

Abstract Submitted
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Wigner High Electron Correlation Regime of Nonuniform Electron Density Systems: A Quantal Density Functional Theory (QDFT) Study¹ DOUG ACHAN, LOU MASSA, VIRAH T SAHNI, The Graduate School CUNY — We investigate the Wigner regime of the nonuniform electron density system of the Hooke’s atom characterized by the “fat attractor” profile via QDFT. We determine the quantal sources: the density; the nonlocal Fermi and Coulomb hole charges; and the single-particle and Dirac density matrices. From these sources we obtain, respectively, the Hartree, Pauli, Coulomb, and Correlation-Kinetic fields. The work done in these fields leads to the corresponding components of the local electron-interaction potential of the noninteracting fermions that reproduce the density. The corresponding components of the total energy are determined by the respective integral virial expressions in terms of the fields. We discover that Correlation-Kinetic effects are very significant. We propose that in addition to a high electron-interaction energy, the Wigner regime also be characterized by a high Correlation-Kinetic energy.

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