学术报告

Lattice density functional theory at finite temperature with strongly density–dependent exchange–correlation potentials

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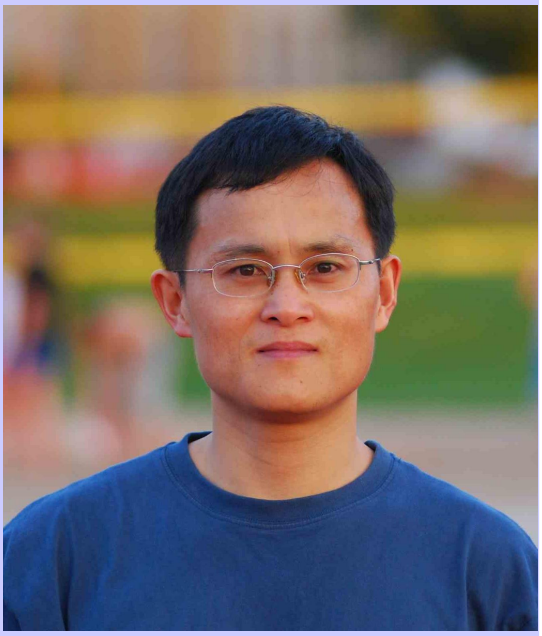

Abstract:
The derivative discontinuity of the exchange-correlation (xc) energy at an integer particle number is a property of the exact, unknown xc functional of density functional theory (DFT) which is absent in many popular local and semilocal approximations. In lattice DFT, approximations exist which exhibit a discontinuity in the xc potential at half-filling. However, due to convergence problems of the Kohn-Sham (KS) self-consistency cycle, the use of these functionals is mostly restricted to situations where the local density is away from half-filling. Here a numerical scheme for the self-consistent solution of the lattice KS Hamiltonian with a local xc potential with rapid (or quasidiscontinuous) density dependence is suggested. The problem is formulated in terms of finitetemperature DFT where the discontinuity in the xc potential emerges naturally in the limit of zero temperature. A simple parametrization is suggested for the xc potential of the uniform one-dimensional (1D) Hubbard model at finite temperature which is obtained from the solution of the thermodynamic Bethe ansatz. The feasibility of the numerical scheme is demonstrated by application to a model of fermionic atoms in a harmonic trap. The corresponding density profile exhibits a plateau of integer occupation at low temperatures which melts away for higher temperatures.

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