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# Spin-hole model for magnetic phase diagram and pairing mechanism in copper-oxide superconductors

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**Abstract.** A model of spins and holes for weakly coupled $CuO_2$ layers is constructed to study the temperature-concentration phase diagrams of doped $La_2CuO_4$ and $YBa_2Cu_3O_6$. For the undoped system we assume antiferromagnetic couplings between Cu magnetic moments and weak Ising anisotropy with canting. Addition of holes, localized on the O sites, induces a transformation of couplings from antiferromagnetic to ferromagnetic nature. The Néel temperature is reduced by doping while spin glass behavior develops. The insulator-metal (I-M) transition occurs when the correlations in the paramagnetic phase switch from antiferromagnetic to ferromagnetic character and the correlation length vanishes. Also there, with the change in sign of the average isotropic exchange coupling, the system develops (canted) $XY$ anisotropy, the vortex magnetic excitations occurring in this regime capture otherwise mobile charges, and the pairing of these occurs via the Kosterlitz-Thouless mechanism.

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## 1. Introduction

As the result of both experimental and theoretical efforts [1] it has become increasingly clear that magnetism plays an essential role in determining the transport properties of electric charge in the $CuO_2$-based superconductors. The salient features of these materials have been integrated into a general scheme and phase diagram that constitutes an important guide for the modelling and understanding of high-$T_c$ superconductivity. Thus: i) The large anisotropies observed in the properties of the three families of compounds, La-based, so-called "123" and Bi- (and closely related Tl) -based copper oxides, imply quasi two-dimensional motion of electrons as well as antiferromagnetic (AF) order associated to spin correlations within the $CuO_2$ planes, ii) Doping of $La_2CuO_4$ with Sr and/or Ba or reduction of the oxygen deficiency in $YBa_2Cu_3O_6$, creates holes, predominantly [2,3] localized on the O sites in the $CuO_2$ planes. iii) The introduction of holes transforms the local exchange cou

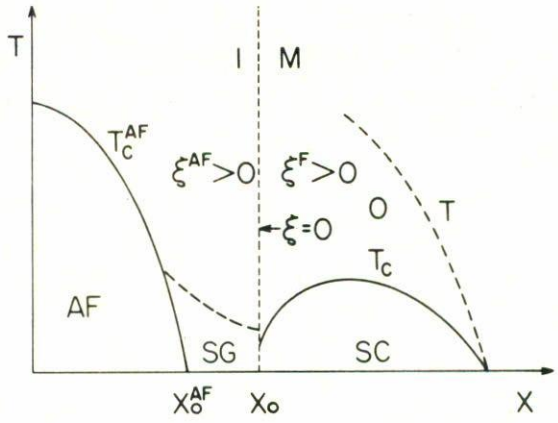


FIGURE 1. Schematic phase diagram for $La_2CuO_4$, as a function of dopant fraction $x$. AF = antiferromagnetic; SG = spin glass; I = insulator; M = metal; SC = superconductor; O = orthorhombic; T = tetragonal. According to our model, at $x = x_0$ the system switches from antiferromagnetic to ferromagnetic (F) character and the correlation length $\xi$ vanishes. Since an F background favours charge conductivity whereas an AF one does the opposite we identify the line $x = x_0$ as the I-M transition line.

pling between Cu spins from antiferromagnetic to ferromagnetic (F) [1,4], and the resulting frustration rapidly reduces the Néel temperature $T_c^{AF}$ with dopant additions. iv) Holes appear to be localized up to a critical concentration at which an insulator-metal (I-M) transition takes place. v) At higher dopant cocentration, beyond the I-M transition, superconducting (SC) behavior develops. vi) Structural transitions from tetragonal (T) to orthorhombic (O) symmetry take place in the La-based and in the 123 families of compounds, however only that of the 123 compound family appears to be related to the ordering of the dopant (in the CuO basal planes). The identification of the charge disbalance agent in the Bi-based materials has not been clearly identified at present, and therefore the manipulation of the degree of doping, and the subsequent observation in them of the above-described phase progression, has not been achieved yet. However, there are indications [5] that this family of materials behaves in a way similar to that of others. vii) Anomalous variations of the lattice parameters above and at the superconducting transition temperature $T_c$ have been observed for both the La-based and the 123 compound families in the highly doped regime [6,7]. Structural data [6] for $La_{1.85}Ba_{0.15}CuO_{4-y}$ show a monotonic increase in the orthorhombic strain with decreasing $T$ until a departure downwards occurs in close proximity to $T \sim 70$ K, the strain decreases until a discontinuity in its slope occurs at $T_c$. The lattice parameters of $YBa_2Cu_3O_{7-y}$ with $y \sim 0$ show a few abrupt decreases near certain temperataures above $T_c$. In Fig. 1 we show the phase diagram for doped $La_2CuO_4$ that illustrates the above description.

