Abstract Submitted for the MAR13 Meeting of The American Physical Society

Temperature and doping dependence of spectral features in determinant quantum Monte Carlo studies of the three-orbital Hubbard model of cuprate superconductors Y.F. KUNG, E.A. NOWADNICK, SIMES, SLAC and Stanford University, S. JOHNSTON, University of British Columbia, C.-C. CHEN, APS, Argonne National Laboratory, B. MORITZ, Northern Illinois University and University of North Dakota, T.P. DEVEREAUX, SIMES, SLAC and Stanford University — Studying temperature and doping trends in strongly correlated materials is integral to understanding how their properties emerge and develop, and possibly can be tuned. To this end, determinant quantum Monte Carlo simulations are used to investigate spectral features in the three-orbital Hubbard model as applied to the cuprate superconductors. Spectral functions relevant to photoemission measurements are calculated and various spectral features, such as the indirect charge-transfer gap and Zhang-Rice singlet band, are shown to vary with doping and temperature. These orbitally resolved calculations help shed light on the applicability of the Zhang-Rice singlet picture at high hole doping levels. The density of states is also compared and contrasted with exact diagonalization studies as well as recent x-ray absorption spectroscopy measurements.

> Yvonne Kung SIMES, SLAC and Stanford University

Date submitted: 28 Dec 2012

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