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A Different Time-Dependent Variational Principle Approach: Going Beyond Wave Packet Molecular Dynamics PAUL GRABOWSKI, Los Alamos National Laboratory, ANDREAS MARKMANN, Yale University, MICHAEL MURILLO, Los Alamos National Laboratory, FRANK GRAZIANI, Lawrence Livermore National Laboratory, CIMARRON COLLABORATION —
During inertial confinement fusion, matter evolves from a solid condensed matter phase through the warm dense matter (WDM) regime to a hot dense matter. In WDM, quantum mechanical effects are important because of both Fermi-Dirac statistics and the rate of electrons transitioning in and out of bound states is large. The time-dependent temperature and quickly changing local environment require a time-dependent quantum method. A converged dynamical quantum simulation is intractable for more than a few particles. Instead, we take as a feasible goal to match the statistical properties of a warm dense plasma. The time-dependent variational principle gives a framework for producing equations of motion. A commonly used ansatz is a Hartree product of isotropic Gaussian wave packets (wave packet molecular dynamics). The resulting dynamics do not produce the right statistics. We therefore introduce a plane wave basis and discuss its advantages and test its ability to reproduce radial distribution functions produced by hyper-netted chain calculations.

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