Abstract Submitted
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Application of partition density-functional theory to model systems[1] LARRY BOYER, George Mason University, MICHAEL MEHL, Naval Research Laboratory — Elliott et al.[2] have introduced a method called partition density-functional theory (PDFT) for expressing the Kohn-Sham charge density as a sum of overlapping fragment densities, which promises accuracy and efficiency along with a framework for developing and testing useful approximations for kinetic-energy functionals, T[n]. They illustrate their method using results obtained for non-interacting electrons in a one-dimensional model potential. Following their approach, we apply PDFT to similar models which examine its usefulness in developing approximations for T. We also discuss how PDFT compares with the self-consistent atomic deformation[3] method.

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[2]P. Elliott, K. Burke. M. H. Cohen and A. Wasserman, Phys. Rev. A **82**, 024501 (2010)
[3]L. L. Boyer, H. T. Stokes, M. M. Ossowski and M. J. Mehl, Phys. Rev. B **78**, 045121 (2008)

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