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Intralayer correlation enhancement and interlayer coherence loss in CuO_2 bilayers

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The role of the interlayer magnetic coupling between CuO_2 planes on bilayer-group high-T_c superconductors is studied within a simple randomly decorated bilayer Ising model and a Bethe-lattice approach. We show that for weak interlayer coupling an enhancement of the intralayer hole-hole correlations is developed at finite temperatures. This phenomenon is related to the loss of interlayer coherence between defects and the consequent strengthening of the antiferromagnetic background.

In the last few years, much attention has been given to the study of the properties of disordered magnetic systems since frustration effects were proposed to be relevant to explaining the behavior of the doped copper-oxide high-T_c superconductors.[1] In these compounds the supercurrent is supposed to flow in the CuO_2 planes[2] which develop intraplane antiferromagnetic order when undoped. Doping introduces charge carriers which, for a large range of doping concentrations, are localized basically on the oxygen ions of such planes.[3] The net $\frac{1}{2}$ spin of each charge carrier interacts with its neighboring $\frac{1}{2}$ spin Cu atoms strongly enough to change the original antiferromagnetic coupling into an effective ferromagnetic one.[4] The resulting frustration effect due to the presence of these competing interactions induces an attraction between the charge carriers that may lead to Cooper pairing.[1] It has also been observed, as for example in Tl compounds, that the superconducting transition temperature is an increasing function of the number of closely spaced interacting CuO_2 layers present in the material.[5] Although this phenomenon has been related with a quantum-well confinement effect,[6] the role played by the coupling between these CuO_2 planes is still to be clarified.[7] Furthermore, since a new fractional quantum Hall effect was predicted to occur,[8] and was experimentally observed,[9] on coupled two-dimensional electron systems, a better understanding of the interplay between in-plane and interplane correlations on systems with mobile particles are clearly desirable.

Recently, within a simple randomly decorated Ising model and a Bethe lattice approach, it was shown that two distinct mechanisms of attraction actually appear in magnetically disordered systems:[10,11] a strong one due to frustration effects, and another due to the enhancement of magnetic fluctuations as the antiferromagnetic order is broken down. Although rather strong, the frustration component is not enough to promote a phase separation instability.[12] It was also pointed out that the transition to the superconducting phase appears to occur experimentally at a line of constant hole-hole correlation in the temperature versus hole-concentration space.[11]

In this paper we show how the coupling between disordered Ising models affects the intralayer hole-hole correlations. We obtain that in the ground state the intralayer correlations are quite insensitive to interlayer coupling. Nevertheless, an enhancement of the hole-hole correlations is developed at finite temperatures for weakly coupled layers. We relate this phenomenon with the loss of interlayer hole-hole coherence and the consequent strengthening of the antiferromagnetic order.

The model we study consists of a bilayer system. As it was shown that, in the range of temperatures and hole concentrations of interest for superconductivity, a Bethe lattice approach reproduces qualitatively and quantitatively well the hole-hole correlations in a square lattice,[11] in our model each layer is represented by a Bethe lattice. The layers have at each site Ising spins that represent the localized Cu spins. Although the high-T_c superconductors are actually better described by a two-component XY spin,[13] we believe that the main magnetic properties due to frustration may be reproduced by this simple Ising approach. The hole spin is represented by a mobile $\frac{1}{2}$ Ising spin randomly located on the oxygen ions. The Hamiltonian for the model is

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_{\text{int}} , \tag{1}$$

where,

$$\mathcal{H}_0=-J\sum_{i,j,l}\left\{(1-n_j^l)S_i^lS_j^l+n_i^l[\gamma S_i^lS_j^l+\alpha\sigma_j^l(S_i^l+S_j^l)]\right\} -\mu\sum_{j,l}n_j^l , \tag{2}$$

