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A MEAN-FIELD DESCRIPTION OF THE ANTIFERROMAGNETISM OF CuO_2 LAYERS

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Abstract: Antiferromagnetic (AF) ground state properties of CuO_2 layers are calculated at the mean-field level within a slave-boson approach to a multiband Hubbard model which includes a minimal number of Cu and O orbitals.

1. Introduction

Purpouse of this work is to provide a description of the antiferromagnetism of CuO_2 layers via a *mean field* which is suited to describe strongly correlated systems with partly itinerant electrons.

Specifically we consider a two-dimensional square lattice of Cu atoms bridged by O atoms, and describe the electronic phenomena occuring within the plane by a multiband Hubbard model that includes the $d_{x^2-y^2}$ orbital for Cu and the p_x and p_y orbitals for O:

$$\begin{aligned} H = & \sum_{ij}\sum_{\nu\sigma} t_1 \left(d^\dagger_{i\sigma} p_{j\nu\sigma} + H.c. \right) + \sum_{jj'}\sum_{\nu\nu'\sigma} t_2 \left(p^\dagger_{j\nu\sigma} p_{j'\nu'\sigma} + H.c. \right) \\ & + \varepsilon_d \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma} + \varepsilon_p \sum_{j\nu\sigma} p^\dagger_{j\nu\sigma} p_{j\nu\sigma} \\ & + U_d \sum_i d^\dagger_{i\uparrow} d_{i\uparrow} d^\dagger_{i\downarrow} d_{i\downarrow} + U_p \sum_{j\nu} p^\dagger_{j\nu\uparrow} p_{j\nu\uparrow} p^\dagger_{j\nu\downarrow} p_{j\nu\downarrow} \end{aligned} \tag{1}$$

Here, the lattice sums are limited to neighboring sites, the index ν distinguishes the p orbitals, σ is the spin projection, $\varepsilon_p - \varepsilon_d = \Delta$ is the separation between p and d hole energy levels, and U_d and U_p are the Coulomb repulsions at the Cu and O sites, respectively. The Cu-O hopping t_1 and the O-O hopping t_2 can be obtained by a tight-binding fit to a conventional band structure. For La_2CuO_4 one gets $t_1 \cong 1.4$ eV

and $|t_2/t_1| \cong 1/4 \div 1/2$. The value of Δ is rather controversial: reported values for La_2CuO_4 differ by an order of magnitude ranging from .5 eV to 5 eV. We shall take Δ as a free parameter in the following. Reasonable estimates for U_d and U_p are 10 eV and 2 eV, respectively.

These estimates suggest that a conventional Hartree-Fock decoupling, which replaces the two-body interaction term in (1) by a one-body operator upon factorization of its average value, is reliable only for the O sites where $U_p/t_1 \cong 1$. A different approach is, however, required for the Cu site since $U_d/t_1 \gg 1$. We shall limit ourselves to consider a mean-field solution in the following.

Before describing the approach, it is worthed to comment on its limitations and the way to overcome them. Since we consider a strictly two-dimensional system, our results will be meaningful at zero temperature although the mean-field approximation provides an AF solution even at finite temperature. We should mention in this context that there have appeared recently several arguments in favor of the existence of AF order in two dimensions for spin 1/2 at zero temperature. In addition, quantum fluctuations are also neglected by our mean-field solution that assumes a Néel state. To overcome the limitations of our two-dimensional mean-field approach one could (i) include the interlayers coupling to obtain an AF temperature which compares favorably with the experimental value even at the mean-field level, and (ii) include the fluctuations about the mean field by relaying on its definition as the saddle point of a functional.

