Correlation in Antiproton Capture by Atoms and Molecules

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Antiprotonic ($\bar{p}$) atoms are formed in low-energy collisions between antiprotons and normal atoms or molecules. There is renewed interest in this subject due to upcoming experiments (ASACUSA Collaboration), which, for the first time, can directly measure the energy-dependent cross sections. This can be done for capture by the hydrogen molecule *and* atom, as well as for capture by the noble-gas atoms. The only existing accurate capture cross sections calculated purely quantum mechanically are for the hydrogen atom below 10 eV. They are in good agreement with a number of other more approximate calculations. Comparison between theory and experiment for this simplest system will be important in confirming that most captures occur after the $\bar{p}$ has been slowed to a kinetic energy less than or comparable to the target ionization potential. This problem can be interpreted as a case of a resonant state embedded in an electronic continuum, *a la* the Fermi Golden Rule.

However, there are other fundamental effects due to correlation and the additional degrees of freedom in multielectron atoms and molecules. The fermion molecular dynamics (FMD) method has enabled us to go beyond the atomic hydrogen target and study electron-correlation effects with noble-gas targets and molecular effects with isotopic molecular hydrogen targets. FMD is a quasiclassical method for treating quantum-mechanical systems using classical equations of motion with momentum-dependent model potentials added to the usual Hamiltonian to simulate quantum-mechanical effects. These model potentials constrain the motion to satisfy the Heisenberg uncertainty and the Pauli exclusion principles. In this method, correlation and rearrangement are simple.

The differences between capture by H_2 and the H atom are found to be dramatic. The effects due to the two-center structure, rotational motions, and vibrational motions are distinguished. Of particular importance, the vibrational degree of freedom enables the molecule to capture antiprotons

having lab energies above 100 eV, whereas atomic capture cuts off sharply above the ionization threshold of 27 eV (in the lab system). The largest molecular cross sections are obtained when the negative projectile mass best matches a nuclear mass in the molecular target. The vibrational degree of freedom is found to be most important in distinguishing capture by H_2, HD, and D_2, but the effects of rotations, two-center electronic charge distribution, and nonadiabaticity are also significant.

Antiproton captures by helium, neon, argon, krypton, and xenon atoms have also been treated using the FMD method. The residual electrons are generally left in a shake-up state. When capture is accompanied by multiple ionization, the second and later electrons are seen to escape with increasing kinetic energies, a process which is not well described as quasiadiabatic. In agreement with experiments on muonic and pionic atoms (none exist for antiprotons yet), the capture probabilities are found to increase with increasing numbers of electrons. This is opposite the trend predicted by a recent theoretical treatment using a quantum-mechanical *one-electron* method and provides evidence of the importance of electron-electron correlation.

The important electronic continua and molecular dissociation are easily, and perhaps accurately, treated quasiclassically. However, the quasiclassical method does not quantize the final states, so the effects of shake-up electronic states, excited ro-vibrational levels, and associated resonances may not be treated adequately. In addition to presenting some surprising results, I hope to initiate a dialog on what features will be important for a completely quantum-mechanical description and what possibilities exist for such capabilities.