Efficient Simulation of Electron Quantum Dynamics using the Kepler Predictor-Corrector Algorithm for One-Over-R Potentials

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Abstract

Explicit simulations of electrons-proton multiscattering processes in high-density plasmas provide valuable insights and guidance for current experimental efforts at the National Ignition Facility. However, serious numerical problems typically arise in classical and semiclassical simulations when particles gravitate into each other and the potential gradients (or accelerations) diverge. Here, we introduce an accurate and efficient algorithm for dynamics simulations of particles with attractive 1/r singular potentials to be implemented in the massively parallel molecular dynamics (MD) code ddcMD, developed at Lawrence Livermore National Laboratory within the multi-institutional Cimarron Project. The method is applied to semiclassical dynamics simulations of electron-proton scattering processes in the Wigner-transform time-dependent picture, showing excellent agreement with full quantum dynamics calculations. Rather than avoiding the singularity problem by using a pseudopotential, the algorithm predicts the outcome of close encounter two-body collisions for the true 1/r 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). The resulting symplectic integration is time-reversal symmetric and can be applied to the general multibody dynamics problem featuring close encounters as occur in electron-ion scattering events, particle-antiparticle dynamics, as well as in classical simulations of charged interstellar gas dynamics and gravitational celestial mechanics.