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Towards a semiclassical theory of electronic structure[1] ATTILA CANGI, DONGHYUNG LEE, Department of Chemistry, University of California, Irvine, PETER ELLIOTT, Department of Physics, University of California, Irvine, KIERON BURKE, Department of Chemistry, University of California, Irvine —
Modern density functional theory (DFT) -formulated in the context of the Kohn-Sham scheme- evolved from "old" Thomas-Fermi theory to an accurate theory for predicting various properties of molecules and solids. We discuss the interrelation of semiclassical physics[1] with the fundamental gradient approximation, which is the basis of all functional construction. We speculate that applying semiclassical methods in the context of a DFT-like theory is a path towards more accurate and efficient approximations to electronic properties of condensed systems.[2]

[1] M. V. Berry and K. E. Mount, Reports of Progress in Physics 35, 315 (1972).
[2] P. Elliott, D. Lee, A. Cangi, and K. Burke, Phys. Rev. Lett. 100, 256406 (2008).

[1]National Science Foundation, CHE-0809859

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