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Atomic and Molecular Collisions using a Time-Dependent Close-Coupling Method[1]

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A non-perturbative time-dependent close-coupling method has been developed to handle quantal many-body Coulomb breakups found in photon-impact, electron-impact, and ion-impact ionization of atoms, molecules, and their ions. For atoms the time-dependent Schrodinger equation is solved using a 2D or 3D numerical lattice and an expansion in coupled spherical harmonics. For molecules the time-dependent Schrodinger equation is solved using a 4D numerical lattice and an expansion in rotational functions. For highly charged atomic ions the time-dependent Dirac equation is solved using a 2D numerical lattice and an expansion in coupled spin-orbit eigenfunctions. Theoretical cross sections are compared to experiment for a variety of atomic and molecular collisions, including the triple photoionization of the Li atom.

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