Antiferromagnetism in the undoped and weakly coupled $CuO_2$ layers of $La_2CuO_4$ arises through the anisotropic [8] superexchange interaction and a $2D$ Heisenberg

Hamiltonian with weak, and canted, Ising anisotropy is the corresponding representation. As it is known [9], the $2D$ Heisenberg ferromagnet is extremely sensitive to anisotropy, and vanishingly small amounts are sufficient to overrule the required absence of long range order (LRO) and to lift the spontaneous magnetization transition to finite values. A well known example [9] is the $2D$ Ising AF behavior of the perovskite $K_2NiF_4$ isostructural to $La_2CuO_4$. This material has tetragonal symmetry and exhibits only $2D$ magnetic order because each Ni ion is coupled to four equidistant nearest-neighbor Ni ions in each adjacent plane, therefore frustrating LRO normal to the planes. On the other hand, $La_2CuO_4$ is orthorhombic below 500 K due to the buckling of the $CuO_2$ planes generated by the rotation of the $CuO_6$ octahedra [10], and for this reason nearest-neighbor Cu ions on adjacent planes are not all equidistant. The $3D$ AF ordering observed in $La_2CuO_4$ is due to the disbalance in the weak interlayer coupling introduced by the orthorhombic symmetry, and a large value for $T_c^{AF}$ is obtained in spite of the weak interlayer spin couplings because of the unusually large in-plane correlation lengths [1,10]. The rotated $CuO_6$ octahedra in the orthorhombic phase imply an antisymmetric superexchange term in the Cu-Cu spin interaction [8] which is responsible for the observed canting of the spins out of the plane by a small angle [8]. Similar quasi-$2D$ magnetism occurs in the 123 compounds [11], although the differences in structure between the two families of compounds imply different ways by means of which anisotropic superexchange leads to canted Ising components. In what follows we discuss specifically the La-based compounds for which more information is available, but our arguments can be readily adapted to the 123 type superconductors.

Here we present a simple model, in terms of classical spins, for the magnetic interactions that take place in the $CuO_2$ planes. Our model shares several features of, and was motivated by, earlier spin-hole models for the same system (see Refs 1,2 and 4 and references therein). These earlier models indicated the way in which the basic antiferromagnetic phase behavior of the copper oxides can be understood and helped visualize possible mechanisms by means of which their magnetic and charge transport properties may relate to each other. The effect on the free energy of some nonclassical features like the degree of localization and high mobility of holes are introduced only as phenomenological ingredients. A main feature of the model is that it considers explicitly the effect of doping on the thermodynamics of the underlying $2D$-Heisenberg model, including changes in the degree of anisotropy implied by the antisymmetric superexchange Hamiltonian. As discussed below, we propose that doping not only introduces ferromagnetic Cu-Cu couplings but also generates $XY$ anisotropy at sufficiently high dopant fractions (when the holes are no longer firmly trapped and can migrate freely). We obtain the phase boundary for the AF transition as well as an expression for the correlation length for both spins and holes. We identify the loci of the I-M transition as that in which the correlation length of the system vanishes and a change in the nature of the hole-hole correlation occurs. Beyond this critical doping concentration the system is appropriately described by ferromagnetically-coupled Cu spins with canted $XY$ anisotropy. The vortex excitations of this system capture charges from the uniform delocalized background, and, as temperature is further reduced, these charges be-

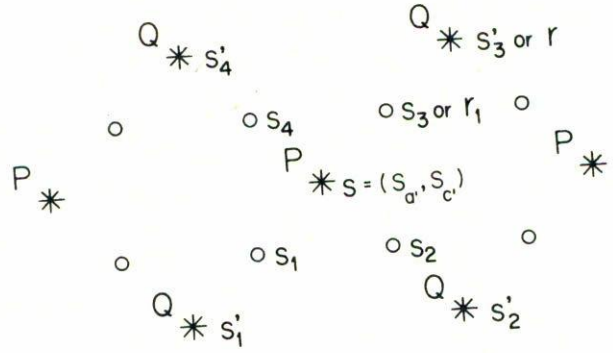


FIGURE 2. Sublattices for Cu (*) and O (o) sites in the $CuO_2$ layers. Cu spins are antiferromagnetically coupled in the absence of an electron hole at the intermediate O site. Otherwise their coupling is ferromagnetic.

