Abstract Submitted
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Superconconductivity and antiferromagnetism for the one-band Hubbard model of the cuprates including inter-plane hopping[1] SIMON VERRET, Universite de Sherbrooke, Quebec, Canada, CHUCK-HOU YEE, KITP, UCSB, DAVID SENECHAL, Universite de Sherbrooke, Quebec, Canada, A.-M.S. TREMBLAY, Universite de Sherbrooke, Quebec, Canada and CIFAR, Canada — While the overall features of the zero-temperature phase diagram of the cuprates are well described by the two-dimensional Hubbard model, the quest for a quantitative theory must include three-dimensional effects to account for differences between materials. To this end, using first-principles calculations [1,2], we obtain realistic parameters for the one-band Hubbard model that include hopping between planes. We then solve the resulting Hubbard Hamiltonian using the Variational Cluster Approximation [3] and Cellular-Dynamical Mean-Field Theory with an exact diagonalization impurity solver [4,5]. For single-layer materials, the effect of the inter-plane hopping is not sufficient to explain all the differences between the experimental phase diagrams for the various materials. We suggest other avenues of investigation. [1] Weber et al., Europhysics Lett. 100 37001 (2012) [2] Souza et al, Physical Review B 65 035109 (2001) [3] Sénéchal et al, Phys. Rev. Lett. 94 156404 (2005) [4] Caffarel and Krauth, Phys. Rev. Lett.72 1545-1548 (1994) [5] Sénéchal, Theoretical methods for Strongly Correlated Systems, eds: Mancini, Avella (Springer series, 2011)

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