Abstract Submitted for the MAR14 Meeting of The American Physical Society

Study of the multi-orbital Hubbard model at finite temperature ANAMITRA MUKHERJEE, Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA, SHUAI DONG, Department of Physics, Southeast University, Nanjing 211189, China, GONZALO ALVAREZ, Center for Nanophase Materials Sciences and Computer Science & Mathematics Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA, EL-BIO DAGOTTO¹, Department of Physics and Astronomy, University of Tennessee, Knoxville, Tennessee 37996, USA — Research in pnictide superconductors have clearly established the need for the study of multi-orbital Hubbard models. With this motivation, here we apply a combination of the real-space Exact Diagonalization and Classical Monte Carlo (ED+MC) method, widely used in manganites, with the standard Hartree-Fock mean field (MF) theory to investigate the properties of multiorbital models as a function of temperature. In this approach the MF parameters are treated via a classical MC and the fermions moving in the MF background are solved by exact diagonalization. The temperature dependence of the dynamical spin susceptibility $S(\vec{q}, \omega)$, orbital resolved single particle spectral function $A(\vec{k}, \omega)$, optical conductivity, and real space charge/spin/orbital density maps are calculated at different dopings. These results are relevant in understanding the role of the multiple degrees of freedom in governing the magnetic and transport properties of the Fe based superconductor materials.

¹Materials Science and Technology Division, Oak Ridge National Laboratory, Oak Ridge, Tennessee 37831, USA

Anamitra Mukherjee University of Tennessee, Knoxville

Date submitted: 14 Nov 2013

Electronic form version 1.4