Uniform semiclassical approximations for many-particle systems

RAPHAEL RIBEIRO, KIERON BURKE, Department of Chemistry, University of California Irvine — Semiclassical analysis is used to construct uniform asymptotic approximations to the quantum one-body and kinetic energy densities of a system of noninteracting particles in a 1D potential well in the limit of infinite particle number. The approximations encode the appropriate limiting behavior of the electron density at the bulk, edge and classically-forbidden regions. High accuracy is obtained even when far from the limits assumed in the derivations. The field of density functional theory [1] is impacted in at least two ways. First, the semiclassical kinetic energy density is orbital-free, thereby providing a rare analytical development that is not based on the gradient expansion to the kinetic energy functional. Second, several results are obtained on the global and local asymptotic behavior of the quantum density and kinetic energy density everywhere in configuration space which might be established as new guiding principles for the development of approximate functionals in Kohn-Sham DFT.

[1] A. Cangi P. Elliott, D. Lee and K. Burke. Semiclassical origins of density functionals. *Phys. Rev. Lett.*, 100(25):256406

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