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Gradient corrections to finite-temperature exchange-correlation functionals[1] TRAVIS SJOSTROM, JAMES DUFTY, University of Florida — In principle, the only approximation in Kohn-Sham DFT is for the exchange-correlation (XC) energy. As such, about 40 years of development for the zero-temperature XC density functional has resulted in a ladder of functionals from simple LDA (based on essentially exact QMC results) to orbital-dependent functionals including virtuals. The non-zero temperature situation is different. To date, a handful of $T \neq 0$ K XC functionals have been introduced based on approximate electron gas calculations or interpolations. Except for a finite-T gradient expansion of X, all are local density approximations. Here we present calculations for the XC energy of the electron gas in the dielectric formalism, specifically with approximate local field corrections (LFC). Analysis of the LCF is used to evaluate the first term of the gradient expansion of the XC energy in the slowly varying limit. The resulting gradient expansion finite temperature XC functional will be presented and possible generalized gradient approximations will be considered.

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