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Systematic Results in Finite Temperature DFT¹ TAMAS GAL,

JAMES DUFTY, Department of Physics, University of Florida — An exact representation for the non-interacting free energy density functional is identified from the thermodynamics of a non-uniform, finite temperature system of particles in an external potential. A formally exact functional density expansion whose leading term is the Thomas-Fermi approximation is described to second order in the density non-uniformity. The familiar Perrot form [Phys. Rev. A 20, 586 (1979)] is recovered from a subsequent smooth gradient expansion. A related formal expansion about the Thomas-Fermi plus von Weizsacker functional to second order is also described and discussed.

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