Abstract Submitted
for the MAR07 Meeting of
The American Physical Society

Asymptotic Near Nucleus Structure of the Electron-Interaction Potential in Local Effective Potential Theories VIRAHT SAHNI, The Graduate School, CUNY, ZHIXIN QIAN, Peking University — In previous work, it has been shown that for spherically symmetric or sphericalized systems, the asymptotic near nucleus structure of the electron-interaction potential is $v_{ee}(r) = v_{ee}(0) + \beta r + \gamma r^2$. In this paper we prove via time-independent Quantal Density Functional Theory[1](Q-DFT): (i) correlations due to the Pauli exclusion principle and Coulomb repulsion do not contribute to the linear structure;(ii) these Pauli and Coulomb correlations contribute quadratically; (iii) the linear structure is *solely* due to Correlation-Kinetic effects, the coefficient β being determined analytically. By application of adiabatic coupling constant perturbation theory via QDFT we further prove: (iv) the Kohn-Sham (KS-DFT) 'exchange' potential $v_x(r)$ approaches the nucleus linearly, this structure being due *solely* to lowest- order Correlation-Kinetic effects: (v) the KS-DFT 'correlation' potential $v_c(r)$ also approaches the nucleus linearly, being *solely* due to higher-order Correlation-Kinetic contributions. The above conclusions are equally valid for system of arbitrary symmetry, provided spherical averages of the properties are employed.
1 *Quantal Density Functional Theory*, V. Sahni (Springer-Verlag 2004)

Viraht Sahni
The Graduate School, CUNY

Date submitted: 17 Nov 2006 Electronic form version 1.4