B.1.3. Do v/2 Electrons Imply the Saddle Point Mechanism for Ion Impact Ionization of Atoms?--*Emil Sikdy, Clara Illescas and C.D. Lin*

In Section B.1.2 we showed that the momentum distributions obtained from our quantum mechanical calculations do not agree with the calculations of Macek and Ovchinnikov [1]. Since there are no experimental data and no other theoretical calculations available for comparison, we decided to collaborate with Dr. A. Riera's group in Spain [2], who has been examining the ionization dynamics using a different version of the classical trajectory Monte Carlo method (CTMC). Using an initial distribution which reproduces the ground state density distribution of the hydrogen atom, they performed the CTMC calculations and were able to show that the resulting total ionization cross sections agree quite well with the recent measurements of Shah *et al.*, [3] in the low-energy region of a few keV. In their work they also addressed the "explosion" of the free electrons, which actually is the free expansion of the ionized electrons.

Since it is relatively straightforward to obtain electron momentum distributions from the classical calculations, we were able to obtain the longitudinal and transverse momentum distributions from the CTMC calculations and compare the results with what we have obtained using the quantum formulation. The comparison is given in Fig. 1. The plots show qualitative agreement, even in some fine details, with the CTMC results tending to give narrower distributions. Both results differ from those reported by Macek and Ovchinnikov [1] in that we did not see any rapid oscillations in the transverse distributions between 5 and 15 keV. Of course the final answer to the discrepancy has to wait for experimental confirmation.

In addition to the calculated or measured electron momentum spectra, it is an interesting question to ask what is the mechanism for ionization at low energies. In our early paper [4] using a three-center atomic orbital close-coupling calculation, we discovered the importance of the potential saddle (which was used as the third center) in ionization at low energies. In the CTMC calculations by Olson at higher energies [5] it was found that there is a concentration of electrons at v/2, where v is the collision speed. It has since been understood by many groups that a peak in the momentum distribution near v/2 is direct evidence that the potential saddle plays a major role in the ionization process. Since the 1980's there have been many experiments performed at relatively high energies searching for the v/2 electrons with the goal of proving the importance of the saddle point mechanism for ionization, in contrast to our earlier studies which showed that saddle point mechanism decreases in importance as the collision energy is increased. These experiments have been summarized in a recent monograph [6].

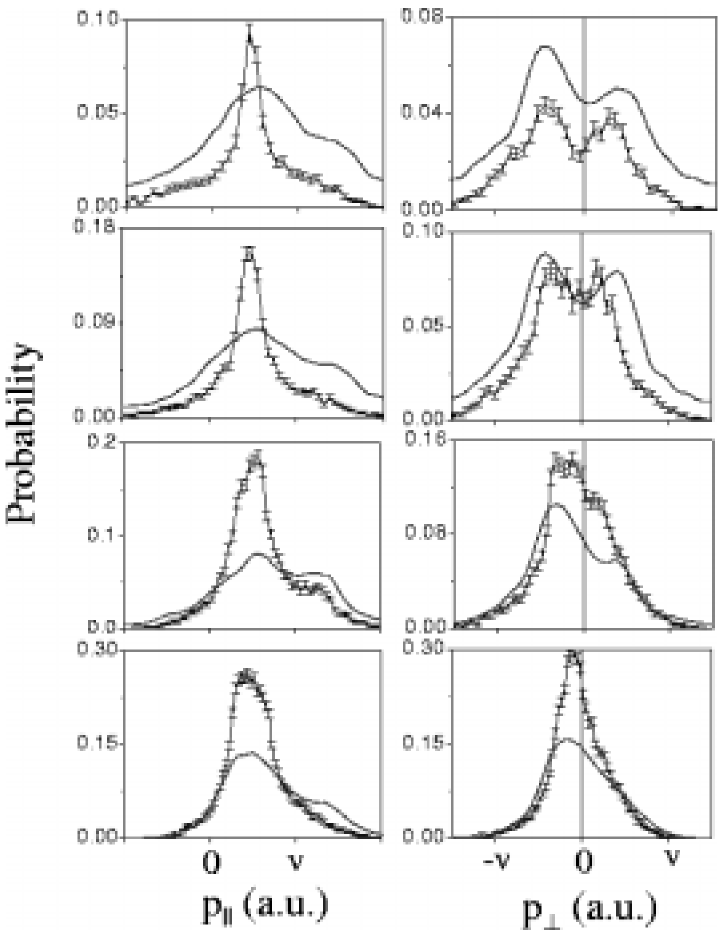

Figure 1. Projection of classical (thin line with error bars) and quantum mechanical (thick line) ejected electron distributions parallel, $p_{\parallel}$, and transverse, $p_{\perp}$, (in collision plane) to projectile motion. The collision system is proton on hydrogen at 10, 15, 25 and 50 keV (from top to bottom).

Thus one of the important issues is whether it is possible to find an experimental signature that can prove the importance of a saddle point mechanism for ionization. In a slow collision, it is very difficult for the electron to get ionized when the electron is close to either proton since the strong Coulomb attraction can pull the electron into bound states. An electron can remain free only if it is sitting near the potential saddle where it experiences zero force along the direction of the internuclear axis. These electrons are bound at finite internuclear separations and they are ionized as the potential saddle is pushed up, when the two nuclei recede from each other.

