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MODEL STUDY OF ANTIFERROMAGNETISM IN HIGH-T_c SUPERCONDUCTING OXIDES

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The antiferromagnetic ground state in high-T_c superconducting oxides (HTSO) is studied with a two-band model Hamiltonian by using a Hartree–Fock approximation and the Gutzwiller ansatz. It is found that the magnetic moments of Cu atoms and the antiferromagnetic gap agree well with the available experimental data for HTSO.

1. Introduction

The understanding of antiferromagnetic (AF) order in high-T_c superconducting oxides (HTSO) is one of the important questions in the search for the microscopic mechanism of superconductivity. The AF phase of these compounds is interesting in itself. It is highly anisotropic with large exchange constant within CuO_2 planes $J \approx 1300$ K [1] and weak magnetic coupling between the planes. It is therefore important to understand the magnetic properties of a CuO_2 plane. In doped systems ($La_{2-x}Sr_xCuO_4$ and $YBa_2Cu_3O_{6+x}$, $x > 0$) antiferromagnetism disappears quickly with the increasing number of holes N within CuO_2 planes. In the localized picture one may understand that as a consequence of frustration caused by ferromagnetic interactions induced by holes [2]. The observed magnetic moments of $0.4–0.6\mu_B$ per Cu atom agree then also with what is expected for a two-dimensional Heisenberg magnet where quantum fluctuations are significant.

In spite of this qualitative success of the localized picture, the evidence increases that the *itinerant description of* HTSO *is more appropriate*. The Cu(3d) holes are localized only if both U (Coulomb interaction) and D (the energy cost of a charge fluctuation $d^9 \rightarrow d^{10}$ + p-hole) are larger than the p–d hybridization V [3]. The analysis of electron spectroscopy data [4], as well as a direct calculation of these parameters within the local spin density formalism [5] give that $U/V \approx 5$, but $D/V < 1$. Therefore, the *charge degrees of freedom are important* in HTSO. Below we discuss the results obtained by an itinerant description of the AF phase of HTSO.

2. Model Hamiltonian and antiferromagnetic ground state

We use the following two-band model Hamiltonian for HTSO

$$H = \epsilon_d \sum_{i\sigma} d^+_{i\sigma} d_{i\sigma} + \epsilon_p \sum_{m\sigma} a^+_{m\sigma} a_{m\sigma} + V \sum_{im\sigma} (d^+_{i\sigma} a_{m\sigma} + \text{h.c.}) + U \sum_i n_{i\uparrow} n_{i\downarrow}, \qquad (1)$$

with $D = \epsilon_p - \epsilon_d$. It describes holes in $Cu(3d_{x^2-y^2})$ and $O(2p_{x(y)})$ orbitals within a CuO_2 plane and has three parameters: D/V, U/V and the number of holes per unit cell N [3].

The AF phase is studied in the Hartree–Fock approximation (HFA) by solving a Hamiltonian H_0 in place of H, where the interaction term proportional to U is replaced by an alternating field $v_{i\sigma} = \mp v \exp(i\mathbf{Q}\cdot\mathbf{R}_i)$ with a wave vector $\mathbf{Q} = (\pi/a, \pi/a)$ characteristic of the two-sublattice AF structure observed in HTSO; the signs correspond to $\sigma = \uparrow$ and $\downarrow$. From the diagonalization of H_0 one obtains an AF band structure and the energy minimization gives $v = Um$, where m is a magnetic moment per one Cu atom related to the local hole densities by $n_{i\sigma} = \langle d^+_{i\sigma} d_{i\sigma} \rangle = \frac{1}{2}[n_d \pm m \exp(i\mathbf{Q}\cdot\mathbf{R}_i)]$.

In HTSO $U/V \gg 1$ [4,5] and electron correlations are important [6]. Therefore, one has to go beyond the HFA to get a more realistic description of the AF phase. A mean-filled theory in the case of strong correlations is obtained by using the Gutzwiller ansatz (GA). We analyzed the kinetic and interaction energy for the lattice built by Cu

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and O atoms in a similar way to that used for the periodic Anderson model [7,8]. The reduction of kinetic energy may be described by introducing the following effective Hamiltonian

$$H_{\rm eff} = \sum_{i\sigma} (\epsilon_{\rm d} - \mu_{i\sigma}) d^{+}_{i\sigma} d_{i\sigma} + \epsilon_{\rm p} \sum_{m\sigma} a^{+}_{m\sigma} a_{m\sigma} + \sum_{im\sigma} V_{i\sigma}(n_{i\sigma}, n_d, d)(d^{+}_{i\sigma} a_{m\sigma} + \text{h.c.}), \quad (2)$$

where $V_{i\sigma}(n_{i\sigma}, n_{\rm d}, d) = q^{1/2}_{i\sigma}(n_{i\sigma}, n_{\rm d}, d)V$,

$$q_{i\sigma}(n_{i\sigma}, n_{\rm d}, d) = \frac{1}{n_{i\sigma}(1-n_{i\sigma})} \left\{ \left[(1 - n_{\rm d} + d)(n_{i\sigma} - d) \right]^{1/2} + \left[d(n_{\rm d} - n_{i\sigma} - d) \right]^{1/2} \right\}^2, \quad (3)$$