come bounded in pairs via the Kosterlitz-Thouless mechanism for the formation of vortex-antivortex excitations [12]. We propose this to be the magnetic setting, and vehicle, albeit here only rudimentarily described, from which superconductivity arises in the $CuO_2$ materials.

## 2. Heisenberg model with antisymmetric exchange

We consider the planar decorated lattice shown in Fig. 2 where the square sublattice of primary sites is occupied by Cu and the square sublattice of secondary sites (the bond midpoints between nearest-neighbor primary sites) are occupied by $O^{2-}$ or $O^{-}$ (*i.e.* holes). We find it convenient to subdivide the primary sites in turn into two interwoven sublattices of sites of types $P$ and $Q$, since this facilitates the description of magnetic order with canting of the Cu spins (Fig. 2).

The antisymmetric superexchange interactions in the Cu-O-Cu complex are represented by the spin Hamiltonian [8,13] (for the undoped system)

$$\mathcal{H} = \sum_{\langle i,j \rangle} \mathbf{S}_i \cdot \mathbf{J} \cdot \mathbf{S}_j, \tag{1}$$

where

$$\mathbf{J} = \begin{pmatrix} J_{aa} & 0 & 0 \\ 0 & J_{bb} & J_{bc} \\ 0 & -J_{bc} & J_{cc} \end{pmatrix},$$

and where $\mathbf{S}_i$ and $\mathbf{S}_j$ represent Heisenberg spins on the Cu sites, and **a**, **b** and **c** indicate the $La_2CuO_4$ unit cell directions, with **b** normal to the basal plane. Eq. (1) can be written in the form

$$\mathcal{H} = \sum_{\langle i,j \rangle} \left\{ J\mathbf{S}_i \cdot \mathbf{S}_j + K_{a'} S_i^{a'} S_j^{a'} + K_{b'} S_i^{b'} S_j^{b'} + K_{c'} S_i^{c'} S_j^{c'} \right\}, \tag{2}$$

where $\langle i,j \rangle$ indicates summation over nearest-neighbor pairs only and where

$$J = \frac{1}{3}[J_{aa} + J_{bb} + J_{cc}], \tag{3a}$$

$$K_{a'} = \frac{1}{3}[2J_{aa} - J_{bb} - J_{cc}], \tag{3b}$$

$$K_{b'} = \frac{1}{3}[2J_{bb} - J_{aa} - J_{cc} + 2J_{bc}^2 (J_{bb} + J_{cc})^{-1}], \tag{3c}$$

and

$$K_{c'} = \frac{1}{3}[2J_{cc} - J_{aa} - J_{bb} + 2J_{bc}^2 (J_{bb} + J_{cc})^{-1}]. \tag{3d}$$

In Eq. (2), $S_i^{a'}$, $S_i^{b'}$ and $S_i^{c'}$ are the components of $S_i$ in a Cartesian frame of reference $(a'b'c')$ obtained from that defining the unit cell $(abc)$ through rotation by an angle $\varphi$ in the **b** direction away from **c** when site $i$ is of type $P$ and by an angle $-\varphi$ when site $i$ is of type $Q$. The angle $\varphi$ (in radians) is given by

$$\varphi = J_{bc}(J_{bb} + J_{cc})^{-1}. \tag{4}$$

The relative values of $K_{a'}$, $K_{b'}$ and $K_{c'}$ determine the type of anisotropy imprinted on the $2D$ Heisenberg magnet. This has been quantified [13] for undoped $La_2CuO_4$ for which one obtains weak Ising anisotropy along the $\mathbf{c}'$ axis with a small canting angle $\varphi \sim 0.003$. We assume that doping affects not only the sign [1,4] and value of the isotropic coupling $J$ but also (via concomitant structural changes) the values of $K_{a'}$, $K_{b'}$ and $K_{c'}$ between every pair of nearest-neighbor Cu spins where a hole has been created at their intermediate O site.

