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Comparison of Finite Temperature Hartree-Fock and Density Functional Theory for Confined Systems[1] TRAVIS SJOSTROM, S.B. TRICKEY, Quantum Theory Project, University of Florida, FRANK E. HARRIS, Quantum Theory Project, University of Florida and Physics Dept. University of Utah — Warm dense matter (WDM) at elevated temperatures (*e.g.*, $T \approx 1$ to several eV) and densities (*e.g.* one or more orders of magnitude denser than equilibrium) is of growing importance. So far, the most detailed studies of WDM use Born-Oppenheimer molecular dynamics with ground-state density functional theory (DFT) approximations. Little, however, is known about the behavior of the free energy over the temperature and density ranges of interest. In the case of DFT, this deficiency is a barrier to assessing the validity of proposed approximate free-energy functionals. For insight into this problem, we have undertaken systematic numerical study of the thermal Hartree-Fock (THF) approximation. We report progress on application of THF to the problem of eight one-electron atoms at arbitrary positions in a hard-walled box. We discuss the physics which emerges for both high- and low-symmetry ionic arrays, including molecular binding transitions. In addition, we compare the THF results directly with approximate DFT results, including approximate finite-temperature orbital-free kinetic and exchange functionals.

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Travis Sjostrom
Quantum Theory Project, University of Florida

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