Abstract Submitted
for the MAR08 Meeting of
The American Physical Society

Properties of high-T_C superconductors from spin-phonon coupling and band models. THOMAS JARLBORG, DPMC, University of Geneva, CH1211 Geneva 4, Switzerland — An understanding of the rich doping- and $(\vec{q},\omega)$-dependences of spin excitations in high T_C materials is essential since the mechanism of high-T_C superconductivity might be linked to spin fluctuations. Ab-initio band calculations show important spin-phonon coupling (SPC), i.e. antiferromagnetic fluctations are enhanced when they co-exist with $\vec{q}_x$-phonons involving O, Cu or La distortions. Parameters for these "1-dimensional" (1D) electron-phonon and spin-wave couplings are obtained from band calculations for long supercells containing phonon distortions and/or staggered fields. The characteristic 2-D q-dependence of the excitations are calculated for a free-electron like band with the use of the ab-initio parameters. The q-variation depend on the strength of the SPC, which leads to a linear relation between $\vec{q}$ and doping, x, for x$\leq$0.15. The SPC is strongest for in-plane O-modes, weaker for modes involving the heavy atoms, and smallest for apical O, which together with SPC for the phonons at the characteristic frequency lead to a q-dependent excitation spectrum. These and other properties coming from SPC in the band/free-electron model compare favorably with observations.

Thomas Jarlborg
DPMC, University of Geneva, CH1211 Geneva 4

Date submitted: 23 Nov 2007 Electronic form version 1.4