## 3. Ising anisotropy regime

We denote by $M^P$ and $M^Q$ the magnetizations for the spins associated to the Cu sites on sublattices $P$ and $Q$, respectively. Positive magnetization is defined for spins that point their axis of anisotropy (hereafter refered to as the spin direction) in the $\mathbf{c}'$ direction ($\uparrow$) on $P$ sites and (inversely) for spins in the $-\mathbf{c}'$ direction ($\downarrow$) on $Q$ sites. We find it convenient to consider two bond states, $\rightarrow$ and $\leftarrow$, on the secondary sites that represent the sequences of copper and oxygen spins $P$ $Cu^{\uparrow}$–$^{\downarrow}O^{\uparrow}$–$Cu^{\downarrow}$ $Q$

and $P$ $Cu^{\downarrow}$–$^{\uparrow}O^{\downarrow}$–$Cu^{\uparrow}$ $Q$, respectively. (Alternative sequences of spins for the two bond states are $P$ $Cu^{\uparrow}$–$^{\uparrow}O^{\downarrow}$–$Cu^{\downarrow}$ $Q$ and $P$ $Cu^{\downarrow}$–$^{\downarrow}O^{\uparrow}$–$Cu^{\uparrow}$ $Q$). Thus, independently of the sign of the coupling $J_1$ between a copper spin and an adjacent oxygen spin $\sigma$ one obtains antiferromagnetic Cu–Cu configurations for both kinds of bond states ($JS_i \cdot S_j \approx -|J_1|(S_i + S_j) \cdot \sigma$). We denote by $m^b$ the (auxiliary) order parameter associated to the bond states and take it to be positive when the symbol points towards a $P$ site. When a hole is created and localized on a secondary site there is only one oxygen spin that couples with exchange $J_2$ to the neighboring Cu spins, and the corresponding magnetization $m^h$ is taken to be positive when the spin of the hole points in the $\mathbf{c}'$ direction. We note that irrespective of the sign of $J_2$ a hole always leads to a ferromagnetic effective exchange between the Cu spins (now $JS_i \cdot S_j \approx |J_2|(S_i + S_j) \cdot \sigma$). We denote by $n_b$ and $n_h$ the occupation numbers for bonds and holes, respectively, on the secondary sites. We shall consider in our model a repulsion $\Lambda$ between nearest neighbor holes representative of Coulomb interactions.

Because we are interested in obtaining expressions for the correlations of our spin model we require the free energy $F$ for general nonuniform states [14]. From Fig. 2 we note that we can write $F$ as a sum only over $P$ sites provided we include in each term the entropy contribution and all interactions involved within a cluster of the four secondary and the four $Q$ sites sorrounding each site $P$. In Fig. 2 we give the notation for their positions. It is straightforward now to write the free energy in mean field approximation, and from it the associated Euler-Lagrange equations that determine the equilibrium states. For reasons of space we write here only the linearized expressions for the latter, from which the location of second order transitions and the behavior of the correlation length in the paramagnetic phase can be determined. We have

$$kTm^b(\mathbf{s}_l) - J_1[M^P(\mathbf{s}) + M^Q(\mathbf{s}'_l)] = 0, \qquad (5a)$$

$$kTm^h(\mathbf{s}_l) - J_2[M^P(\mathbf{s}) - M^Q(\mathbf{s}'_l)] + \Lambda n_h^2[m^h(\mathbf{s}_{l+1}) + m^h(\mathbf{s}_{l-1})] = 0, \qquad (5b)$$

$$kTM^P(\mathbf{s}) - J_1 n_b \sum_l m^b(\mathbf{s}_l) - J_2 n_h \sum_l m^h(\mathbf{s}_l) = 0 \qquad (5c)$$

and

$$kTM^Q(\mathbf{r}) - J_1 n_b \sum_l m^b(\mathbf{r}_l) + J_2 n_h \sum_l m^h(\mathbf{r}_l) = 0. \qquad (5d)$$

