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Temperature-Dependent Behavior of Confined Many-electron Systems in the Hartree-Fock Approximation[1] TRAVIS SJOSTROM, FRANK HARRIS, SAMUEL TRICKEY, University of Florida — Many-electron systems at substantial finite temperatures and densities 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. As a result, it is difficult to assess the validity of proposed approximate free-energy density functionals. Here we address, at least in part, this need for detailed results on well-characterized systems for purposes of testing and calibration of proposed approximate functionals. We present results on a comparatively simple, well-defined, but computationally feasible model, namely thermally occupied Hartree-Fock states for eight one-electron atoms at arbitrary positions in a hard-walled box. We discuss the main technical tasks (defining a suitable basis and evaluation of the required matrix elements) and discuss the physics which emerges from the calculations. In addition the Hartree-Fock results are compared directly to approximate density functional results including finite temperature orbital-free kinetic and exchange functionals.

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Travis Sjostrom
University of Florida

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