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Prospects of density-potential functional theory for 2D materials

We propose a versatile variant of orbital-free density functional theory, density-potential functional theory (DPFT), for calculating various properties of systems in one, two, and three dimensions. Large particle numbers and long-range interactions of interacting many-body systems like quantum gases and solid states in various dimensions pose formidable challenges even to state-of-the-art theoretical methods. With the aid of Wigner's phase space formulation we establish semiclassical approximations of energies and particle densities for interacting fermion systems. The position-space formulation of DPFT yields self-consistent interacting particle densities in a spirit similar to the Kohn-Sham scheme, but cirumventing the need for orbitals. By design these single-particle densities can be improved systematically beyond the Thomas-Fermi approximation and can be used to efficiently address inhomogeneous interacting systems like p-n junctions and electron-hole puddles. DPFT also has the potential to tackle a variety of open problems in momentum space like, for instance, interacting band structures and band gap renormalization. Here, dispersion relations for any choice of interaction are self-consistently obtained from the corresponding noninteracting dispersion.