Eqs. (1) admit two types of uniform sublattice solutions. One corresponds to the onset of AF LRO, when $M^P = M^Q = M$, for which one obtains $kT_c^{AF} = (8J_1^2 n_b)^{1/2}$, here $m^h$ always vanishes and $m^b$ is nonzero below $T_c^{AF}$. The second type of solution relates to the onset of F LRO, when $M^P = -M^Q = M$, and $kT_c^F = (\Lambda^2 n_h^4 + 8J_2^2 n_h)^{1/2} - \Lambda n_h^2$, in this case $m^b$ always vanishes and $m^h$ is nonzero below $T_c^F$. We note that the hole-hole repulsion $\Lambda$ depresses $T_c^F$ and vanishes when $\Lambda \to \infty$. Thus we arrive at a proper description for the onset of AF LRO at low $T$ with $T_c^{AF}$ decreasing with increasing doping (Fig. 1). $T_c^{AF}$ above corresponds to

$2D$ Ising behavior (like that in $K_2NiF_4$), in the following section we indicate how the observed $3D$ AF transition is obtained from the model. The appearance of F LRO is a *spurious* solution of the model because it arises from the assumptions that holes remain localized and Ising anisotropy persists with increased doping which, as we shall argue below, is not the case. In the paramagnetic phase the two types of effective AF and F Cu-Cu spin couplings are randomly distributed throughout the lattice bonds. This positional distribution of AF and F interactions leads through frustration to spin glass behavior at low temperature (provided $T_c^{\mathrm{AF}} \approx 0$).

We incorporate the quantum delocalization energy of holes phenomenologically into the model by replacement of the hole density $n_h$ by an effective quantity $n_h^{\mathrm{eff}}$ that is no longer identical to the dopant fraction $x$, but given by $n_h^{\mathrm{eff}} = \alpha + tx$, where $\alpha$ is a measure of the degree of Ising anisotropy (its value would depend on $x$ and $T$, with $\alpha = 0$ for pure Ising and $\alpha = 1$ for pure Heisenberg) and $t$ is proportional to the Hubbard hopping integrals. The bond density $n_b$ is replaced too by $n_b^{\mathrm{eff}} = 1 - n_h^{\mathrm{eff}}$. According to the expression above for $T_c^{\mathrm{AF}}$, the effect of reducing Ising anisotropy is to reduce $T_c^{\mathrm{AF}}$, also large hole delocalization energies destroy AF LRO at low $T$. The percolation thresholds for both AF and F LRO in our mean-field treatment are (unrealistically) given by $n_h^{\mathrm{AF}} = 1$ and $n_h^{\mathrm{F}} = 0$, respectively. Resolution of our model beyond mean field would improve their values and yield $n_h^{\mathrm{AF}} < 1$ and $n_h^{\mathrm{F}}$, 0, in which case, the phenomenological parameter $\alpha$ will have a maximum value $\alpha_0 < 1$ for the pure Heisenberg limit. In Fig. 1 we denote by $x_0^{\mathrm{AF}}$ the value of $x$ that corresponds to percolation of holes, $n_h^{\mathrm{AF}}$, and AF LRO at $T = 0$ is no longer possible.

## 4. The correlation length

The dependence of the correlation length $\xi$ of the spin model on $T$, $x$, and the other parameters in the model can be obtained by differentiation of the nonuniform free energy, or, equivalently, via a linear response analysis of Eqs. (5). In the paramagnetic phase these equations have solutions of the form

$$\begin{aligned} \delta m^P(\mathbf{s}) &= M_0^P u^{s_{a'}+s_{c'}}, \qquad \delta m^b(\mathbf{s}_1) = m_1^b u^{s_{a'}+s_{c'}}, \\ \delta m^h(\mathbf{s}_1) &= m_1^h u^{s_{a'}+s_{c'}}, \qquad \delta M^Q(\mathbf{s}_1') = M_1^Q u^{s_{a'}+s_{c'}}, \end{aligned} \tag{6}$$

where $\delta M^P$, etc. represent fluctuations form the vanishing equilibrium values, and $u = \exp(-1/\xi)$. Substitution of Eqs. (6) into (5) (with $\Lambda = 0$) leads to

$$\begin{aligned} kTm_1^b &= J_1(M_0^P + M_0^Q), & kTm_1^h &= J_2(M_0^P - M_0^Q), & M_1^Q &= M_0^Q, \\ kTm_{2,4}^b &= J_1(M_0^P + uM_0^Q), & kTm_{2,4}^h &= J_2(M_0^P - uM_0^Q), & M_{2,4}^Q &= uM_0^Q, \\ kTm_3^b &= J_1(M_0^P + u^2M_0^Q), & kTm_3^h &= J_2(M_0^P - u^2M_0^Q), & M_3^Q &= u^2M_0^Q, \end{aligned} \tag{7}$$

and to the "dispersion" relation

$$R^2 - S^2(1-u)^2(1+u^{-1})^2 = 0, \tag{8}$$

$$R = (kT)^2 - 4(J_1^2 n_b^{\text{eff}} + J_2^2 n_h^{\text{eff}}) \quad \text{and} \quad S = (J_1^2 n_b^{\text{eff}} - J_2^2 n_h^{\text{eff}}). \tag{9}$$

