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Contributions to the Non-interacting Free Energy Density Functional[1] S.B. TRICKEY, Physics, QTP, U. Florida, JAMES DUFTY, Physics, U. Florida, T. SJOSTROM, Physics, QTP, U. Florida — Phenomenological models for the T=0 non-interacting kinetic energy density functional often use a linear combination of the von Weizsäcker (vW) and Thomas-Fermi (TF) functionals. A more systemmatic approach, for any temperature follows from extracting the vW functional from the exact free energy density functional, and analyzing the remainder in a local density approximation. We show that the vW functional is a lower bound for the free energy functional, extending a well-known T=0 result and indicating its priority in the decomposition. The exact remainder involves gradients of the off-diagonal one-body Fermi density matrix, for which a local density approximation is ambiguous. We discuss the extent to which a TF contribution can be extracted. Extension of the original vW phenomenological approach gives complementary insight. Modeling the orbitals as modulated plane waves, with coefficients identified in terms of the density and its gradients leads to vW and TF functionals plus higher-order gradient and temperature corrections.

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