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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 \( \beta \) 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)

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