From Eq. (8) we obtain two meaningful branches (*i.e.* $0 < u < 1$) with correlation lengths given by

$$\xi^{\text{AF}} = -\left\{ \ln \left[ \left( \frac{R}{2S} - 1 \right) - \sqrt{\left( \frac{R}{2S} - 1 \right)^2 - 1} \right] \right\}^{-1}, \tag{10a}$$

and

$$\xi^{\text{F}} = -\left\{ \ln \left[ \left( -\frac{R}{2S} - 1 \right) - \sqrt{\left( -\frac{R}{2S} - 1 \right)^2 - 1} \right] \right\}^{-1}, \tag{10b}$$

where $\xi^{\text{AF}}$ corresponds to antiferromagnetic-like fluctuations, *i.e.* $M_0^P = M_0^Q$, and $\xi^{\text{F}}$ to ferromagnetic ones, $M_0^P = -M_0^Q$. A given paramagnetic state with temperature $T$ and dopant fraction $x$ selects a correlation length $\xi$ from one of the branches, at low dopant concentration it does so from the AF-branch, whereas for large $x$ it is given by the F-branch. At fixed tempereature $\xi = \xi^{\text{AF}}$ decreases as $x$ increases and vanishes at $x_0$ given by $S = 0$, explicitly, when $\alpha = \alpha_0$, by

$$x_0 = \frac{J_1^2(1-\alpha_0) - J_2^2\alpha_0}{t(J_1^2 + J_2^2)}, \tag{11}$$

there it changes character from AF to F behavior and then increases as $x$ increases. The $3D$ AF ordering in orthorhombic $La_2CuO_4$ is driven by the interlayer coupling $J'$ and the $3D$ transition temperature can be obtained from Eq. (10$a$) via [1] $kT_c^{\text{AF}} \sim J'(\xi^{\text{AF}})^2$.

## 5. $XY$-anisotropy regime

We identify the loci at which the correlation length of the system vanishes and a change in the nature of the hole-hole correlation occurs as the model's representation of the insulator-to-metal transition in the copper oxides (Fig. 1). There, the strongly coupled spins behave, on average, as independent spins (since $\xi = 0$) and the overturning of spins that the AF environment imposes to hole translation disappears. Beyond $x_0$, the prevailing F-like correlations enhance hole conductivity. Holes are strongly correlated (Eqs. (7) for $m_l^h$) when $x > x_0$ ($M_0^P = -M_0^Q$) but

not when $x < x_0$ ($M_0^P = M_0^Q$). An interesting experimental indication that a ferromagnetic background favours conductivity of charges whereas an antiferromagnetic one does the opposite, is the discovery of field-induced ferromagnetism (allowed for by the canted nature of the spins) in undoped $La_2CuO_4$ and its effect in charge transport [8].

On the other hand, large and sudden changes in hole conductance can have a strong effect in the magnetic properties of the system. According to our model, once the holes acquire a high mobility (due to an overall majority of F spin couplings in the lattice) our picture of randomly distributed, and permanent for practical purposes, AF and F spin couplings gives way to one of *averaged* and *uniform* couplings. A simple mean-field estimate of such averaged diagonal coupling $\Delta J_{aa}$ at dopant fraction $x > x_0$ is $\Delta J_{aa} = (1-x)J_{aa}^{\mathrm{AF}} + xJ_{aa}^{\mathrm{F}}$, and similarly for $\Delta J_{bb}$ and $\Delta J_{cc}$ (where the superindices indicate the AF and F values of a local coupling when there is no hole and when there is a hole at the intermediate oxygen site, respectively). We assume [1,4] $|J_{aa}^{\mathrm{AF}}| < |J_{aa}^{\mathrm{F}}|$, etc., so that the average isotropic coupling $\Delta J = 1/3(\Delta J_{aa} + \Delta J_{bb} + \Delta J_{cc})$ is ferromagnetic when $x > x_0$, and small when $x \sim x_0$. However, recalling that the antisymmetric term $J_{bc}$ arises from the rotation of the $CuO_6$ octahedra in the orthorhombic phase, and because the La-based system exhibits appreciable and similar orthorhombic strains both before and after the I-M transition, we expect the antisymmetric coupling $\Delta J_{bc}$ to have a weak dependence on $x$ and to remain of the order of $|J_{bc}^{\mathrm{AF}}| \sim |J_{bc}^{\mathrm{F}}|$ throughout the I-M transition. It is possible that $J_{bc}^{\mathrm{AF}}$ and $J_{bc}^{\mathrm{F}}$ have both the same sign. Accordingly, when the orthorhombic strain decreases near the O-T transition $\Delta J_{bc}$ should decrease too and vanish at and beyond the O-T transition.

