Classical Trajectory Monte Carlo Calculation of the Fully Differential Cross Section for Ionization of $H_2$ by Positron Impact

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Abstract. The possibility of performing kinematically complete measurements of ionization collisions by positron impact brings about the promise of encountering new unexpected phenomena, which otherwise would be impossible to foresee. In this communication, we employ the classical trajectory Monte-Carlo method to explore $H_2$ ionization fully differential cross section (FDCS), depending on the relative momentum of the electron-positron continuum dipole and the deflection angle of its center of mass. We find a strong structure in the FDCS at non-zero deflection angles. Finally, we discuss some of these new effects, and the possibility of observing them in actual experiments.

1. Introduction
In the early sixties experimental techniques reached a stage where it was possible to measure double differential cross sections (DDCS) on the energy and angle of the electrons ejected in ion-atom collisions. This technical breakthrough opened the way to the discovery of new unforeseen phenomena. The most conspicuous was a pronounced peak that occurred when the electron-projectile relative momentum $k$ approached zero [1, 2, 3]. Many years later this cusp, first thought to be due to spurious electrons [1], was identified and explained in terms of an electron capture to the continuum (ECC) mechanism [4]. In positron impact collisions, this peak is spread out in the DDCS by the deflection of the much lighter projectile [5, 6], and only becomes visible if the projectile scattering angle is also measured, as demonstrated by Kövér and Laricchia in 1998. Further experiments [7, 8] disclosed another interesting effect: The ECC cusp was not centered at $k = 0$. While $k = 0$ corresponds to electron and positron matching energies, it was experimentally observed that the cusp maximum is shifted to lower values of the electron energy and higher values of the positron energy.

2. Classical Trajectory Monte Carlo (CTMC) Simulations
The natural conclusion of these few examples is that by increasing the dimension of the cross section, new effects are discovered. Thus, the possibility of performing kinematically complete measurements of ionization collisions by positron impact brings about the possibility of encountering new phenomena, which otherwise would be impossible to foresee. With this
premise in mind, let us explore the Fully Differential Cross Section (FDCS) for ionization of molecular hydrogen by positron impact. To this end we employ “Classical Trajectory Monte Carlo” (CTMC) simulations with more than $2 \times 10^8$ trajectories [9]. We study the ionization of H$_2$ molecules by the impact of 50 keV positrons using a simple three-body model [9]. The obtained cross sections correspond to averaged values over all possible orientations of the molecule. By rotational symmetry and momentum and energy conservation, this FDCS is fully characterized by four out of the nine variables associated to the three-body final state [10]. A convenient choice to study the ECC cusp features is the reduced electron-positron momentum $k = (k_e - k_P)/2$ and the direction of the momentum $K$ of the positron-electron center-of-mass respect to the residual target ion.

Figure 1 shows the cartesian projections of the cross section in $k$-space. The three upper maps correspond to the center-of-mass (CM) of the electron-positron system restricted to moving within 5 degrees of the direction of the initial positron velocity $v$, while in the lower maps the CM has been deflected in $45 \pm 5$ degrees.

![Figure 1. Cartesian projections of the distribution of the electron - positron relative momentum $k$ for the ionization of H$_2$ molecules by 50 keV positron impact. The orthogonal components of $k$ are defined as follows: $k_z$ is parallel to the momentum $K$ of the electron-positron center-of-mass with respect to the residual target ion; $k_{\parallel}$ and $k_{\perp}$ are parallel and perpendicular to the plane formed by $K$ and the initial velocity $v$, respectively. The figures correspond to angles of $0^\circ$ and $45^\circ$ between $K$ and $v$ as indicated, within an uncertainty of $5^\circ$.](image)

The momentum distribution in figure 1 is peaked at $k = 0$ and $k \approx -0.8 \hat{z}$ a.u., but blurred to some extent by the resolution employed to visualize the CTMC simulation. The first cusp corresponds to the aforementioned ECC effect, while the second can be related to the excitation
of the electron to a low-lying continuum state of the target. Another conspicuous feature of this momentum distribution is a strong orientation of the electron-projectile pair away from the forward direction \((k_Z > 0)\), an effect that can be ascribed to the Coulomb interaction with the receding ion. It was recently proposed that this effect might explain why, while centered at \(k = 0\) as it was just explained, the ECC cusp exhibits an apparent deviation towards lower electron energies when it is convoluted with the experimental acceptance [11]. In figure 2 we show this shift of the ECC cusp at \(0^\circ\) for the FDCS as a function of the electron energy and angle and the positron angle. The cross sections for larger final angles of the electron and the positron in a coplanar geometry show increasingly larger displacements. While the cusp should be located at exactly the same energy for all angles by energy and momentum conservation, this increasing shift represents a characteristic fingerprint of the strong orientation of the electron-projectile continuum dipole previously described.

Figure 2. Normalized cross sections for the ionization of \(\text{H}_2\) molecules by 50 keV positron impact. The electron is ejected in the plane determined by the initial and final positron momenta in the Lab frame. The electron and the positron are detected in the same direction at an angle \(\theta\) with respect to the positron incident velocity direction. The plane is determined in all cases with an uncertainty of 30\(^\circ\). \(E_0\) is the energy corresponding to the kinematical position of the cusp, obtainable only for infinitesimal resolution. The cusp should be located at exactly this energy for all emerging angles.

These are only some of the structures observed in figure 1. While at \(0^\circ\) the cross section is relatively simple due to the rotational symmetry of the collision process, it becomes very complex at non-zero deflection angles, up to the point that any subjacent structure is difficult to apprehend. In cases like this, rotating the point of view might help to get a clearer visualization, as shown in the video accompanying the online version.

Structures like the one described above are not only difficult to identify and visualize in CTMC and Quantum Mechanical calculations, but also very hard to measure. However, they might still leave observable fingerprints in lower-dimension cross sections. For instance, the DDCS in the recoil ion momentum exhibits a threshold structure that can be related to the ECC cusp at \(k=0\), as shown in figure 3. This threshold has even an effect on the cross section singly differential in the parallel component [12], as it can be seen in the upper panel of figure 3, a structure than becomes sharper whenever the transversal component is restricted to a narrow region in momentum space, (see figure 4). These results might represent good opening experiments for future positron cold-target recoil-ion momentum spectroscopy (ColTRIMS) setup.

3. Conclusions
We have calculated the FDCS for the ionization collisions by positron impact by means of CTMC simulations. We have discussed some effects observed in this very complex cross section. They display some structures, some very well known, such as the ECC cusp, some novel, such as the
Figure 3. The gray scale map displays the DDCS for the ionization of H$_2$ molecules by 50 keV positron impact as a function of the components of the recoil-ion momentum $K_R$ parallel ($||$) and perpendicular ($\perp$) to the initial projectile velocity $v$. The upper and right side graphs show the cross sections single differential in $K_{R||}$ and $K_{R\perp}$, respectively.

orientation of the electron-positron system. It is noteworthy that this orientation is reproduced in simulations for ionization at higher incident energies, though the effect is less pronounced. Also, calculations on ionization of helium by impact of 50 eV positrons show a similar effect. Finally we discussed how these effects might affect lower dimension cross sections, making it feasible to observe them in actual experiments.

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Figure 4. Normalized cross section for the ionization of $\text{H}_2$ molecules by 50 keV positron impact, single differential in the recoil ion momentum component parallel to the initial velocity $v$. The threshold becomes sharper for decreasing acceptances $\Delta K_{R\perp}$ of the transversal momentum component. In the limit of perfect resolution the cross section presents a discontinuity in the threshold.

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