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Monte Carlo-Mean Field approach for the one band Hubbard model NIRAVKUMAR D. PATEL, ANAMITRA MUKHERJEE, The University of Tennessee, Knoxville, Tennessee 37996, USA, SHUAI DONG, Southeast University, Nanjing 211189, China, STEVE JOHNSTON, ADRIANA MOREO, ELBIO DAGOTTO, The University of Tennessee, Knoxville, Tennessee 37996, USA — Multiorbital model Hamiltonians are crucial to understand iron-based superconductors. We employ a recently developed "Monte Carlo-Mean Field" (MC-MF) method [1] to study single and multiband Hubbard models. The focus here is on the single band case at half filling. We start with a mean-field (MF) decomposition of the Hubbard hamiltonian and then promote the MF parameters to classical variables studied via MC simulations, while fermions are exactly diagonalized in the background of those classical variables. We present the Hubbard U vs. temperature phase diagram on large three and two dimensional clusters. Our MC-MF method can capture the nonmonotonicity of T_N with U, local moment physics above T_N, and the two peak behavior of specific heat, as compared with Determinantal Quantum Monte Carlo (DQMC). Results for the $t - t'$ Hubbard model in two dimensions show that our approach can capture ground state and finite temperature properties reliably where DQMC fails due to sign problems. These one-band results set the stage for extending the MC-MF method to multiband Hubbard models of relevance to the Pnictide superconductors.

[1] Mukherjee et.al. arXiv:1409.6790 (to appear in Phys. Rev. B)

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