# Finite Temperature Hartree-Fock and Density Functional Theory Calculations on Confined Hydrogen Systems

Travis Sjostrom, S.B. Trickey, and Frank E. Harris

*Quantum Theory Project, Dept. of Physics and Dept. of Chemistry,*

*University of Florida, Gainesville FL 32611*

Warm dense matter (WDM) at temperatures up to several eV and densities one or more orders of magnitude above equilibrium, is of growing importance. Hydrogen is a particularly important example. 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 in the temperature-density domain of WDM. 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 finite-temperature Hartree-Fock (ftHF) approximation [1 ]. We report progress on application of ftHF to the problem of eight and more hydrogen atoms at arbitrary positions in a hard-walled box. We discuss the physics which emerges for both high- and low-symmetry ionic arrays, with respect to compression and heating, including molecular binding transitions. In addition, we compare the ftHF results directly with approximate DFT results, including approximate finite-temperature orbital-free kinetic and exchange functionals.

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[1] T. Sjostrom, F.E. Harris, and S.B. Trickey, arXiv:1106.4792v2 (2011);
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