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Approximate treatment of the three-band Hubbard model

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Abstract

An approximate treatment of the three-band Hubbard model is developed which allows the calculation of spectral functions on the CuO_2 planes of superconducting cuprates. The lattice is divided into CuO_2 clusters (trimers), on which the Hamiltonian can be diagonalized. The hole concentrations on both orbitals and the amplitude of the staggered magnetization are obtained as a function of the total number of holes through a linear interpolation of the Green functions. The stoichiometric compound is a charge transfer insulator in the antiferromagnetic phase. Magnetic order is destroyed at different concentrations for electron and hole doping.

The CuO_2 planes of superconducting cuprates are considered to be responsible for most of their peculiar electronic properties. These oxides are insulating in the stoichiometric phase, where the copper sublattice shows an antiferromagnetic (AF) order [1, 2]. It is widely agreed that high-T_c superconductivity is induced in these oxides as carriers are introduced into the planes.

A realistic description of these compounds is given by the three-band Hubbard Hamiltonian, which takes into account both local electronic correlations and covalence [3, 4]. In this communication we develop an approximate solution of the three-band Hubbard model which accounts for the essential features of the electronic states of superconducting oxides. In the paramagnetic phase, the stoichiometric system (one hole per CuO_2 unit) is metallic, whereas in the AF phase a narrowing is observed in some bands and the Fermi level falls into the charge transfer (CT) gap.

The present approximation takes advantage of the exact diagonalization of the Hamiltonian on the basic CuO_2 trimer. The two-dimensional lattice is built up as the trimers are linked together via the hopping between copper and oxygen in different trimers, which is treated as a perturbation. The energy levels of the isolated trimer give rise to narrow bands. As carriers are added, a redistribution of spectral weight occurs, as expected by Eskes et al. [5].

We write the three-band Hubbard Hamiltonian as

$$\mathscr{H} = \sum_{ix\sigma} (\mathscr{H}^0_{ix\sigma} + V_{ix\sigma}), \tag{1}$$

where the trimer Hamiltonian is

$$\begin{aligned}\mathscr{H}^0_{ix\sigma} = {} & \Delta(n^a_{ix\sigma} + n^c_{ix\sigma}) + \tfrac{1}{2} U_d n^d_{ix\sigma} n^d_{ix\sigma} \\ & + \tfrac{1}{2} U_p (n^a_{ix\sigma} n^a_{ix\sigma} + n^c_{ix\sigma} n^c_{ix\sigma}) \\ & - t(a^\dagger_{ix\sigma} d_{ix\sigma} + d^\dagger_{ix\sigma} a_{ix\sigma} - c^\dagger_{ix\sigma} d_{ix\sigma} - d^\dagger_{ix\sigma} c_{ix\sigma})\end{aligned} \tag{2}$$

and the inter-trimer hopping term is

$$\begin{aligned}V_{ix\sigma} = {} & -t(c^\dagger_{ix\sigma} d_{i+1,x,\sigma} - a^\dagger_{ix\sigma} d_{i,x+1,\sigma} \\ & + d^\dagger_{ix\sigma} c_{i-1,x,\sigma} - d^\dagger_{ix\sigma} a_{i,x-1,\sigma}).\end{aligned} \tag{3}$$

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In Eqs. (2) and (3), $b^{\dagger}_{i\alpha\sigma}$ ($b_{i\alpha\sigma}$) is the operator that creates (annihilates) a hole with spin σ on a b-site of the trimer ($i\alpha$) ($b = a, d$ or c, where d stands for copper states and a and c for the oxygen p-states). Δ is the energy difference between p and d orbitals, U_p and U_d are the Coulomb repulsive interactions on copper and oxygen ions, respectively, and t is the hopping between neighboring p and d orbitals.

The analytical evaluation of all the eigenvalues and eigenvectors of the Hamiltonian $\mathscr{H}^0_{i\alpha}$ is greatly simplified if one makes the simple assumption that $U_d = U_p + 2\Delta$, which is not far from realistic parameter values. We have considered $\Delta = 2.6t$ and $U_p = 4.6t$.

The trimer's Green functions $g^{(n)}_{bb'}(\omega)$ for a fixed number of particles n (= 0, 1 or 2) per unit cell are obtained by the spectral representation, after evaluation of all matrix elements involving the corresponding ground state. The ground state degeneracy for $n = 1$ is resolved by the presence of an infinitesimal magnetic field h.

The unperturbed Green functions $g^{\sigma}_{bb'}$ must be defined in the whole range of concentrations n. A linear interpolation is the simplest choice and we write

$$g^{\sigma}_{bb'} = \begin{cases} (1-n)g^{(0)}_{bb'} + ng^{(1)\sigma}_{bb'} & \text{if } 0 \le n \le 1, \\ (2-n)g^{(1)\sigma}_{bb'} + (n-1)g^{(2)}_{bb'} & \text{if } 1 < n \le 2, \end{cases} \tag{4}$$

with $b, b' = a, d$ or c.

