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Method to compute wave function evolution from microscopic to macroscopic distances JAMES STERNBERG, University of Tennessee — The treatment of loosely bound and continuum electrons in atomic collisions has provided challenges for calculations of these systems. These challenges have not been fully overcome for ion- atom collisions since electron wave functions evolve from microscopic to macroscopic distances. One major source of difficulty is that solutions to the time-dependent Schrödinger equation contain an essential singularity at infinity which makes numerical modeling of these systems difficult for large distances. We have identified this essential singularity and developed a method to treat these systems which is extremely efficient and stable. The method is Gallelian invariant, which avoids any ambiguity about what the proper frame of reference should be. It also avoids numerical inaccuracies induced by reflection or absorption at finite boundaries. Wave functions can easily be propagated out to macroscopic distances instead of only approximately 100 au. Finally, the results are consistent with the hidden crossing theory at low impact energies and the Born theory at high energies. In both regimes the electron distribution agree qualitatively with experiment.

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