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Abstract for an Invited Paper for the MAR16 Meeting of the American Physical Society

Semiclassical origins of density functionals¹ KIERON BURKE, UC Irvine

By careful numerical analysis of non-relativistic atomic correlation energies, we show that (a) the local density approximation becomes relatively exact for the correlation energy as the atomic number approaches infinity, (b) we find the leading correction, which is about 38.5 milliHartrees per atom, (c) show how this correction dominates for larger atoms and (d) how to construct a generalized gradient approximation that respects this limit (See KB, A. Cancio, T. Gould, S. Pittalis, arXiv:1409.4834).

The relevance to density functional calculations will also be explained.

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