We have not found a convenient way to analyze the time evolution of the ionized electrons in the quantum formulation, thus we decided to explore the role of saddle point in ionization classically. First we identified all the electrons that are ionized at R=500, i.e., those electrons that have positive total energies with respect to either center. We then backtrack these electrons to smaller R, to examine how they are eventually ionized. An example of the momentum distributions of these electrons at R=30 for collisions at 15 keV and impact parameter 1.2 a.u. is shown in Fig. 2. The striking feature is that there is a lack of electrons near both the target and projectile velocities. To estimate roughly the minimum momentum that an ejected electron needs to have with respect to the target or the projectile for it to be ionized, we assume that the ejected electron primarily exhibits a free expansion. Thus its distance from the center is proportional to the momentum of the electron p, and t is measured from the distance of closest approach. Thus the distance r =(R/v) p. By requiring that the total energy with respect to either center be zero, the smallest momentum for the electron to be ionized with respect to that center may be found as

$$\frac{p^2}{2}-\frac{Z}{(R/v)p}=0; \qquad p_{ion}=\left(\frac{2vZ}{R}\right)^{1/3}. \tag{2}$$

where ν is the projectile velocity and Z is the nuclear charge. The two circles drawn in Fig. 2 are from this equation. Among the electrons we further distinguish two groups. The first group is for electrons that have positive energies with respect to both centers. These kinetic electrons are considered ionized at this R. In the second group, the electron energy is negative with respect to either proton. These electrons need the potential from the other proton to get free. They rely on the long range potential from the other center to reach the continuum. These are called saddle point (SP) electrons. In Fig. 2 the kinetic electrons are denoted by light dots, and SP electrons are denoted by dark dots. Clearly all the SP electrons are located inside the circles. As the internuclear separation increases, the fraction of SP electrons diminishes. At each fixed R, the fraction of SP electrons decreases with increasing collision velocities.

Our definition of SP electrons allows us to explore quantitatively the importance of the SP mechanism for ionization as well. We found that the SP mechanism plays no role at all internuclear distances at 50 keV. From Fig. 1, however, at this energy the longitudinal electron momentum distribution still shows a v/2 peak. In other words, a v/2 peak does not prove that the saddle point mechanism is important for the ionization. In the 5-15 keV region we do see SP electrons contributing a significant fraction to ionization, about 40% at R=10 a.u. for 10 keV collisions.

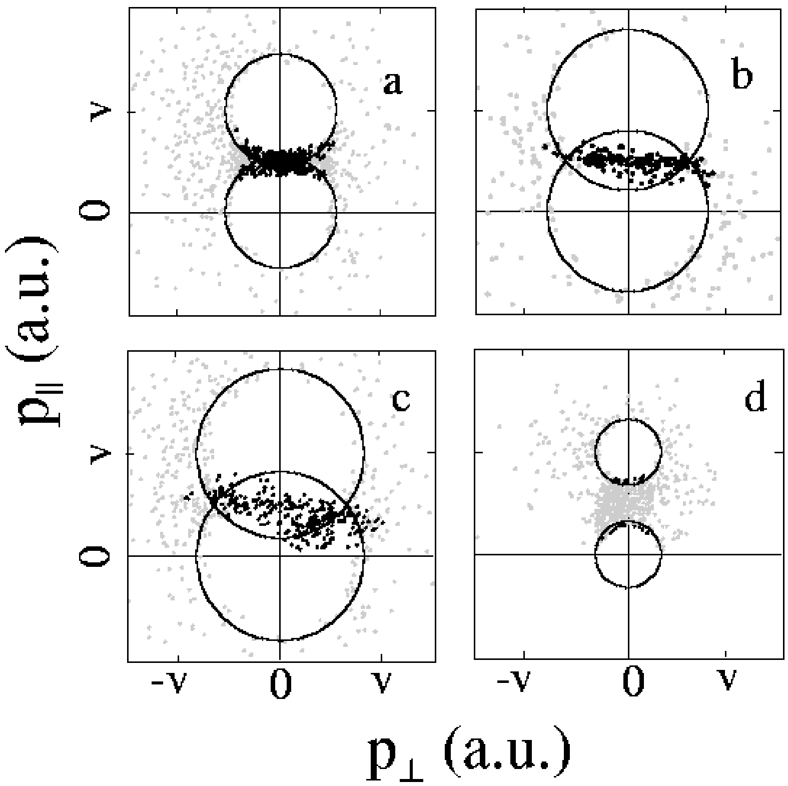

Figure 2. Collision plane scatter plot of ejected electrons, in momentum space, within 0.1 a.u. of the collision plane. Light and dark circles represent kinetic and saddle electrons respectively, see text. (a) 15 keV at z=vt=30 a.u.; (b) 5 keV at z=20 a.u.; (c) 15 keV at z=9 a.u., and (d) 50 keV at z=30 a.u.

References

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