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

— •STEFAN KURTH¹, GAO XIANLONG², A-HAI CHEN², and ILYA TOKATLY¹ — ¹Univ. of the Basque Country UPV/EHU, San Sebastian, Spain and IKERBASQUE, Basque Foundation for Science, Bilbao, Spain — ²Zhejiang University, Jinhua, China

The derivative discontinuity of the exchange-correlation (xc) energy of density functional theory (DFT) at integer particle number 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 but 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 quasi-discontinuous) density dependence is suggested. The problem is formulated in terms of finite-temperature 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 1D Hubbard model at finite temperature obtained from 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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Topic: Focused Session: Frontiers of Electronic Structure Theory
Email: stefan_kurth@ehu.es