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Interaction of Zhang-Rice singlets with the buckling phonons in Cuprates EHSAN KHATAMI, ALEXANDRU MACRIDIN, MARK JARRELL, University of Cincinnati, THOMAS DEVEREAUX, University of Waterloo — Starting from a fully interacting three-band model we derive an effective single-band Hamiltonian which describes the interaction of Zhang-Rice (ZR) singlets[1] with the buckling phonons. Our approach is based on exact diagonalization of small clusters which contain both Cu and O atoms[2]. We study the parametric dependence of the electron-phonon coupling. The coupling to the phonon mode with B_{1g} symmetry is one order of magnitude stronger than the coupling to the A_{1g} phonon mode and there is an anisotropy in the interaction. For the B_{1g} phonon, the antinodes contribute to the interaction more than the nodes, in agreement with weak coupling approaches[3]. By increasing the O-O hopping, the coupling amplitude becomes smaller in antinodal points. We also find that a simpler model, which considers the modulation of the ZR hopping by the corresponding bond phonons, captures the symmetry of the electron-phonon interaction. Reference: [1] F. C. Zhang and T. M. Rice, PRB **37**, 3759 (1988) [2] H. Eskes *et.al.*, Physica C **160**, 424 (1989) [3] T. P. Devereaux *et.al.*, PRL **93**, 117004 (2004)

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