Towards a semiclassical theory of electronic structure\(^1\) \text{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).

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