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Ion scattering from state-selected Rydberg atoms

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Classical-trajectory Monte Carlo calculations have been performed for collisions of protons with state-selected hydrogenic Rydberg atoms. The examples investigated were Rydberg atoms in the $n=10$, $l=9$ level with $m_l=0$ and 9. The collision velocity range was 0.1 to 1.0 a.u. (2.2×10^7 to 2.2×10^8 cm/s). The ionization cross sections were found to be relatively insensitive to changes in the m_l levels. However, the charge-transfer cross sections showed considerable enhancement if the Rydberg electron is orientated in a plane which is parallel to the direction of the incident projectile.

INTRODUCTION

It is quite difficult to examine charge-transfer and ionization cross sections for collisions between ions and state-selected Rydberg atoms using a quantum-mechanical treatment. Therefore we have investigated the problem using the classical-trajectory Monte Carlo (CTMC) technique. Monte Carlo techniques have been thoroughly discussed in the literature and successfully applied to collisions between ions and Rydberg atoms.[1–4]

The application of the CTMC method to collisions involving state-selected atoms requires the use of modified random variables which directly place the Rydberg atom into a specific n,l,m_l state. Once the atom has been orientated, the collision trajectories are calculated with use of standard techniques. In this study, the reactions of interest are

$$A^+ + B(n,l,m_l) \rightarrow A + B^+ \text{ (charge transfer)} \quad (1)$$

and

$$A^+ + B(n,l,m_l) \rightarrow A^+ + B^+ + e^- \text{ (ionization)} \ . \quad (2)$$

Total cross sections are presented for processes (1) and (2). Our studies focused on hydrogenic atoms since classical techniques are directly applicable.

MONTE CARLO METHOD

In applying the classical trajectory Monte Carlo method to state-selected Rydberg atoms, we have made two departures from the five traditional random variables used to define the electron orbit.[2,5] First, instead of choosing the eccentricity of the electron orbit ϵ using

$$\beta = 1-\epsilon^2 \ , \quad (3)$$

with $0\leq\beta\leq1$, as is usually done when using the microcanonical distribution for a given n level, we have randomly selected the square of the eccentricity uniformly in the interval

$$1-(l+1/n)^2 \leq \epsilon^2 \leq 1-(l/n)^2 \ . \quad (4)$$

This is equivalent to choosing a value for the l quantum number $l_{\rm cl}$ in the range

$$l \leq l_{\rm cl} < l+1 \ . \quad (5)$$

Mackellar and Becker[6] have shown that binning $l_{\rm cl}$ in this manner reproduces the quantal weights $(2l+1)/n^2$, and is general for all n and l values, including the microcanonical representation of the $1s$ state.

The second point of departure eliminates one random variable entirely. Instead of choosing the second Euler angle θ (i.e., the rotation from z to z' about x') randomly in the range

$$0 \leq \theta \leq \pi \ , \quad (6)$$

we have defined θ to be

$$\cos\theta = \frac{m_l}{\sqrt{l(l+1)}} \ , \quad (7)$$

where m_l is the magnetic quantum number (the z component of the angular momentum). In effect, we are demanding that the z component and the magnitude of the classical angular momentum be in the same proportion as their quantum counterparts.

In our study, the direction of the incident projectile's velocity is chosen to be the z direction. Therefore the magnetic quantum number will be related to the orientation of the projectile's motion relative to the plane of the electron's orbit.

With these two changes we are able to place Rydberg atoms into an initial n,l,m_l state. All the remaining random variables for determining the electron orbit and the spanning of the two-dimensional impact-parameter space are unchanged from previous descriptions in the literature.[7]

Once the Rydberg atom is placed in an initial state and the impact parameter is specified, the subsequent motion of the system is determined via the Hamiltonian

$$H = \sum_{i=1}^{3}\frac{p_i^2}{2m_a} + \sum_{i=4}^{6}\frac{p_i^2}{2m_b} + \sum_{i=7}^{9}\frac{p_i^2}{2m_c} + V(q_1,\ldots,q_9) \ , \quad (8)$$

and the 18 coupled equations of motion,

$$\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i} \ , \quad (9)$$

$$\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i} \ . \quad (10)$$

In Eq. (8), m_a,m_b,m_c are the masses of the projectile, Rydberg nucleus, and electron, respectively. Z_a,Z_b,Z_c are similarly defined as the charges on the respective particles, q_i and p_i are the generalized coordinates and momenta of the parti-

cles, and V is the Coulomb interaction potential between the particles.

