Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

A new approach to density functional theory KIERON BURKE, PETER ELLIOTT, ATTILA CANGI, DONGHYUNG LEE, University of California, Irvine — I will explain a new way to think about density functional theory, based on a simple principle: asymptotic exactness for large particle number. This explains many features of existing functionals [1], and makes the connection between semiclassical and density functional approximations. It underlies the restoration of the gradient expansion in PBEsol[2]. It also provides a path toward highly accurate, orbital-free, non-local functionals of the potential, for both the density itself and the non-interacting kinetic energy.
[1] J.P. Perdew, L.A. Constantin, E. Sagvolden, and K. Burke, Phys. Rev. Lett. **97**, 223002 (2006).
[2] J.P. Perdew, A. Ruzsinszky, G.I. Csonka, O.A. Vydrov, G.E. Scuseria, L.A. Constantin, X. Zhou, and K. Burke, arXiv:0707.2088 (2007).

Kieron Burke
University of California, Irvine

Date submitted: 30 Nov 2007 Electronic form version 1.4