THE ELECTRONIC HAMILTONIAN FOR CUPRATES

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A realistic many-body Hamiltonian for the cuprate superconductors should include both copper d and oxygen p states, hopping matrix elements between them, and Coulomb energies, both on-site and inter-site. We have developed a novel computational scheme for deriving the relevant parameters *ab initio* from a constrained occupation local density functional. The scheme includes numerical calculation of appropriate Wannier functions for the copper and oxygen states. Explicit parameter values are given for La_2CuO_4. These parameters are generally consistent with other estimates, and with the observed superexchange energy.

Secondly, we address the question: can this complicated multi-band Hamiltonian be reduced to a simpler one with fewer basis states per unit cell? We propose a mapping onto a new two-band effective Hamiltonian with one copper d and one oxygen p derived state per unit cell. This mapping takes into account the large oxygen-oxygen hopping given by the *ab initio* calculations.

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