Abstract Submitted
for the MAR11 Meeting of
The American Physical Society

Reference Calculation of Temperature-dependent Behavior of Confined Many-electron Systems[1] FRANK E. HARRIS, TRAVIS SJOSTROM, University of Florida — Confined many-electron systems at finite temperatures present a major challenge to density functional theory. Very little is known about the free energy behavior over the temperature range of interest, for example, in the study of warm dense matter, and as a result, it is difficult to assess the validity of proposed free energy density functionals. We present preliminary results on a comparatively simple but computationally feasible model, namely thermally occupied Hartree-Fock states for eight one-electron atoms in a box. We discuss the main technical task, evaluation of the required matrix elements, and summarize the results thus far obtained.

[1]We acknowledge support from US DoE Grant DE-SC0002139.

Frank E. Harris
University of Florida

Date submitted: 15 Nov 2010 Electronic form version 1.4