is the Hamiltonian for the uncoupled system. Here n_j^l is the hole occupation number at the bond connecting the site j at layer l to a site located at the previous generation on the same layer. It can assume the values 0 or 1 if the bond is unoccupied or occupied by a hole. J is the antiferromagnetic coupling between the copper spins S in the absence of a hole in the oxygen ion localized between them. In the presence of a hole, the direct coupling between the Cu spins is reduced by a factor γ. Also the hole-spin σ_j^l interacts with the neighbors Cu spins through a coupling αJ, with $\alpha > 1.0$ in the high-T_c compounds. *Ab initio* calculations on finite-size $\mathrm{CuO_2}$ clusters indicate that $\gamma \simeq 0.7$ and $\alpha \simeq 1.9$, and we will use these values in our analysis. As $\alpha > 1.0$, the effective hole-mediated interaction between Cu ions becomes ferromagnetic at low temperatures. μ is a chemical potential per hole that is used as a hidden variable controlling the mean hole concentration per oxygen site $p = \langle n_j^l \rangle$. The hole-hole effective attraction appearing in this model has been extensively studied and its possible connections with the properties of the high-T_c superconductors explored.[10-12] The interaction between such disordered layers can be represented by the Hamiltonian

$$\mathcal{H}_{\mathrm{int}} = -J_\perp \sum_j S_j^1 S_j^2 \ , \tag{3}$$

where $J_\perp$ is the interlayer coupling between neighboring Cu spins. In the present model we do not consider interlayer coupling between hole-hole and hole-Cu spins which we believe to be quite small. The interlayer coupling $J_\perp$ shall not be confused with the weak dipolar interaction between bilayer groups. Actually $J_\perp$ is originated by direct exchange and is much larger than the dipolar interactions. Inelastic neutron scattering experiments indicate that $J_\perp / J \gtrsim \frac{1}{40}$.[14]

The partition function of a similar model Hamiltonian was recently calculated and the magnetic phase diagram obtained as a function of the interlayer coupling.[15] A multiple reentrance was observed and its origin related to the role played by thermal fluctuations on frustration, hole-hole and spin-spin correlation functions. After performing a partial trace over the hole-spin variable, the present model turns into a generalization of the one studied in Ref. 15. Here the hole mediated effective interaction is temperature dependent and the chemical potential is shifted by a temperature dependent function.

The intralayer first-neighbor hole-hole correlations

$$\begin{aligned} C_{1,1} = C_{2,2} &= C(J_\perp / J, k_B T / J, p) \\ &= \langle n_j^l n_i^l \rangle - \langle n_i^l \rangle^2 \ , \end{aligned} \tag{4}$$

can be exactly obtained through the partial partition function technique.[15,16] Its main behavior is plotted in Fig. 1 as a function of temperature and hole concentration for the cases of uncoupled, weakly coupled, and strongly coupled layers. Notice that the picture remains almost the same for uncoupled and strongly coupled layers. The main distinction is on the small correlations regime in which, for high concentrations, the correlations are larger in the strong-coupling limit. However, in the range of temperature and hole concentration of interest for superconductivity, there is no effective enhancement on the hole-hole correlations and consequently the effective attraction between holes is not increased. Nevertheless, for small coupling between layers a maximum is developed at finite temperatures, which is higher than the maximum of the uncoupled system by a factor of order 1.2. This enhancement is in qualitative agreement

