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Finite Temperature Scaling of the Non-interacting Free Energy Density Functional[1] J.W. DUFTY, V.V. KARASIEV, S.B. TRICKEY, Physics, Univ. Florida — The non-interacting free energy density functional is central to formulation of orbital-free DFT, yet its construction remains a challenge. Here, exact scaling relations and related bounds are obtained for guidance. First, that free energy is expressed as a functional of one-body reduced density operators that deliver the same average number density. For a one-component Fermion system, this functional has a minimum at the Fermi operator whose external potential assures the chosen number density. This is the formal definition of the non-interacting free energy density functional. The associated entropy and internal energy functionals are identified directly. A unitary transformation generating spatial scaling then determines how these functionals change under density scaling. As an application, these scaling laws are used to obtain inequalities and bounds for functionals at different values of the density and temperature. Relationships to similar recent work at finite temperatures, and the extensive prior zero-temperature results are noted.

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