RESULTS AND DISCUSSION

Charge-transfer and ionization cross sections were calculated for protons colliding with hydrogenic Rydberg atoms in the $n=10$, $l=9$, and $m_l=0$ and $m_l=9$ excited states. Incident proton velocity v spanned the range

$$1 \leq v/v_e \leq 10 \ , \tag{11}$$

where $v_e = 2.19\times 10^{+8} n^{-1}$ cm/s is the orbital velocity of the Rydberg electron. For this velocity region the CTMC method has demonstrated its ability to yield accurate cross sections for ion-hydrogenic atom collisions.

The charge-transfer cross sections are plotted in Fig. 1 as a function of reduced proton velocity (v/v_e) for the representative cases $m_l=9$ and $m_l=0$. When the reduced velocity is unity, the incident proton is in the neighborhood of the atom for approximately the time it takes the electron to make one orbit, and the charge-transfer cross sections for $m_l=9$ and $m_l=0$ are identical within Monte Carlo statistical errors. At this velocity the major factor determining the magnitude of the cross section is the length of time the proton spends in the region of the atom, not the relative velocities of the electron and incident particle. However, as the velocity increases, the cross sections diverge rapidly, with the charge-transfer cross section for $m_l=9$ decreasing much more rapidly than that for $m_l=0$.

A qualitative understanding of this phenomena can be gained from Fig. 2 which depicts the collision geometry for our two cases. For $m_l=0$ the proton is incident in the direction of the field and sees an "edge view" of the electron orbit. Hence, for impact parameters $b \lesssim 100a_0$, the incident proton can significantly perturb the electron when both particles are on the same side of the nucleus and capture the electron. Consequently, velocity matching becomes a major factor and charge transfer proceeds with high probability. With increasing proton velocity, the length of time the proton spends in the neighborhood of the atom decreases, leading to a rapid decrease in the charge-transfer cross section.

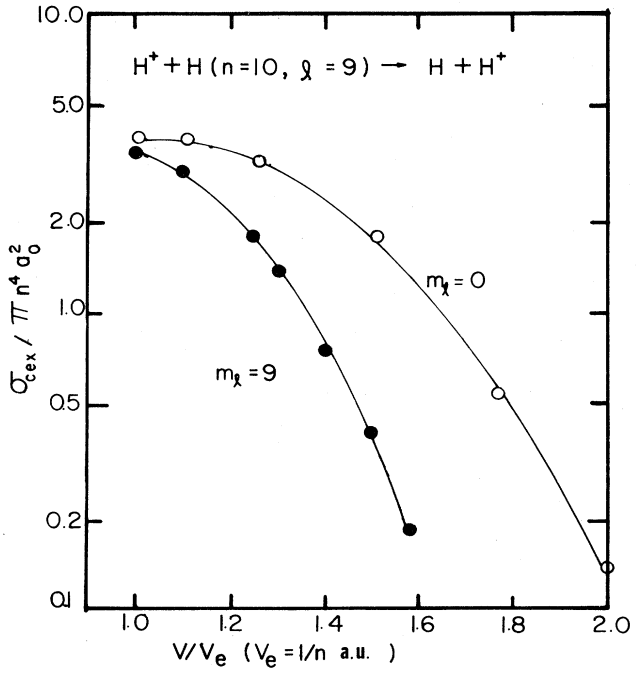

FIG. 1. Charge-transfer cross sections for collisions of protons with hydrogenic Rydberg atoms in the states $n=10$, $l=9$, and $m_l=0$ (open circles) and $m_l=9$ (closed circles). 1-standard-deviation statistical errors are $\leq 10\%$.

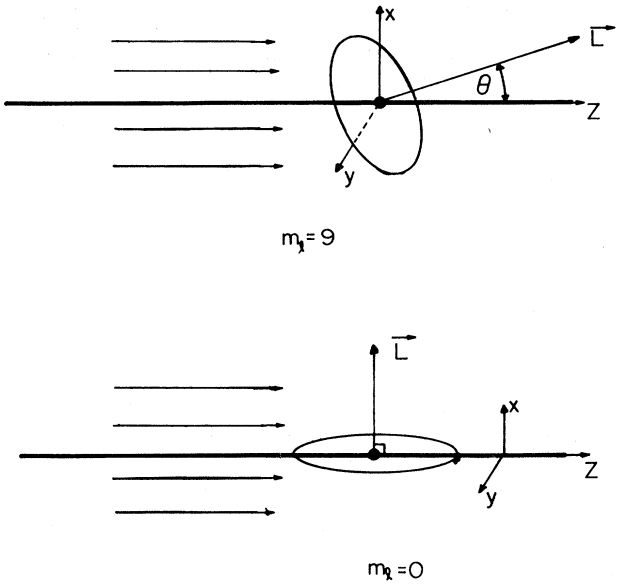

FIG. 2. Schematic of the collision system and the orientation of the Rydberg electron relative to the incident projectile.