2. The method

The method we consider extends to a multiband Hubbard model the treatment by Kotliar and Ruckenstein for a one-band Hubbard model [1]. According to the method, slave bosons which specify empty (e_i) and singly occupied $(s_{i\sigma})$ states are assigned to each Cu site i as additional degrees of freedom to take into account the local environment. [The doubly occupied states need not be considered in the limit $U_d \approx \infty$ we shall assume]. To avoid multiple bosonic occupation at a given Cu site, the physical subspace is selected by the requirement that the operators

$$Q_i^I = e_i^\dagger e_i + \sum_\sigma s_{i\sigma}^\dagger s_{i\sigma} \tag{2a}$$

$$Q_{i\sigma}^{II} = d_{i\sigma}^\dagger d_{i\sigma} - s_{i\sigma}^\dagger s_{i\sigma} \tag{2b}$$

have eigenvalue 1 and 0, respectively. A convenient way to enforce

this requirement is to resort to a functional integral approach for the coupled Bose-Fermi system, where one introduces Lagrange multiplier fields to project onto the physical subspace [1]. The approach provides in turn a mean-field description of the antiferromagnetism of the CuO_2 layers by selecting the saddle-point for the bosonic part of the functional.

The introduction of slave bosons at Cu sites requires one to map the original operator $d_{i\sigma}$ of (1) onto the product $d_{i\sigma} z_{i\sigma}$ where $z_{i\sigma}$ is an appropriate bosonic operator. At the saddle point the introduction of slave bosons results thus into a renormalization of the hopping integral t_1 owing to correlations. This procedure has to be contrasted with the Hartree-Fock decoupling that we have adopted for the O sites, which affects the interaction terms but leaves the hopping t_2 unchanged. The Hamiltonian (1) is then replaced by

$$\begin{aligned} H = &\sum_{ij}\sum_{\nu\sigma} t_1 \left(z^\dagger_{i\sigma} d^\dagger_{i\sigma} p_{j\nu\sigma} + H.c. \right) + \sum_{jj'}\sum_{\nu\nu'\sigma} t_2 \left(p^\dagger_{j\nu\sigma} p_{j'\nu'\sigma} + H.c. \right) \\ &+\varepsilon_d \sum_{i\sigma} d^\dagger_{i\sigma} d_{i\sigma} + \varepsilon_p \sum_{j\nu\sigma} p^\dagger_{j\nu\sigma} p_{j\nu\sigma} + U_p \sum_{j\nu\sigma} [n_0 p^\dagger_{j\nu\sigma} p_{j\nu\sigma} - \frac{1}{2} n_0^2] \end{aligned} \tag{3}$$

with the condition $n_0 = < p^\dagger_{j\nu\sigma} p_{j\nu\sigma} >$ at the O sites.

The identification of the bosonic operator $z_{i\sigma}$ in terms of e_i and $s_{i\sigma}$ is not unique within the physical subspace. Although the choice of $z_{i\sigma}$ would not be an issue for an exact calculation, attention must be paid to this choice when dealing with approximations. In particular, the arbitrairness of $z_{i\sigma}$ must be resolved within the mean-field approximation so as to reproduce known results and to avoid spurious outcomes. It turns out from our calculation that the choice [1]

$$z_{i\sigma} = e^\dagger_i (1 - s^\dagger_{i\sigma} s_{i\sigma})^{-1/2} (1 - e^\dagger_i e_i - s^\dagger_{i\bar{\sigma}} s_{i\bar{\sigma}})^{-1/2} s_{i\sigma} \tag{4}$$

reproduces the AF energy of a Néel state with one hole per Cu site, namely,

$$E_{AF} = N(-4\, t_1^2/\Delta + 16\, t_1^4/\Delta^3 + ...) \tag{5}$$

(N being the number of Cu sites) in the limit of large Δ (i.e., for $\Delta/t_1 \gtrsim 10$), when comparison with perturbation theory in t_1/Δ is meaningful [2]. In addition, the slave-boson method with he choice (4) develops a molecular-like AF state for increasing Δ by suitably renormalizing the hopping for the two spin projections. Specifically, for

an atom of the 'spin up' sublattice $z_\uparrow \sim 1$ and $z_\downarrow \sim 0$ for increasing Δ, so that a hole with spin up tends to be confined near the corresponding site. For these reasons, we adopt confidently the choice (4) for all values of Δ.

