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Low-temperature properties of the half-filled frustrated Hubbard model in high dimensions

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The half-filled single-band Hubbard model has been of fundamental interest for decades and is a benchmark problem for correlated-electron methods. The dynamical mean-field (DMFT) treatment of its fully frustrated version with Bethe density of states, a minimal model for the Mott metal-insulator transition, is the subject of numerous recent studies using, e.g., the density-matrix renormalization group (DMRG) and (projective) quantum Monte Carlo (QMC/PQMC) methods.

In this contribution, 10th order strong-coupling perturbation theory for the Mott insulating phase is extrapolated to infinite order using the recently developed ePT method. The excellent agreement with QMC results both validates the ePT and confirms the high accuracy of our refined QMC scheme. We obtain continuous estimates of energy and double occupancy with unprecedented precision $\mathcal{O}(10^{-5})$ for the Mott insulator above its stability edge $U_{c1} \approx 4.78$ as well as critical exponents. QMC results for the metallic low-temperature phase of similar precision are extrapolated to the ground state. Somewhat surprisingly, the accuracy of these extrapolations is very competitive with numerical ground state methods such as numerical renormalization group (NRG), exact diagonalization (ED), DMRG, and PQMC. Our continuous estimate of the ground state energy contains the first correct prediction of the 4th order coefficient in a weak-coupling expansion.

NB and E. Kalinowski, Phys. Rev. B **71**, 195102 (2005); Physica B **359**, 648 (2005).

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