energy for which the pseudostates were constructed. We show some of these new results here.

### 3. Results

We show a sample of results for antiproton ionization of H(1s). These have been calculated using the 165 state pseudostate set \( \{H(nl), l = 0 \text{ to } 9, n = (l + 1) \text{ to } 21\} \) described in [1]. This set has been constructed to describe the ejection of a 5eV electron. As a benchmark, in some of the figures we make comparison with exact first Born calculations (FBA) for which, in the case of atomic Hydrogen, there is an exact analytic expression for the TDCS, see [1].

First let us look at an impact energy of 30 keV. In figure 1 we show a three dimensional picture of the TDCS for an ejected electron energy of 5 eV. Here we see that the FBA gives a cross section with a large binary peak pointing in the direction of \( \mathbf{q} \), i.e., in the "forward" region. By contrast, the 165 approximation shows a smaller cross section in which the electron is deflected into the "backwards" region, a result of post collisional interaction between the antiproton and ionized electron, a physical effect not represented in the FBA.

Using our new generalised version of (7) [2] we show in figure 2 the 165 state double differential cross section \( d^2\sigma/dE d\Omega_e \) at 30 keV for a range of ejected electron energies up to 5 eV. We see increasing backward repulsion of the electron with decreasing ejected energy. Figure 3(a) shows the single differential cross section \( d\sigma/d\Omega_e \) at 30 keV. This cross section is an integral over all ejected electron energies and, like \( d^2\sigma/dE d\Omega_e \), an integral over all angles of the scattered antiproton. In \( d\sigma/d\Omega_e \) we see a maximum near 70°, a shallow dip near 120° and a subsequent rise to backward ejection. While figure 2 shows a clear preference for backward ejection for the lowest energy electrons, figure 3(a) demonstrates that, overall, the picture is a little bit different, i.e., the higher energy electrons are not so easily stampeded into the backward direction by post collisional interaction. Figure 3(b), which gives \( d\sigma/dE \) at 30 keV, shows that there are plenty of electrons with energies higher than those shown in figure 2, i.e., above 5 eV. Also exhibited in figure 3(a) is the FBA which, as one might expect from figure 1, clearly prefers forward ejection.

There has been much discussion in the literature, e.g., [3], about of the role of the nuclear interaction in differential ionization. The interaction \( V \) between the antiproton and a hydrogen atom is given by

\[
V = \frac{k_f}{\mu} \frac{\rho}{r^2} e^{-r/a} \sin\theta
\]

where \( r = \sqrt{x^2 + y^2 + z^2} \) and \( a \) is the radius parameter. The interaction is attractive for small \( r \) and repulsive for large \( r \). The pseudostates are constructed so that the energy of each state is given by \( \varepsilon^+ + \kappa/2 \). This means that for each ejected electron energy a new set of pseudostates must be constructed and the equations (5) solved. This is highly inconvenient if one needs to average cross sections over experimental energy resolutions or wants to calculate cross sections for comparison with experiment. It is therefore important to see if (7) can be easily extended to a range of ejected energies while using a single set of pseudostates. What if we simply take (7) at face value and forget about the on-energy-shell requirement? Recent new work [2] suggests that this is reasonable provided that we do not move too far away from the particular ejected energy for which the pseudostates were constructed. We show some of these new results here.
Figure 1. TDCS in three dimensions for an ejected electron of 5 eV and an impact energy of 30 keV with \( q = 0.7 \) au. Wire cage, FBA; solid surface, full coupled pseudostate calculation. The antiproton is incident along the z-direction.

Figure 2. Cross section \( \frac{d^2\sigma}{dEd\Omega} \) at 30 keV.