A test of the velocity-matching hypothesis is provided by examining the $m_l=9$ case. Now the orbital angular momentum vector is nearly aligned with the incoming particles's trajectory, giving the incident proton a "view" of the entire electron orbit. However, at no time does there exist the possibility for velocity matching. In order to capture an electron, the incident proton must "shear" the electron away from the nucleus. At higher incident velocities the proton spends little time in the neighborhood of the Rydberg electron and is unable to impart sufficient momentum in the direction required to capture the electron. Thus the cross section for capture from $m_l=9$ is much smaller than for $m_l=0$ (see Fig. 1).

Figure 3 illustrates the ionization cross section for the sublevels $m_l=0$ and $m_l=9$. From the agreement between these two cases it appears that velocity matching is not an important mechanism for ionization since a preferential direction imparted to the ejected electron is not required. Geometrical considerations, however, are important at the higher velocities with the $m_l=9$ results lying slightly above the $m_l=0$ values. The impact-parameter dependence of the transition probabilities reveals that the $m_l=9$ values are larger than those of the $m_l=0$ at large impact parameters, since the entire $m_l=9$ orbit is in the impact-parameter region $b \approx 100a_0$. In contrast, small impact-parameter collisions contribute very little to the ionization of the $m_l=9$

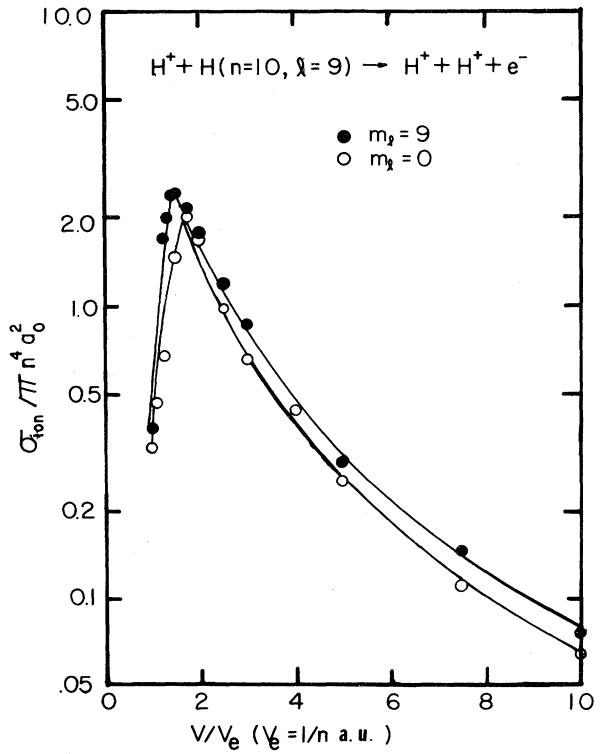

FIG. 3. Ionization cross sections for the collisions of protons with hydrogenic Rydberg atoms in the states $n=10$, $l=9$, and $m_l=0$ (open circles) and $m_l=9$ (closed circles). 1-standard-deviation statistical errors are $\leq 10\%$.

sublevel, since the projectile can pass through the center of the $m_l=9$ orbit. Because the transition probabilities are weighted by the impact parameter in the cross-section evaluation, the net result is that the $m_l=9$ cross sections are slightly larger than those of $m_l=0$.

SUMMARY

In summary, we have introduced a procedure for placing Rydberg atoms into initial n,l,m_l states when using the Monte Carlo method to simulate collisions with state-selected atoms. This prescription was then applied to the cases of protons on atomic hydrogen in the $n=10$, $l=9$, and $m_l=0,9$ states. The importance of velocity matching for charge-transfer cross sections was indicated. If the Rydberg electron's orbit is oriented so it provides an "edge view" to the incident proton, the charge-transfer cross sections are considerably enhanced for velocities $v/v_e > 1.0$. We have also shown that the ionization cross sections are relatively insensitive to the orientation of the Rydberg electron's orbit. An experimental test of these predictions may be possible in the near future with the rapid advances being made in experimental techniques for the measurement of ion–Rydberg-atom cross sections.[8]

ACKNOWLEDGMENT

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