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# MAGNETIC PHASES AND POSSIBLE MAGNETIC PAIRING IN DOPED LANTHANUM CUPRATE

Amnon AHARONY[1-3], R. J. BIRGENEAU[1], A. CONIGLIO[2], M. A. KASTNER[1] and H. E. STANLEY[2]

[1]Physics Department, Massachusetts Institute of Technology, Cambridge, MA, 02139, USA, [2]Physics Department, Boston University, Boston, MA, 02215, USA, and [3]School of Physics and Astronomy, Tel Aviv University, Tel Aviv 69978 Israel

We discuss the temperature-concentration (T-x) phase diagram of $La_{2-x}(Sr_1Ba)_xCuO_4$. The magnetic interactions of the hole spins with the Cu spins yield frustration, explaining the fast decrease in the Néel temperature and yielding a new spin glass phase. The same interactions yield a strong attractive hole-hole potential, which can lead to pairing and superconductivity.

## 1. INTRODUCTION

Both $La_{2-x}(Sr,Ba)_xCuO_{4-\delta}$ and $YBa_2Cu_3O_{6+\delta}$ exhibit antiferromagnetism (AF), with high Néel temperatures, at low doping, and superconductivity (SC), at higher doping. In both cases, there exist strong AF exchange interactions (J~1100 K) between the Cu spins in the $CuO_2$ planes. The possible relevance of magnetism to the SC is thus a topic of much current research.

Since we believe the physics of the two classes of high $T_c$ superconductors is the same, we discuss the simpler case of $La_{2-x}Sr_xCuO_4$, which exhibits the T-x phase diagram shown (schematically) in Fig. 1. Given

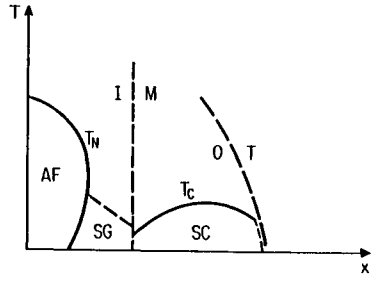


FIGURE 1
Temperature-concentration phase diagram (AF=antiferomagnetic, SG=spin glass, I=insulator, M=metal, O=orthorhombic, T=tetragonal, SC=superconducting).

the experimental fact that for $x \leq 0.05$ the holes are localized (1) on the $O^-$ ions (2,3), we show in Sec. 2 that each hole generates a strong local ferromagnetic (F) Cu-Cu interaction, which competes with the otherwise AF exchange. The consequences of this frustration on the T-x phase diagram are then discussed in Sec. 3.

## 2. FRUSTRATION

For small x, the random potential localizes the extra holes within a localization length $l_0$ of order (2-3)a (1). $l_0$ probably grows gradually as x approaches the I-M transition. There is also evidence that the holes are on the $O^-$ ions (2,3).

Consider first an instantaneous configuration, with the hole on one $O^-$ site. The spin of the hole, $\vec{\sigma}$ will have strong exchange interactions with the two neighboring Cu spins $\vec{S}_1$ and $\vec{S}_2$. Writing $H=-J_\sigma \vec{\sigma} \cdot (\vec{S}_1 + \vec{S}_2)$, it is intuitively clear that, regardless of the sign of $J_\sigma$, the ground state of $H_\sigma$ prefers $\vec{S}_1 \| \vec{S}_2$. Quantum mechanically, the exact ground state of $H_\sigma$ (neglecting the couplings to other Cu spins) indeed has $S_{12}=1$ (where $\vec{S}_{12} = \vec{S}_1 + \vec{S}_2$), i.e. $\langle \vec{S}_1 \cdot \vec{S}_2 \rangle = 1/4$ (4). It is thus reasonable to replace $H_\sigma$ by an F interaction, $\tilde{H}_\sigma = -K(\vec{S}_1 \cdot \vec{S}_2)$, where $K=O(|J_\sigma|) >> |J|$ ($|J_\sigma| >> |J|$ because the Cu-Cu distance is twice that of Cu-O). This replacement is exact for classical spins at low temperatures (4).

Since a strong F bond in the $CuO_2$ plane destroys the local AF order, it also influences the coupling to the neighboring planes. The Cu spins thus feel competing AF and F interactions. Each F interaction arises from one hole sitting on a Cu-O-Cu bond. In the extremely localized case, the concentration of these F bonds would be x. However, for a finite localization length $l_0$, the holes are shared by $(l_0/a)^2$ bonds, hence the F-bond concentration is of order $x(l_0/a)^2$. This is of order 10x for small x, and increases as the I-M transition is approached.

