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"Coherent approach to orbital-free DFT"

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Orbital-free DFT is immensely appealing both for intellectual purity and for the potential for making materials, cluster, and biomolecular simulations much faster. The challenge of OF-DFT commonly is said to be to find a sufficiently accurate approximation for the Kohn-Sham kinetic energy functional T_s. But Perdew's exchange-correlation functional Jacob's ladder raises a concomitant challenge: higher-rung E_{xc} functionals use the KS orbitals explicitly. OF-DFT progress therefore requires pursuit of improved orbital-independent approximations for both T_s and E_{xc}. Consistent treatment of finite temperature $\mathcal{T}$ adds requirements both for temperature dependence of those functionals as well as for the non-interacting (KS) entropy. There are few $\mathcal{T}$-dependent functionals in the literature, yet the temperature range of interest in, *e.g.* warm dense matter, is immense, to $\mathcal{T} \approx 10$ eV or higher.

In this diverse context, I shall discuss three aspects of functional development:

1. Recent work on constraint-based single-point T_s approximations ($\mathcal{T} = 0$) of the modified-conjoint GGA type ("mcGGA") and beyond. Beyond-mcGGA functionals are required to remove nuclear-site singularities in the so-called Pauli term. That raises the issue of how to select fruitful combinations of higher-order derivatives and how to constrain those combinations. In passing, this topic also raises the issue of numerical solution of the OF-DFT Euler equation.

2. Recent improvements in the GGA-type E_{xc} functionals by tightening and refining the enforcement of important, relevant constraints, giving the VMT and VT{84} functionals. VT{84}, in combination with PBE E_c, gives heats of molecular formation with $\approx 50\%$ smaller mean absolute deviation than PBE-PBE with relatively little harm to geometries, while also giving NMR ^{13}C chemical shifts of quality better than those from PW91.

3. Unpublished comparison calculations on the existing $\mathcal{T}$-dependent approximate functionals, on ground-state functionals used at finite $\mathcal{T}$ (a common practice in present studies of warm dense matter), and on finite-temperature Hartree-Fock.

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