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Semiclassical Origin of Density Functionals ATTILA CANGI, PETER ELLIOTT, DONGHYUNG LEE, KIERON BURKE, University of California, Irvine — We use methods of semiclassical physics [1] to study the basic ingredients of DFT in terms of an asymptotic expansion in powers of the particle number. As an example we derive an approximate many-particle density [2] of a general potential in a one-dimensional system with hard walls. If the Fermi level lies above the maximum of the potential, we obtain densities very close to the exact answer, even for a small particle number. Density oscillations due to the effect of the boundaries are also present.
[1] M. V. Berry and K. E. Mount, Reports of Progress in Physics 35, 315 (1972).
[2] W. Kohn and L. J. Sham, Phys. Rev. 137, A1697 (1965).

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