

Abstract Submitted
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Exact condition on the non-interacting kinetic energy for real matter DONGHYUNG LEE, KIERON BURKE, University of California, Irvine
— From the analysis of the asymptotic expansion [1,2] for the total energies of neutral atoms, we suggest a modified gradient expansion approximation to the kinetic energy which satisfies the exact asymptotic condition as the number of electrons $N \rightarrow \infty$. The resulting functional determines the small gradient limit of any generalized gradient approximation, and conflicts with the standard gradient expansion. We apply this new functional to the atoms up to $Z \sim 88$ in comparison with the 2nd and 4th gradient expansion approximations. We also give a modern, highly accurate parametrization of the Thomas-Fermi density of neutral atoms.

[1] Thomas-Fermi model: The second correction, J. Schwinger, Phys. Rev. A **24**, 2353 (1981).

[2] Semiclassical atom, B.-G. Englert and J. Schwinger, Phys. Rev. A **32**, 26 (1985).

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