Developing Laplacian-based kinetic energy functionals for orbital-free density functional theory*

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The goal of Orbital-Free Density Functional Theory is to model the noninteracting kinetic energy (KE) of Kohn-Sham theory as a functional of ingredients derived from the density directly, so as to remove the bottleneck of computing orbitals in large systems. The Perdew-Constantin (PC) KE metaGGA[1] and later improvements[2] 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. We explore several developments of these models with the goal of making them reliable for practical applications. First, 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 de- scription of Poisson's equation, applied to the Laplacian-generated terms in the potential. Secondly, we explore visually how closely the KE den- sity of typical solids can be reproduced as a function of the local density and derivatives. We find that modifications of the PC model lead to a highly accurate description of semiconductor KE densities within a pseudopotential model.

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

[2]A. Cancio, D. Stewart and A. Kuna, JCP 144, 084107 (2016).

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