Finite-temperature orbital-free density functional theory: development, implementation, and applications

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The computational cost of orbital-based Kohn-Sham (KS) density functional theory (DFT) grows rapidly with both increasing system size and increasing temperature. Thus the predictive power of *ab-initio* molecular dynamics driven by KS forces becomes prohibitively costly for practical applications in the warm denses matter regime (typical system temperatures $10^3 \leq T \leq 10^6$ K). In principle, orbital-free DFT (OFDFT) is a computationally effective alternative. It scales almost linearly with increasing system size, and has growing accuracy as T increases without increasing the computational cost.

We present our the most recent progress on development of functionals for OF-DFT at finite temperature (the non-interacting free-energy and exchange-correlation free-energy functionals), software implementation, and applications which demonstrate the importance of the intrinsic temperature dependence in the exchange-correlation and which show the high accuracy of orbital-free functionals at elevated temperatures [1-5].

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1. V.V. Karasiev, and S.B. Trickey, in *Adv. in Quantum Chem.*, J.R. Sabin and R. Cabrera-Trujillo (Eds.), Vol. 71 (Elsevier Academic Press, Amsterdam, 2015) p. 221.
2. V.V. Karasiev, "*Tunable non-interacting free-energy functionals*", (in preparation).
3. V.V. Karasiev, L. Calderín, and S.B. Trickey, "*The importance of finite-temperature exchange-correlation for warm dense matter calculations*", (in preparation).
4. S.B. Trickey, V.V. Karasiev , and D. Chakraborty, Phys. Rev. B, **92**, 117101 (2015).
5. V.V. Karasiev, T. Sjostrom, J.W. Dufty, and S.B. Trickey, Phys. Rev. Lett. **112**, 076403 (2014).
6. V.V. Karasiev, T. Sjostrom, and S.B. Trickey, Comp. Phys. Commun., **185**, 3240 (2014).