Recent developments of zero- and finite-T orbital-free functionals

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Ab initio molecular dynamics for ions driven by forces from Kohn-Sham (KS) density functional theory (DFT) calculations is a standard computational approach for probing both warm dense matter (electon temperatures typically 1 eV or more) and ordinary materials (at near zero temperature). The computational cost of the standard KS approach increases very rapidly with system: at least as the cube of the number of occupied KS orbitals. This cost worsens as the temperature increases because of the growth of the occupied KS orbital manifold. If orbital-independent exchange-correlation approximations are used, the costly scaling comes solely from the explicit KS orbital dependence of the non-interacting kinetic energy. This motivates work on the alternative, orbital-free DFT. This presentation will cover recent advances providing the first generalized-gradient approximation non-interacting orbital-free KE functional that binds crystals properly and its extension to proper non-interacting free-energy functionals. Numerical results and simulation timings will be presented. [See Phys. Rev. B 88, 161108(R)(2013) available at www.qtp.ufl.edu/ofdft]

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