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Density Functional Theory and Semiclassical Methods[1] PETER ELLIOTT, DONGHYUNG LEE, ATTILA CANGI, KIERON BURKE, University of California, Irvine — In this work we explore the relationship between semiclassical methods and density functional theory. There is a rich history between the two, for example, the gradient expansion approximation (GEA), on top of which all common generalized gradient approximations (GGAs) are built, may be derived semiclassically. However methods like Thomas-Fermi and the GEA miss important contributions from quantum oscillations, such as shell structure. In Ref. [1] we showed why these are missing and how, for a simple system, one could derive them . This led to approximations to the density and kinetic energy density which were non-local functionals of just the external potential. Interpreting these in the context of DFT, allows us to understand current approximations and improve them. In fact the potential scaling (re-)introduced in Ref. [1] can be used to derive new exact conditions on the universal functional of DFT and its components. This talk will discuss both the development of potential functionals and how they can be used to understand DFT.
[1] P. Elliott, D. Lee, A. Cangi, and K. Burke, Phys. Rev. Lett. **100**, 256406 (2008).

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