3. Results

A similar calculation for the paramagnetic phase shows that the hopping renormalization parameter z vanishes when $\Delta \geq \Delta_c$ with $\Delta_c \cong 4\sqrt{3}\, t_1$. This indicates that the system is undergoing a transition *a la* Gutzwiller to a Mott insulating state [1]. Although this result represents a nice qualitative feature of the slave-boson mean-field approach, which cannot be obtained within the Hartree-Fock decoupling, it is associated to the vanishing of the ground state energy for $\Delta \geq \Delta_c$, because the Gutzwiller approximation inhibits the electronic fluctuations in the localized phase. A direct numerical comparison of the ground state energies per Cu site in the two phases, to extract an effective exchange integral $J_{eff} \equiv 2(E_P - E_{AF})/N$, results then in too large values for J_{eff} when $\Delta \gtrsim \Delta_c$.

A better estimate for J_{eff} is obtained by interpolating the paramagnetic energy between its asymptotic expression, namely,

$$E_P = N(-4\, t_1^2/\Delta + 18\, t_1^4/\Delta^3 + ...) \tag{6}$$

valid for $\Delta \gtrsim \Delta_c$ when perturbation theory in t_1/Δ can be applied [2], and our numerical results for smaller Δ. The resulting curve $J_{eff}(\Delta)$ has by construction the correct asymptotic form $4\, t_1^4/\Delta^3$ and presents a maximum at intermediate values $\Delta/t_1 \approx 3$, remaining positive down to vanishing Δ. Comparison with the experimental value $J_{exp} \cong .14$ eV for La_2CuO_4 [3] shows that two values, $\Delta/t_1 \cong .5$ and $\Delta/t_1 \cong 4.5$, are consistent with J_{exp} when $|t_2/t_1| = 1/4$. It is interesting to notice that these two values lie within the interval of the reported values for Δ : they correspond possibly to an itinerant and to a localized description of magnetism, respectively. One may also suggest in this context that a direct experimental check on which side of the maximum of the curve $J_{eff}(\Delta)$ the CuO_2 layers of La_2CuO_4 actually lie, could be obtained by measuring the Néel temperature upon applying uniaxial pressure to the layers so as to decrease the ratio Δ/t_1.

Diagonalization of the Hamiltonian matrix (3) (with the addition of terms corresponding to the constraints (2)) results in an effective

one-particle picture whereby a system of independent fermions interacts with a set of classical fields. The associated band structure shows a gap Δ_{AF} at half filling which separates the lowest filled band from the higher bands. In Fig.1 we report Δ_{AF} vs. Δ when $t_2 = 0$. The AF gap is found to be $\cong \Delta$ (the charge excitation gap) for large Δ and to remain finite for vanishing Δ owing to the strong nesting condition in two dimensions at half filling which stabilizes the antiferromagnetism against charge fluctuations. In Fig.1 we also report the width W of the lowest (filled) band which is seen to decrease rapidly for increasing Δ .

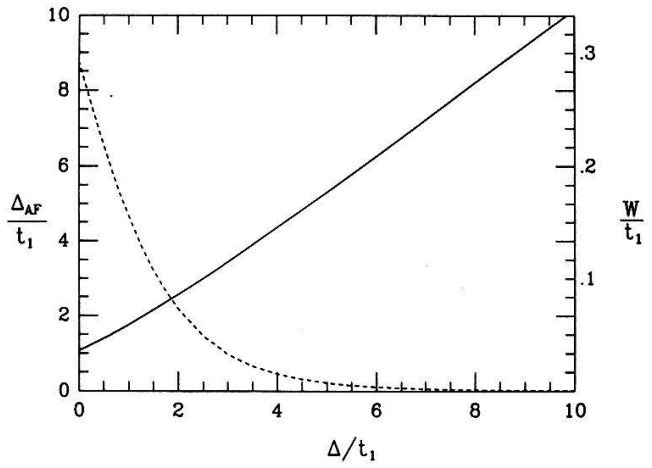

FIGURE 1
AF gap Δ_{AF} (full line) and width W of the lowest band (broken line) for $t_2 = 0$

4. Conclusions

We have calculated several AF ground state properties of CuO_2 layers within a mean-field approach which is specifically conceived to deal with the strong correlation at Cu sites. Future work along these lines may concern the inclusion of fluctuations about the AF saddle point to obtain the spin-wave spectrum and the associated reduction factor of the Cu magnetic moment, as well as the calculation of a possible superconducting pairing interaction starting from the AF mean field.

5. References

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