$\mu_{i\sigma}$ are alternating potentials which fulfill $\mu_{i\sigma} = \mu_{j-\sigma}$ for i and j belonging to different sublattices, $n_{\rm d}$ is the average hole density per Cu site and d is the average number of Cu atoms occupied by two holes. The derived renormalization factor $q_{i\sigma}(n_{i\sigma}, n_{\rm d}, d)$ agrees with that of the Anderson lattice [8] and reduces to the well-known $q_{i\sigma} = [(1 - n_{\rm d})/(1 - n_{i\sigma})]^{1/2}$ at $U = \infty$ [7]. The variational parameters $\{\mu_{i\uparrow}, \mu_{i\downarrow}, d\}$ are found by minimizing the energy $E_0 = \langle H_{\rm eff} \rangle + Ud + \Sigma_{i\sigma} \mu_{i\sigma} \langle d^{+}_{i\sigma} d_{i\sigma} \rangle$. Our effective Hamiltonian (2) interpolates between the band and localized limit and reproduces the exact ground state for a finite cluster consisting of one Cu atom surrounded by four O atoms and filled by two holes.

3. Results and discussion

At $N = 1$ one finds an AF ground state for $U > 0$ which is a consequence of the perfect nesting instability of our half-filled band. Since the results of an mean-field type theory are independent of the actual dimensionality, we have simplified our numerical analysis by considering the AF phase of an alternating Cu–O chain in one dimension (1D). Then we find an analytic formula for the AF gap in the antibonding band

$$\Delta = \tfrac{1}{2} Um + \tfrac{1}{2} \left\{ \left[\left(D_{\rm HF} + \tfrac{1}{2} Um \right)^2 + 8V^2 \right]^{1/2} - \left[\left(D_{\rm HF} - \tfrac{1}{2} Um \right)^2 + 8V^2 \right]^{1/2} \right\}, \quad (4)$$

where $D_{\rm HF} = D - \frac{1}{2} U n_{\rm d}$ is the energy difference between the one-hole levels in HFA. In 2D the gap is anisotropic but its minimum in the (1, 1) direction is given also by eq. (4). If $D_{\rm HF} \to \infty$, $\Delta \to Um$ and only then AF phase of the CuO_2 plane reduces to that of the Hubbard model.

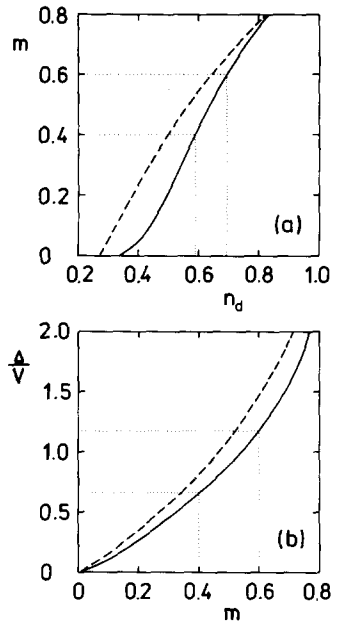

Fig. 1. Magnetic moment m as a function of $n_{\rm d}$ (a) and AF gap Δ/V as a function of m (b) in HFA (dashed) and GA (full lines) for $N = 1$, $U/V = 5$ and $V = 1.8$ eV. Dotted lines indicate the values of $n_{\rm d}$ and Δ/V for $0.4 < m < 0.6$.

Instead of $D_{\rm HF}$, it is more convenient to use $n_{\rm d}$ as a parameter being directly measured by photoemission. The resulting m and Δ are shown in fig. 1. Taking the experimental magnetic moment of $0.4 < m < 0.6$, we find $n_{\rm d} \approx 0.6$ and $\Delta \approx$ V. The GA is a simple way to include electron correlations. Therefore, $n_{\rm d}$ values are *enhanced*, as also found elsewhere for nonmagnetic states [5]. The AF gap Δ is *reduced* and, in spite of the simplifications of our model, agrees with the experimental value of 2.0 eV [9].

The magnetic moment m decreases with increasing number of holes N. In HFA this decrease is slow and the AF ground state disappears only at $N \approx 1.24$; in GA the moment decreases faster and vanishes at $N \approx 1.13$. It is not surprising that the collapse of antiferromagnetism found experimentally is much faster than that. This proves that the correlation effects within uniform AF phase cannot account for the observed breakdown of

long-range order and suggests that the *spin bags* formed by excess holes are important [10]. Indeed, numerical simulation of finite two-dimensional lattice shows that such defects form and condense into domain walls which destroy the AF order [11].

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