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Semiclassical Simulation of Electron Scattering in Attractive Coulomb Potentials ANDREAS MARKMANN, Yale University, FRANK GRAZIANI, LLNL, VICTOR BATISTA, Yale University, CIMARRON COLLABORATION — We study the performance of semiclassical dynamics simulations of electron scattering in the Wigner-transform time-dependent picture at few attractive Coulomb potentials and a two-slit potential. Heisenberg uncertainty and interference are compared to exact quantum dynamics. Serious numerical problems typically arise in classical and semiclassical simulations involving Coulomb potentials when particles approach each other and potential gradients (or accelerations) diverge. We introduce an accurate and efficient algorithm for dynamics simulations of particles with attractive potentials developed within the multi-institutional Cimarron Project. Rather than avoiding the singularity problem by using a pseudopotential, the algorithm predicts the outcome of close encounter two-body collisions for the true Coulomb potential by solving the Kepler problem analytically and corrects the trajectory for multiscattering with other particles in the system by using standard numerical techniques (e.g., velocity Verlet, or Gear Predictor corrector algorithms).

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