

Abstract Submitted
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Constrained Parameterization of Reduced Density Approximation of Kinetic Energy Functionals¹ DEBAJIT CHAKRABORTY, SAMUEL TRICKEY, VALENTIN KARASIEV, Quantum Theory Project, Physics Dept., U. Florida, Gainesville FL 32611 — Evaluation of forces in ab initio MD is greatly accelerated by orbital-free DFT, especially at finite temperature [1]. The recent achievement of a fully non-empirical constraint-based generalized gradient (GGA) functional for the Kohn-Sham KE $T_s[n]$ [2] brings to light the inherent limitations of GGAs. This motivates inclusion of higher-order derivatives in the form of reduced derivative approximation (RDA)[3] functionals. That, in turn, requires new functional forms and design criteria. RDA functionals are constrained further to produce a positive-definite, non-singular Pauli potential. We focus on designing a non-empirical constraint-based meta-GGA[3-5] functional with certain combinations of higher-order derivatives which avoid nuclear-site singularities to a specified order of gradient expansion. Here we report progress on this agenda.

- [1] Phys. Rev. B **86**, 115101 (2012);
- [2] Phys. Rev. B **88**, 161108(R) (2013);
- [3] Phys. Rev. B **80**, 245120 (2009);
- [4] Phys. Rev. B **75**, 155109 (2007);
- [5] Nuc. Phys. A **445** 263 (1985)

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