Towards practical Laplacian-based kinetic energy density functionals[†]

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In recent years interest grown in use of orbital free KED in density functional theory, either for "deorbitalizing" metaGGA functionals or to remove orbitals entirely from the Kohn-Sham formulation. The Perdew-Constantin (PC) KE metaGGA [1] and later variants demonstrate the effectiveness of the use of the Laplacian of the density to model the transition between the slowly varying electron gas to the von Weizsacker or single electron-pair limits in such functionals. Unfortunately, the use of the Laplacian in this context creates unphysically spiky Pauli potentials that are difficult to converge and lead to inherently noisy results. To ameliorate this problem, we construct and test a smoothness measure based on the variational description of Poisson's equation, applied to the Laplacian-generated terms in the potential. Optimization of this measure is used to develop smoother models of the electron localization transition. Secondly, we explore the effect of the self-consistent replacement of the Laplacian of the density by its convolution with a binomial distribution, which filters out unphysically rapid features in the potential. Combined, these measures applied to PC-family models can substantially remove unphysical features in the Pauli potentials of small atoms.

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[1] J. P. Perdew and L. A. Constantin, Phys. Rev. B 75, 155109 (2007).