B. ATOMIC PHYSICS WITH HIGHLY CHARGED IONS: THEORY

B.1. Ion-Atom Collision Theory

B.1.1. Solution of the Time-Dependent Schrödinger Equation in Momentum Space--*Emil Sidky and C.D. Lin*

The motivation of this program was to address issues originating from experiments carried out with the COLTRIMS apparatus.

Ionization is one of the possible reaction processes in any ion-atom collision. While the theory is trivial in the high-energy regime where the Born approximation is valid, the theory for ionization at intermediate and lower energies is not on a solid footing. In the past few years we have used distorted wave theories like the so-called CDW-EIS approximation [1] to obtain electron momentum distributions in ion-atom collisions in the intermediate energy region with good success, but the theory clearly fails in the lower energy region. Thus an alternative approach is needed in order to tackle ionizations at low energies. At lower energies, charge transfer and excitation processes in general dominate. The semiclassical close-coupling theory has been found to be quite successful in treating excitation and charge transfer, however, it does not treat ionization processes adequately. Using pseudostates as basis functions, one can obtain reliable total ionization cross sections, as we have done in the past [2], but the method cannot obtain the ejected-electron momentum distributions which are being determined by experimentalists using the COLTRIMS apparatus.

In the past grant period we have initiated a new theoretical approach aimed at obtaining the momentum distributions of the ionized electrons directly in a broad range of collision energies. The method we adopted is the direct solution of the time-dependent Schrödinger equation in momentum space (see Publication #23). The momentum wavefunction is expanded as

$$\Phi(\vec{p},t) = \sum_{l,m} \tilde{T}_{l,m}(p,t) Y_{l,m}(\hat{p}) + e^{-i(\vec{p}\cdot\vec{R} - \frac{1}{2}v^2 t)} \sum_{l,m} \tilde{P}_{l,m}(q,t) Y_{l,m}(\hat{q}), \qquad \vec{q} = \vec{p} - \vec{v}\,. \qquad (1)$$

Here T and P are radial momentum wavefunctions with respect to each collision center, and Y's are the spherical harmonics in momentum space. The phase factor in front of the second term on the right side is the plane-wave electron translational factor (ETF). The summation over the angular momentum quantum numbers can be truncated. The radial functions are expanded further in terms of B-splines functions.

It is not practical to perform calculations in the momentum space directly since the time-dependent Schrödinger equation in momentum space is an integral equation and the kernel in the integral equation is not convenient to evaluate. We Fourier transform Eq.(1) to coordinate space and perform the integration of the time-dependent Schrödinger equation in the coordinate space directly. To avoid the evaluation of two-center matrix elements we solve the time-dependent equation on numerical grids. The algebraic equations are solved using a linear least-squares fitting procedure for propagation forward in each time step. At the end of the integration which is chosen at R=30 a.u. one can project the bound states on the projectile and on the target. The remaining wavefunction then represents the ionization. Since the momentum basis functions are calculated the momentum distributions of the ionized electrons are obtained directly.

We have checked that the excitation and electron capture probabilities thus obtained are in good agreement with those obtained from the close-coupling calculations. We further checked that the total ionization probability at each impact parameter is also in good agreement with the result of the close-coupling calculation. After these have been checked we can examine the ejected momentum distributions.

In Fig. 1 we show an example of the momentum distributions thus calculated. The collision velocity is 1 a.u. and the impact parameter is 2.5 a.u. The upper frame is for protons colliding with atomic hydrogen, the lower frame is for collisions with antiprotons. The velocity distribution is plotted after

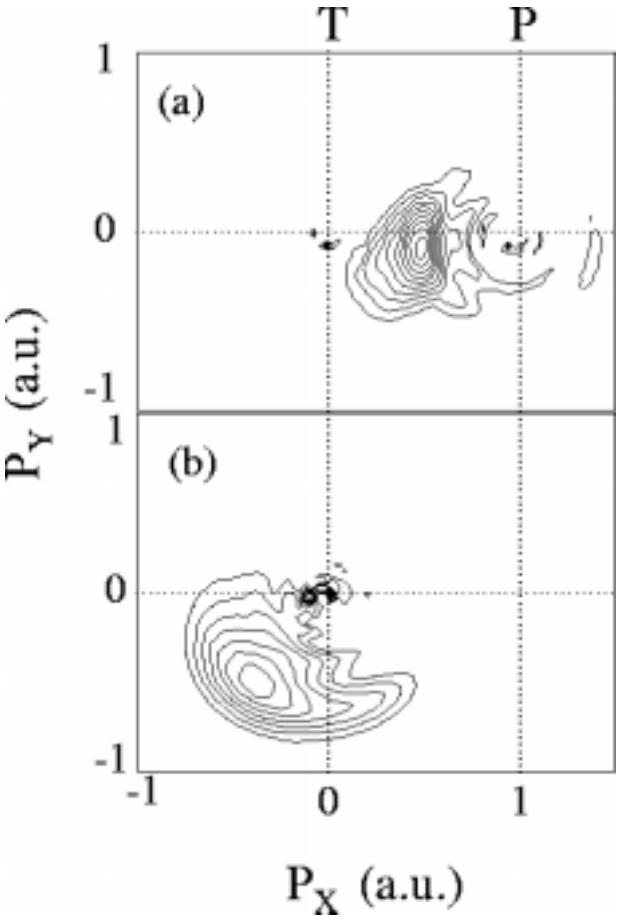

Figure 1. The ejected-electron momentum distributions projected onto the collision plane for (a) proton on hydrogen collisions and (b) antiproton on hydrogen collisions. The collision velocity is 1 a.u. and the impact parameter is at 2.5 a.u. (Publication #23).

integrating over the direction perpendicular to the collision plane. The results in this figure are not unexpected. For proton-hydrogen collisions the ionized electrons are concentrated near v/2, away from the two collision centers where capture and excitation are more likely to occur. For antiproton collisions the electrons are concentrated near the target and away from the side where the antiproton enters the collision (on the +y side). These results are consistent with our intuitive understanding of the collision.

By using the two-center expansion and a fitting procedure we have been able to perform these calculations on personal computers. Direct integration of the time-dependent Schrödinger equation in coordinate or in momentum space without the two-center expansion often requires much more computational resources [3,4]. These latter calculations have not been attempted to extract the ejected electron momentum distributions so far.

References

1. See for example, Y.D. Wang *et al*., Phys. Rev. A 53, 3278 (1996).
2. Y.D. Wang, C.D. Lin, N. Toshima and Z. Chen, Phys. Rev. A 52, 2852 (1995).
3. J. Wells *et al*., Phys. Rev. A 54, 593 (1996).
4. K. Momberger, A. Belkacem and A. Sorensen, Phys. Rev. A 53, 1605 (1996).