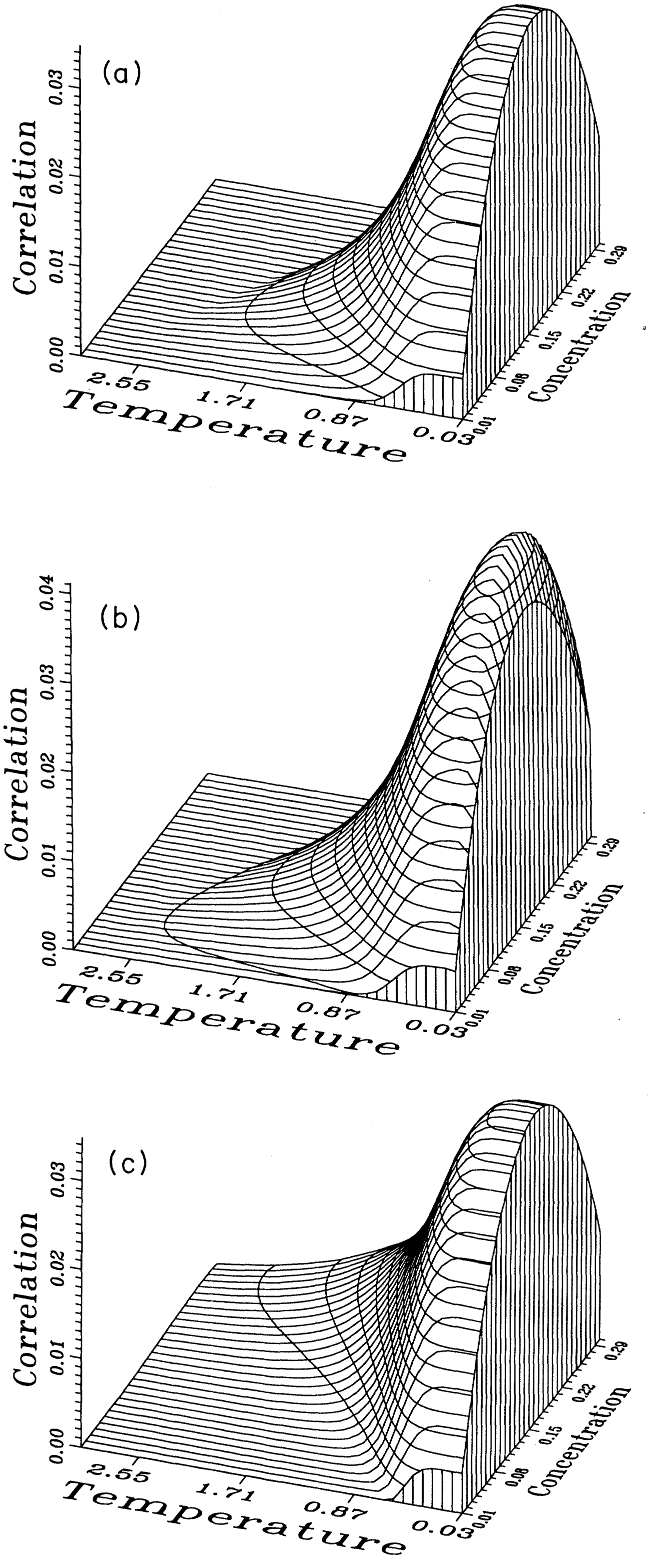

FIG. 1. Intralayer hole-hole correlation vs temperature ($0.03 < k_B T / J < 3.0$) and hole concentration ($0.01 < p < 0.30$) for (a) uncoupled layers $J_\perp = 0$; (b) weakly coupled layers $J_\perp / J = 0.1$; (c) strongly coupled layers $J_\perp / J = 10.0$, with $\alpha = 1.9$ and $\gamma = 0.7$. Notice that a maximum is developed at finite temperatures in the weak-coupling regime.

with the relative increase of the superconducting transition temperature observed in Tl compounds with two interacting CuO_2 planes when compared with the transition temperature of the monolayer system.[5]

A better understanding of the role played by the interlayer coupling can be achieved by looking at the interlayer hole-hole and spin-spin correlations defined as

$$C_{1,2}=\langle n_j^1 n_j^2\rangle-\langle n_j^l\rangle^2 , \tag{5}$$

$$C(S_1,S_2)=\langle S_j^1 S_j^2\rangle-\langle S_j^l\rangle^2 , \tag{6}$$

which revealed themselves as an important tool to explain the multiple reentrant nature of the magnetic phase diagram.[15] It can be observed in Fig. 2 that these correlations at the ground state are $C_{1,2}=p-p^2$, and $C(S_1,S_2)=1-m^2$, where m is the mean magnetization per site. This means that both the hole and spin configurations are the same on each layer. This one-to-one correspondence between hole position and spin orientation makes the system behave like a single layer at the ground state whenever one is concerned with correlations of the interlayer disorder distribution. As temperature is increased this coherence between layers is lost. In the weak-coupling case, the hole-hole correlation decays with increasing temperature faster than the spin-spin correlation. In the regime of strong spin-spin and weak hole-hole correlation, the antiferromagnetic order can be transferred from one layer to the other. This leads to an enhancement of the antiferromagnetic background that makes the frustration induced effective attraction between holes stronger. Similar strong fluctuations of defect lines have also been proposed for the high-T_c superconducting materials that have weak interplanar couplings.[17] As stronger couplings are considered the coherence between hole positions is lost only at temperatures in which the thermal fluctuations inhibit the order enhancement effect. Also, as temperature is increased, the hole-hole correlation decays as fast as the spin-spin correlation so that no order can be effectively transferred between layers. Notice also that, contrary to the low-temperature picture where frustration induces both hole positional and spin orientational interlayer coherence, near the magnetic transition only spin orientational coherence is induced by magnetic fluctuations. Although this effect is interesting by itself, and is actually the reason for the difference between the correlation of the uncoupled and strongly coupled systems [see Figs. 1(a) and 1(c)], it is irrelevant for superconductivity as it is effective only in the weak-correlation regime.

