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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, MIKE SURH, Lawrence Livermore National Laboratory, 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 variational form 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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