Abstract Submitted for the CAL11 Meeting of The American Physical Society

Sorting Category: 4. (C)

The Great Quantum Conundrum: Electronic Phase Diagram of the Layered Copper Oxide Perovskites PAUL GRANT, W2AGZ Technologies — In the months following the publication of the discovery of the quasi-planar CuO "high temperature" superconductors in September, 1986, it was noticed that their electronic properties as a function of temperature and applied magnetic field depended strongly on carrier concentration. This dependence can be universally characterized by a "electronic phase diagram" of temperature vs. carrier concentration identifying separate and overlapping regions of electronic order...insulating antiferromagnetic, non-Fermi liquid, Fermi liquid and superconducting. We computationally explore this phase diagram by applying density-functional-theory to tetragonal rocksalt CuO as a "proxy," or "surrogate" representing the essential structural properties of all layered copper oxide perovskites [1] as a function of coulomb correlation (Hubbard U) on both Cu and O sites as well as carrier density. In the Fermi liquid limit of small U and optimal doping, we compute values of electron-phonon coupling and discuss with respect to various bipolaron-mediated pairing models [2].

[1] P. M. Grant, J. Phys.: Conf. Series <u>129</u>, 012042 (2008).

[2] K. A. Mueller, J. Phys.: Condens. Matter 19, 251002 (2007).

X	Prefer Oral Session
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Date submitted: 30 Sep 2011 Electronic form version 1.4