In conclusion, we have studied the effect of interlayer coupling on the hole-hole intralayer correlation on a randomly decorated bilayer Ising model within a Bethe lattice approach and its relevance on the effective hole-hole interaction in high-T_c superconductors. We obtained that the ground-state has the same intralayer correlations as the single-layer system, since both hole and spin distributions are the same on each layer. Nevertheless, at finite temperatures and small interlayer couplings of order $J_\perp/J\approx 0.1$, a maximum in the hole-hole correlations is developed, whose increase is of the same order of magnitude as the increase of the superconducting transition temperature observed in Tl compounds. This phenomenon is related with the strengthening of the antiferromagnetic order which is transferred from one layer to the other as the interlayer hole-hole coherence is lost. For stronger couplings $J_\perp/J\gtrsim 1.0$, the loss of hole-hole coherence takes place together with the loss of spin-spin coherence so that no order enhancement effectively appears. The present model can be generalized to a n-layer system. The n dependence of the enhancement of the hole-hole correlations is of particular interest and we expect it to show a fast saturation behavior as revealed in experiments.[5,6] This is a subject of current investigation.

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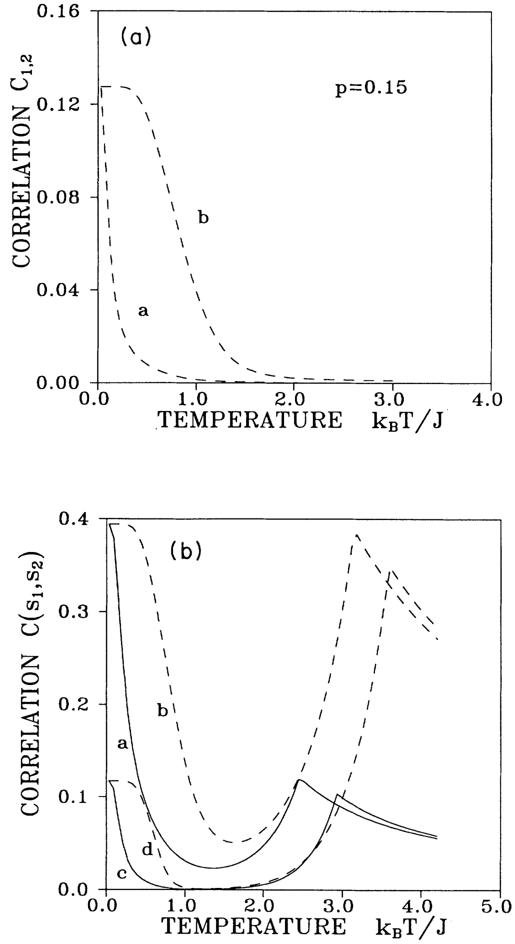

FIG. 2. (a) Interlayer hole-hole correlation for $J_\perp/J=0.1$ (line labeled a) and $J_\perp/J=1.0$ (line labeled b) at $p=0.15$. (b) Interlayer spin-spin correlation for a, $p=0.15$ and $J_\perp/J=0.1$; b, $p=0.15$ and $J_\perp/J=1.0$; c, $p=0.05$ and $J_\perp/J=0.1$; and d, $p=0.05$ and $J_\perp/J=1.0$. Notice that for $p=0.15$ and $J_\perp/J=0.1$ the hole-hole correlation decays faster than the spin-spin correlation as temperature is increased. Near the antiferro to paramagnetic phase transition one sees clearly the spin orientational coherence effect induced by magnetic fluctuations.

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