## 3. PHASE DIAGRAM

Competing AF and F interactions are known to yield a sharp decrease in $T_N$, a spin glass (SG) phase (5) and a re-entrance from the AF to the SG phase upon cooling, because of frozen random local moments (6). This yields the magnetic parts of Fig. 1. In the isostructural $K_2Cu_xMn_{1-x}F_4$, the Cu ferromagnetism is lost at $x \simeq 0.8$ (7), corresponding to a concentration 0.36 of the very weak Cu-Mn and Mn-Mn AF bonds. Renormalizing this by $(l_0/a)^2$, and remembering that we have $K >> |J|$, explains why in $La_{2-x}Sr_xCuO_4$ thw SG phase appears at $x \simeq 0.02$ (8,9).

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Both the re-entrance (10) and the existence of frozen spins at low T for $.02 \le x \le .05$ (8,9) have now been confirmed experimentally.

## 4. PAIRING POTENTIAL

A strong F bond between two Cu spins turns them parallel, against the AF coupling to the other Cu spins. The details of the resulting spin configuration depend on the symmetry of the spins. At low temperatures, the spins order along the orthorhombic c axis, indicating a weak Ising anisotropy (11). Assuming this anisotropy dominates the ground state, the K-bond will simply flip one of its spins (Fig. 2a), with an energy gain of $(K-7|J|)S^2$ (compared to the AF state without the hole).

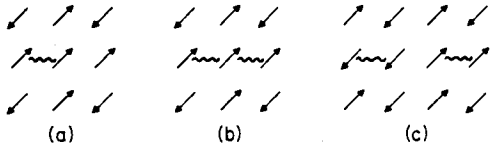


FIGURE 2
Ising ground state with (a) One K bond (wiggly line), (b) Two nn K bonds, (c) Two nnn K bonds.

When two K bonds are placed next to each other (Fig. 2b), flipping the central spin yields a gain of $(2K-6|J|)S^2$, which is larger by $8|J|\,S^2 = 2|J|$ than that of two isolated holes. This implies an attractive potential energy between the holes. Similarly, a gain of $4|J|\,S^2 = |J|$ results for next nearest neighbor bonds (Fig. 2c). Comparison of Figs. 2b and 2c shows, however, that the two hole spins are parallel (triplet) in the former, and antiparallel (singlet) in the latter.

In the Ising case, similar arguments can be applied to each of the 22 neighboring bonds shown in Fig. 3. The singlet state is unfavorable for the six bonds denoted 1,2, and favorable (with energy gain $|J|$) for the remaining 16 bonds. A similar, albeit weaker, attraction will occur between neighboring planes.

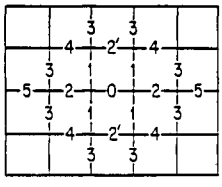


FIGURE 3
Neighboring K bonds: All except 1,2 attracted to 0.

We next consider the Coulomb repulsion. Using a Thomas-Fermi estimate, we find a bare screening length of 1-2Å, yielding a repulsion of ~.04eV at 6Å, assuming a dielectric constant ~10. This is much smaller than the effective attraction there, $|J|$~.12eV.

So far, we have calculated the attractive energy of K bonds in a completely ordered AF background. In fact, for $x>0.05$ the AF correlation length decays as $\xi \sim 3.78x^{-1/2}$ (12). Thus, the above attractive interaction is reduced by a factor $\exp(-r/\xi)$, causing a decrease of the attractive energy.

An attractive potential for singlet pairing can also be derived when the spins have XY or Heisenberg symmetry. Instead of the finite range potential derived above, one obtains a dipole-dipole potential, which decays as $1/r^2$, with an oscillation $\exp(i\vec{Q}\cdot\vec{r})$, where $\vec{Q} = (\pi/a, \pi/a)$ (4). Since the factor $\exp(-r/\xi)$ eliminates the distant K-bonds, the resulting potential is qualitatively similar to the one discussed above, i. e. repulsion at bonds 1,2 and attraction at bonds 2',3,5.

## 5. SUPERCONDUCTIVITY

Having established a strong attractive potential between the holes, one can then find either real space bound pairs, which undergo Bose condensation, or correlated BCS pairing. $T_c$ should grow from zero above the I-M transition, with the number of mobile holes, and then decrease due to the decrease in $\xi$. This qualitatively agrees with the shape of $T_c(x)$ in Fig. 1. A more detailed discussion of the consequences of our model to superconductivity will be given in Ref. (12).

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