Generalized Gradient Approximation for Exchange-Correlation Free Energy

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Matter under extreme conditions (temperature of thousands to millions Kelvin; compressions to four or more times ambient density) usually is treated by means of *finite-temperature* density functional theory (DFT). Practical implementation in either conventional Kohn-Sham or orbital-free form requires reliable approximations for the exchange-correlation (XC) *free-energy*. An under-appreciated aspect is the intrinsic temperature dependence in the XC functional. This should be taken into account in addition to the implicit dependence via the density. The first rung XC free-energy functional developed within the local density approximation (LDA) [1] captures that explicit T-dependence for the homogeneous electron gas. To go beyond that, we analyze the finite-T gradient expansion for X and C, extract from it the appropriate reduced density gradients for X and C with explicit T-dependence, introduce the next-rung generalized gradient approximation XC free-energy functionals, and discuss their behavior and properties.

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1. V.V. Karasiev, T. Sjostrom, J. Dufty, and S.B. Trickey, Phys. Rev. Lett. 112, 076403 (2014).