When the couplings in Eqs. (3) are replaced by the above estimates for the average uniform couplings, we notice that for small $x - x_0 > 0$ the terms quadratic in $\Delta J_{bc}$ would dominate over the other terms in the anisotropic couplings $K_{a'}$, $K_{b'}$ and $K_{c'}$ in Eq. (2), *i.e.* $K_{b'} \approx K_{c'} > K_{a'}$, and *one obtains* canted $XY$ anisotropy. The known properties of the $2D$ $XY$ magnet [12] are inherited by our model $CuO_2$ layer in this regime. Therefore, the Cu spins of our model cannot exhibit conventional F LRO at any temperature in the absence of an applied field when $x > x_0$. The Mermin-Wagner-Hohenberg theorem tells us that the magnetization (order parameter) is zero for finite $T$ [12]. Instead, vortex-like spin fluctuations (Fig. 3) are present in thermal equilibrium because their energy only increases logarithmically with the size of the system. (This is not possible in a $3D$ spin system and it is a very special property of the $2D$ $XY$ model). The vortex excitations play a central role in configuring a low temperature phase. At sufficiently low temperatures, they form tightly bound vortex-antivortex pairs whose effect cancels each other out, so that for most intents and purposes their presence does not have appreciable energy cost. As the temperature is increased, these pairs become widely separated until eventually they become free. The detailed theory [12] of such phase transition, the unbinding of vortex pairs, shows that their density is always very low, even at the transition, however they impress a power law decay to the spin correlations in the low temperature phase which is characteristic neither of a conventional long range order nor of a high temperature phase which has exponential decay of correlations.

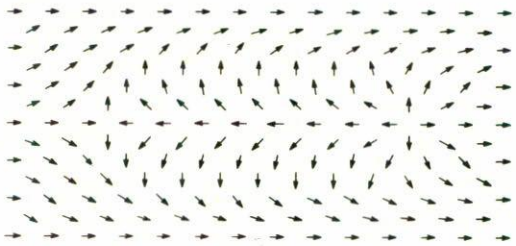

FIGURE 3. A vortex-antivortex pair excitation characteristic of the low-temperature phase in the ferromagnetic $XY$ anisotropy regime. when charges are trapped by the antiferromagnetic environment at their centers they become paired themselves. The repulsion of these charges is overcomed by the logarithmic attraction between the magnetic vortices.

As can be seen in Fig. 3, the spin configuration at the center of a vortex of the ferromagnetic $XY$ system is locally antiferromagnetic, therefore we expect these vortices to trap charges, in the same way that the antiferromagnet with Ising anisotropy had them localized. The Coulomb repulsion between the vortex charges is overcome by the logarithmic [12] attraction between vortices and one obtains vortex pairs with short center-to-center separations. Our model also indicates that the spins of the charges pinned by the vortices would point in opposite directions in a vortex-antivortex pair. Thus, under the above considerations, our model leads in a natural way to a magnetic mechanism for the pairing of charges in doped $La_2CuO_4$. Superconductivity may be derived now from the application of Bardeen-Cooper-Schrieffer theory to these circumstances, or, alternatively, from Bose condensation of the vortex pairs dressed with charges. The critical temperature $T_c(x)$ for the onset of superconductivity does not necessarily coincide with that for the Kosterlitz-Thouless transition. This latter transition refers only to the pairing of charges and it may appear broadened due to the weak interlayer couplings. Because the pairing of charges in our model has been linked to the appearance and permanence of $XY$ anisotropy for a range of dopant fractions, and this in turn has been related to: i) the mobility of the charges in a ferromagnetic background, and, ii) the buckling of the $CuO_2$ planes and the ensuing orthorhombicity and canting of spins, the variation of the critical temperature $T_c$ for the onset of superconductivity will be expected to become different from zero at $x = x_0$, then increase with $x$, but when the O-T phase boundary is approached, it should begin to decrease and then vanish again from there on. This agrees with experiment (Fig. 1).