Figure 3. Cross sections (a) \( \frac{d\sigma}{d\Omega_e} \) and (b) \( \frac{d\sigma}{dE} \) at 30 keV.

\[
V = -\frac{1}{R} + \frac{1}{|R - r|} \tag{9}
\]

where \( \mathbf{R}(\mathbf{r}) \) is the position vector from the proton to the antiproton (electron). Because of the
Figure 4. Cross sections (a) \(d^2\sigma/dEdq\) for an ejected electron of 5 eV, and (b) \(d\sigma/dq\), at 2 keV.

correspondence (6) between the wave treatment and the impact parameter approximation it is clear that the approximation (7) includes a proper representation of the interaction between the antiproton and the atomic nucleus (the \(-1/R\) term in (9)). In antiproton scattering the nuclear interaction becomes more and more important as the impact energy is reduced, this is perhaps not surprising since in the low energy limit we approach the onset of significant protonium formation [4]. To illustrate the importance of the nuclear interaction we show in figure 4(a) the cross section \(d^2\sigma/dEdq\) for antiproton ionization of H(1s) at an impact energy of 2 keV and for an ejected electron energy of 5 eV. Here we see that the FBA cross section collapses very rapidly with increasing momentum transfer \(q\). From (1) and (9) the first Born amplitude for ionization is

\[
 f_{ion}^{B1} = -\frac{1}{2\pi} \langle e^{ik_f \cdot R} \psi^-_0 | e^{-ik_f \cdot R} \psi^+ \rangle - \frac{1}{R} + \frac{1}{|R - r|} \langle e^{ik_f \cdot R} \psi^-_0 | e^{-ik_0 \cdot R} \psi^+_0 (r) \rangle \tag{10}
\]

Due to the orthogonality of \(\psi_0\) and \(\psi_-\) the nuclear interaction \(-1/R\) disappears from the approximation which can therefore only represent scattering of the antiproton by the electron. The light electron is unable to provide large momentum transfers to the antiproton and so the FBA declines rapidly with increasing \(q\). Initially the 165 coupled pseudostate approximation falls like the FBA but then, with increasing \(q\), quickly reaches a sharp minimum and then rises to a pronounced maximum and continues to show a sustained cross section up to large values of \(q\). In the initial fall of the 165 state cross section we see the longer range interactions which are included in the FBA, but in the minimum and subsequent maximum we see the nuclear interaction start to exert its influence.

Figure 4(b) shows the single differential cross section \(d\sigma/dq\). This is obtained by integrating \(d^2\sigma/dEdq\) over all allowed ejection energies for a given allowed \(q\), i.e.,

\[
 \frac{d\sigma}{dq} = \int_0^{(qv_0 + \varepsilon_0 - \varepsilon^+)} \frac{d^2\sigma}{dEdq} dE \tag{11}
\]

\[
 q \geq q_{min} = \frac{\varepsilon^+ - \varepsilon_0}{v_0} + O \left( \frac{1}{\mu} \right) \tag{12}
\]

Note that \(d\sigma/dq\) is zero at the threshold \(q = q_{min}\), figure 4(b), unlike \(d^2\sigma/dEdq\) which is non-zero at the minimum \(q\) allowed for the given ejected electron energy, figure 4(a). Apart from
rising from zero at $q = q_{\text{min}}$ the FBA and 165 cross sections of figure 4(b) are similar to those of figure 4(a). This similarity is perhaps not a surprise since the nuclear effect is probably not that different for each ejected electron energy.

Figure 5 shows $d\sigma/dE$ at 2 keV. As at 30 keV, figure 3(b), and as in the FBA, the 165 pseudostate cross section is greatest at zero ejected energy. However, the shape of the cross section is different. being mainly convex upwards at the lower energies while the other cross sections are concave downwards which seems to be a feature of the FBA and therefore of the higher impact energy regime.

4. Conclusions
In [1] and [2] a powerful method based on impact parameter pseudostate close coupling has been introduced. This method can give fully differential cross sections able to describe any aspect of coincidence measurements using heavy projectiles. Here we have shown but a few simple examples from antiproton impact ionization of atomic hydrogen. Results for ionization by carbon and gold ions have also been obtained but will be published elsewhere.

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