The remaining one-particle term $V_{i\alpha\sigma}$ in Eq. (1) is included by assuming Dyson-like equations for the lattice Green functions $G^{\sigma}_{bb'}(i\alpha; j\beta)$ describing the propagation of an electron from site b' of a given trimer ($j\beta$) to site b of trimer ($i\alpha$). The details of the calculation will be presented elsewhere [6]. Here, we restrict ourselves to the discussion of the main results.

The local densities of states (LDOS) on Cu and O sites exhibit a number of bands that originate from the one-particle energy levels of the CuO_2 trimer. By comparing with the spectral functions obtained from exact diagonalization on a Cu_4O_{13} cluster [8], we find good agreement in the position of the bands, considering the differences in the parameter values employed in both methods. We observe the presence of a narrow band, with predominant O character, that might correspond to the Zhang–Rice singlet band [7, 8].

In order to study the AF phase, we eliminate the "down spin" trimers (marked by grey circles in Fig. 1) by using the Green function equations. In the new lattice all trimers are equivalent and each one is connected to eight neighbors (its nearest-neighbor and next-nearest-neighbor trimers) through renormalized hopping matrices.

The LDOS determine $\langle n^d_\sigma \rangle$, $\langle n^a_\sigma \rangle$ and also the Fermi energy that corresponds to the given n ($= \sum_\sigma (\langle n^d_\sigma \rangle + 2\langle n^a_\sigma \rangle)$). The Cu(3d) and O(2d) hole densities and the magnetization on the Cu sites are

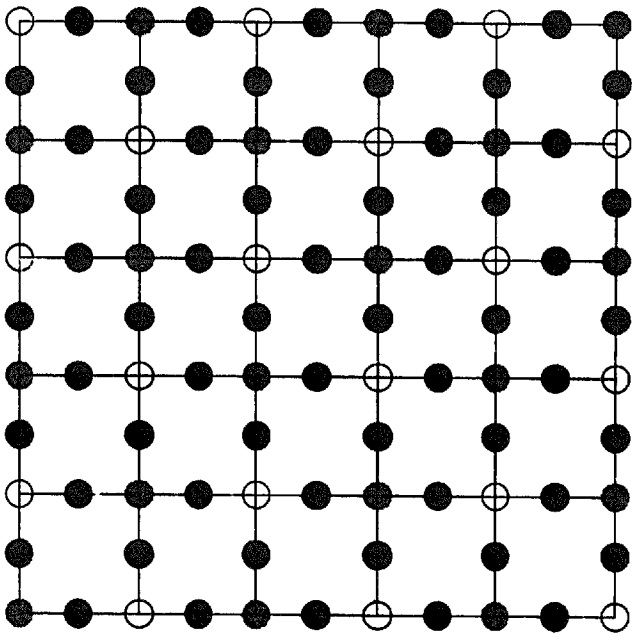

Fig. 1. The CuO_2 lattice. Black circles are O sites; white and grey circles are Cu sites with up and down magnetic moments, respectively.

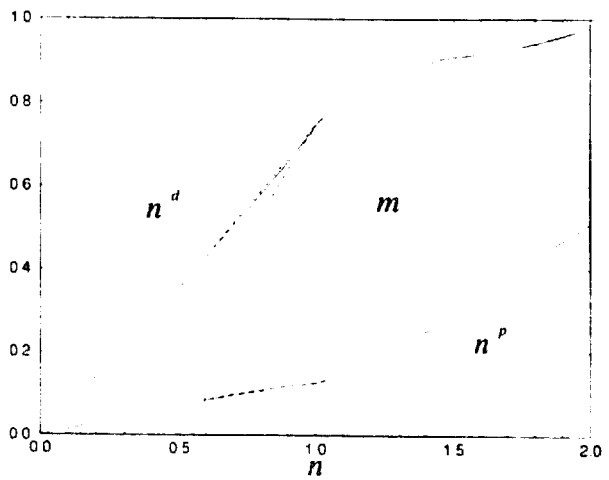

Fig. 2. Hole concentrations on Cu and O sites in the paramagnetic (solid lines) and AF (dotted) phases, and the staggered magnetization (dashed) as a function of the total number n of holes per unit cell.

shown in Fig. 2 as a function of the total number of holes per trimer.

There is an intrinsic asymmetry between electron and hole doping. For $n < 1$, the AF (dotted) curves n^d and n^p in Fig. 2 are very close to the corresponding paramagnetic solutions (solid lines). The magnetization curve

exhibits a typical second-order transition at $n \approx 0.60$. For $n > 1$, when $n \approx 1.40$ is attained, the dotted and solid curves are very far apart, so that the transition to the nonmagnetic state is abrupt. Doped holes go mostly to O sites, whereas added electrons prefer the Cu ions. If the paramagnetic phase could be stabilized, for low doping levels, one would get a completely different situation where practically all added holes would go to the Cu sites. The critical carrier concentrations are expected to be reduced if one includes the direct hopping t_{pp} between O orbitals [9].

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