## 6. Summary

We have presented a model of spins and holes for weakly coupled $CuO_2$ planes with which we represent the main known features of the copper-oxide superconductors. We have especialized our description to the particular case of the $La_2CuO_4$-based family of compounds, but we believe that the main ideas can be applied to the case of the 123 superconductors, and when more information becomes available, also to the more recently discovered Bi- and Tl-based superconductors. Our model has elements in common with those outlined in Refs. [1] and [2] and with the analogous results of the calculations carried out in Ref. [4]. However, it explores the thermodynamic consequences of an important additional ingredient, the anisotropy of the superexchange interaction that has its origin in the orthorhombic strain of the crystal. This, together with the consideration that doping can not only change the sign of the magnetic couplings for Cu spins but also the degree and type of anisotropy of the underlying Heisenberg Hamiltonian leads to a specific magnetic mechanism for the pairing of charges that differs from those proposed in Refs. [1,2] and [4].

According to our model, if holes are firmly trapped, as it is the case of the insulating low dopant fraction limit, we obtain a Heisenberg model with Ising anisotropy where one has a random distribution of AF and F couplings, and the thermodynamic behavior is reminiscent of that of binary alloys when an AF component is diluted with F impurities. On the other hand, if holes are considered to be highly mobile, as it is the case of the highly-doped conducting phase, the model system is better represented by uniform average couplings with values that depend on the dopant fraction. These average couplings have F character and the associated Heisenberg Hamiltonian adopts $XY$ anisotropy. Thus, the picture that we endorse for the $CuO_2$ superconductor is one of a close realization of the $2D$ Heisenberg model with a small degree of anisotropy that can be manipulated either way, Ising or $XY$, with doping (or with temperature). The model reproduces all the phase boundary features shown in Fig. 1 (here only within the mean-field approximation, or via heuristic arguments). The key element in this diagram is the critical dopant fraction $x_0$ at which the correlation length vanishes, our contention is that at $x_0$ the system switches from AF to F character, from Ising to $XY$ anisotropy, and from an electrical insulator to a conductor. Superconductivity is taken to originate in the magnetic interactions taking place in the $CuO_2$ planes. Despite the repulsion between conduction charges, these can be paired via the net attraction of the vortex excitations to which they become associated. There is already some recorded [15] experimental evidence pointing to Kosterlitz-Thouless behavior in the resistive transition in 123-type materials. However, more measurements relevant to the specific mechanism proposed are required in this and the other copper oxide superconductors. Also, some of our assumptions about the relationship between the symmetry of the Hamiltonian with orthorhombicity and with the degree of doping, as well as our conclusions in relation to the phase diagram and the pairing of charges, need to be derived with more care and detail. The anomalous variations and discontinuities of the lattice parameters observed in these systems [6,7] may have a role in the enrichment or modification of the points of view presented here.

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**Resumen.** Construimos un modelo de espines y huecos que representan planos de $CuO_2$ para estudiar los diagramas de fases temperatura vs. concentración de drogado de los compuestos $La_2CuO_4$ y $YBa_2Cu_3O_6$. Suponemos acoplamientos antiferromagnéticos entre momentos magnéticos del Cu para el sistema sin drogar con una anisotropía débil de Ising y canteado. La creación de huecos, localizados en las posiciones de los oxígenos, inducen una transformación de acoplamientos de naturaleza antiferromagnética a ferromagnética. El drogado progresivo reduce la temperatura de Néel y genera comportamiento de vidrio de espín. La transición aislante-metal ocurre cuando las correlaciones en la fase paramagnética cambian de carácter antiferromagnético a carácter ferromagnético y la longitud de correlación se anula. En esta situación, cuando cambia de signo el acoplamiento de intercambio isotrópico promedio, el sistema genera anisotropía XY canteada, y las excitaciones magnéticas de tipo vórtice capturan cargas móviles y el apareamiento de éstas toma lugar por medio del mecanismo de Kosterlitz y Thouless.