

Abstract Submitted  
for the MAR15 Meeting of  
The American Physical Society

**N Dependence of the Equilibrium Free Energy from the Canonical Ensemble**<sup>1</sup> DEBAJIT CHAKRABORTY, QTP, Department of Physics, University of Florida, JAMES DUFTY, Department of Physics, University of Florida — Free-energy density functional theory conventionally is formulated in the Grand Canonical ensemble but implemented computationally in the Canonical ensemble. To investigate the effects of this disjuncture, the equilibrium free energy per particle for a uniform non-interacting gas is calculated from the Canonical ensemble for given particle number  $N$  and fixed volume. The same calculation is performed from the Grand Canonical ensemble for the corresponding average  $\bar{N}$  and same volume. In dimensionless forms the latter depends only on the reduced temperature,  $t = T/T_F$ . In contrast, of course, the Canonical result depends on both  $t$  and  $N$ . The results are compared for  $1 < N < 100$ . Next, the same calculations are performed for a non-uniform gas generated by an external ion using a regularized Coulomb potential. The number dependence is explored for positions near and far from the ion. The implications for free-energy density functional theory are discussed.

<sup>1</sup>Research supported by US DOE Grant DE-SC0002139

Debajit Chakraborty  
QTP, Department of Physics, University of Florida

Date submitted: 11 Nov 2014

Electronic form version 1.4