

Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

The importance of local band effects for ferromagnetism in hole doped La_2CuO_4 . BERNARDO BARBIELLINI, Department of Physics, Northeastern University, Boston, Massachusetts 02115, USA, THOMAS JARLBORG, DPMC, University of Geneva, CH-1211 Geneva 4, Switzerland — Doping is of vital importance for cuprates, since only about 0.15 holes per Cu atom is sufficient to transform them from antiferromagnetic insulators to the best known superconductors. The doping is usually made through substitution of the ternary element (Sr for La etc.), and the effects are typically described by rigid band filling of the CuO band. However, results of band calculations for supercells of $\text{La}_{(2-x)}\text{Ba}_x\text{CuO}_4$ show that the rigid band model for doping is less adequate than what is commonly assumed. In particular, weak ferromagnetism (FM) can appear locally around clusters of high Ba concentration. The clustering is important at large dilution and averaged models for magnetism, such as the virtual crystal approximation, are unable to stabilize magnetic moments. These results give a support to the idea that weak FM can be the cause of the destruction of superconductivity at high hole doping.

Thomas Jarlborg
DPMC, University of Geneva, CH1211 Geneva 4

Date submitted: 28 Nov 2007

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