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Study of multi-orbital Hubbard model at finite temperature using the Monte Carlo-Mean Field approach ANAMITRA MUKHERJEE, NIRAVKUMAR D. PATEL, University of Tennessee, Knoxville, SHUAI DONG, Southeast University, China, STEVE JOHNSTON, ADRIANA MOREO, ELBIO DAGOTTO, University of Tennessee, Knoxville — The phenomenology of iron-based superconductors suggest the need to use multi-orbital Hubbard models. For this reason, here we apply a recently developed technique, the "Monte Carlo-Mean Field" (MC-MF) method, to single and multiband Hubbard models [1]. In this approach, first a mean field approximation is used. The MF parameters are then treated via a finite-temperature classical MC as opposed to usual self consistency. In this talk, we show that the MC-MF results substantially improve on the naive finite-temperature MF approach and are in very good agreement with Determinantal Quantum Monte Carlo (DQMC) data for the single orbital case, both in weak and strong Hubbard U coupling. In the case of multiorbital models, phase diagrams for the parent compounds will be presented, varying U at fixed Hund coupling. Region of preformed local moments above the ordering temperatures will be discussed. Results for dynamical quantities such as the orbital resolved single particle spectral function $A(\vec{k}, \omega)$, optical conductivity, and real space charge/spin/orbital density maps are also presented.

[1] A. Mukherjee et al., arXiv:1409.6790, to appear in PRB

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