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Semiclassical origins of density functional theory[1]

KIERON BURKE, University of California, Irvine

Until the seminal work of Hohenberg, Kohn, and Sham of the mid 60's, most density functional theory (DFT) was derived from semiclassical approximations. This non-empirical approach shows an intrinsic difference between solids (for which DFT was originally developed) and molecules, and explains many of its more mysterious manifestations. For example, the success of DFT for molecules has nothing to do with the uniform gas. Results include [1] a derivation of the empirical parameter in the B88 exchange functional, [2] PBEsol, a new GGA that restores the exchange gradient expansion and improves lattice constants in solids, [3] a novel approach to "orbital-free" DFT that, in preliminary tests, is 40 times more accurate than its DFT counterpart. The talk is aimed at a general theoretical audience. Detailed technical knowledge of DFT is neither needed, nor desirable.

[1] J.P. Perdew, L.A. Constantin, E. Sagvolden, and KB, Phys. Rev. Lett. 97, 223002 (2006).
[2] J.P. Perdew, A. Ruzsinszky, G.I. Csonka, O.A. Vydrov, G.E. Scuseria, L.A. Constantin, X. Zhou, and KB, Phys. Rev. Lett. 100, 136406 (2008).
[3] Peter Elliott, Donghyung Lee, Attila Cangi, KB, Phys. Rev. Lett. 100, 256406 (2008).

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