

Ab-initio simulation of ultracold atomic gases

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Abstract:

The successful validation of experiments on bosons in optical lattices has been followed by similar efforts for fermions. While for bosons direct numerically exact ab-initio simulations of quantum gases with millions of particles are easily possible and excellent agreement with experiments is achieved, fermions pose a bigger challenge. Supercomputer simulations using cluster extensions of dynamical mean field theory for the Hubbard model can accurately calculate properties of fermions in deep optical lattices at temperatures down to the Néel temperature. To simulate shallow optical lattices and non-equilibrium dynamics we have generalized Kohn-Sham density functional theory (the workhorse for materials simulations) to ultracold quantum gases and I will present results for ground states and dynamics of repulsively interacting fermions.