

Density functional theory: A great success story?

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Density functional theory began with the work of Thomas and Fermi, at about the same time as Schroedinger wrote his famous equation. It is a bizarre approach to the quantum mechanics of many particle systems. Its unreasonable utility for electronic structure problems is slowly transforming the world we live in, as was recognized by the 1998 Nobel prize in chemistry. At least 20,000 scientific papers apply it every year, in fields as diverse as biochemistry and astrophysics.

In this general talk, I will explain in broad terms what density functional theory is, and why it is so annoying. Over 40 years ago, Lieb and Simon demonstrated that the Thomas-Fermi approximation becomes relatively exact in a certain, unusual semiclassical limit. I will explain why I believe this holds the key to a systematic treatment of modern DFT approximations.

An introduction for anyone with a background in quantum mechanics can be found in "DFT in a nutshell" (KB and Lucas O. Wagner, *Int. J. Quant. Chem.* 113, 96-101 (2013)) and a more recent perspective on the subject can be found in *J. Chem. Phys.* 136, 150901 (2012).