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LETTER TO THE EDITOR

An effective spin model for the magnetism of oxide superconductors

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Abstract. Assuming localized Cu^{++} magnetic moments to survive for low enough doping in systems like $La_{2-x}Sr_xCuO_4$, an effective spin model is constructed in order to understand the magnetic structures characterizing the CuO_2 planes. A field-theoretic treatment calls for two separate non-linear-σ-model descriptions, below and above a specific threshold in doping, within which the fluctuations of magnetic correlations can be properly accounted for. An interesting new mechanism for superconductivity might ensue within a faithful, though qualitative, description of the phase diagram.

A successful model and mechanism for high-temperature superconductivity must account for the peculiar magnetic properties of the novel oxide superconductors [1,2]. In the more controlled systems of the $La_{2-x}Sr_xCuO_4$ family, it is found that distinct incommensurate magnetic structures characterize the spin fluctuations in the CuO_2 planes for dopings above the superconducting threshold $\delta_s \sim 0.05$. At the same time, no incommensurate structure is detected by neutron-scattering experiments below δ_s. The existence of such threshold behaviour for incommensurate 'spiral' spin phases contrasts with the mean-field explanations offered by existing $t-J$ model calculations [3]. In this letter it is argued that further understanding can be gained by abandoning itinerant electronic model calculations for an effective long-range spin-model analysis that can more efficiently take into account the fluctuations of the doped antiferromagnetic (AFM) background. The spin-off of such models might be the identification of a novel Cooper pair formation mechanism mediated by the quantum of a field associated with the frustration of the background itself.

Consider a doped CuO_2 plane and imagine that the itinerant hole degrees of freedom are neglected, *except* for their frustrating effects on the background of the localized Cu^{++} spins. If $\delta = 0$ this reduces to a nearest-neighbour quantum Heisenberg superexchange Hamiltonian, which has been demonstrated to correctly account for the spin fluctuations within the La_2CuO_4 magnetic planes [4]. When $0 < \delta \ll 1$ many arguments [5] suggest that the motion of holes in the AFM background induces trails of frustrated bonds which, in some mean-field sense, results in a spiral spin structure having incommensurate inverse pitch $\Delta \propto \delta$ [3]. Such a mean-field structure of the spins can be immediately accounted for by making use of an effective frustrated

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quantum Heisenberg Hamiltonian:

$$\mathcal{H} = -\frac{1}{2}\sum_{i,j} J_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j = -\frac{1}{2}J\sum_{<ij>}\boldsymbol{S}_i\cdot\boldsymbol{S}_j - \frac{1}{2}\sum_{i,j}\mathcal{J}_{ij}\boldsymbol{S}_i\cdot\boldsymbol{S}_j \tag{1}$$

where the $\boldsymbol{S}_i$ are the quantum $s = \frac{1}{2}$ Cu^{++} spins on a square lattice, $J < 0$ is the nearest-neighbour superexchange coupling and $\mathcal{J}_{ij}(\delta)$ is a suitably long-range further-neighbour interaction mimicking the frustrating effect of hole motion. A proper, yet problematic, derivation of the form of $\mathcal{J}_{ij}$ should follow from an appropriate realistic multi-band itinerant model containing both spin and charge degrees of freedom. However, here I take the stance that a phenomenological model is needed in order to make further progress, perhaps justifying the form proposed below as corresponding to some indirect oscillating RKKY-type interaction [6] between the localized spins mediated by the mobile vacancies and appropriate for the two-dimensional geometry. Fine details of the interaction should not qualitatively change the conclusions of this work; in the worst possible scenario, the following is just an interesting statistical-mechanics model. Denoting by the integer coordinates (l, m) a certain shell of neighbours of a given spin, and by $\nu(l, m)$ (= 4 or 8) its coordination number, I consider the model

$$\mathcal{J}_{0,0;l,m}(\delta) = (-1)^{l+m}\frac{4CJ\delta^2}{\nu(l,m)\sqrt{l^2+m^2}} \tag{2}$$

for $l^2 + m^2 > 1$ and with $\mathcal{J} = 0$ for $a\sqrt{l^2+m^2} > \Lambda(\delta)$, with Λ a suitably divergent range of the interaction for $\delta \to 0$. Hence, there is an oscillating effective $\sim \delta^2/r$ type interaction with C some positive constant and a the lattice spacing. For small δ the classical mean-field spin configuration appropriate for the model will be an incommensurate spiral defined in an arbitrary plane and deviating slightly from perfect Néel ordering. With the classical parametrization

$$\boldsymbol{\sigma}(\boldsymbol{R}_i) = s\big(\hat{\boldsymbol{x}}_1\cos(\boldsymbol{k}_0\cdot\boldsymbol{R}_i+\theta) + \hat{\boldsymbol{x}}_2\sin(\boldsymbol{k}_0\cdot\boldsymbol{R}_i+\theta)\big)$$

for the spin, the incommensurate spiral wavevector $\boldsymbol{k}_0$ maximizes $J(\boldsymbol{k}) = \sum_j J_{ij}\exp(\mathrm{i}\boldsymbol{k}\cdot\boldsymbol{R}_{ij})$ [7]. Calculating to the appropriate lowest order in δ, a true maximum is found for $\boldsymbol{k}_0 = \pi/a \pm \boldsymbol{\Delta}$ with the inverse spiral pitch $\Delta \simeq \delta/a$ for model (2).

Though the mean-field structure of [3] is thus recovered, the task now is to study its stability to quantum and thermal fluctuations. This can be done by means of an efficient path-integral approach to the non-linear-σ-model description of the low-energy spin dynamics [8, 9]. The quantum partition function $\mathcal{Z} = \int\mathcal{D}\sigma\exp(-\mathcal{S})$ calls for the low-temperature ($\beta = 1/k_BT \to \infty$) arbitrary-$s$ effective action for the classical local magnetization field $\boldsymbol{\sigma}_i(\tau)$

$$\mathcal{S} = \frac{1}{2}\int_0^\beta \mathrm{d}\tau\sum_i\boldsymbol{\sigma}_i\cdot\boldsymbol{\Omega}_i - s\int_0^\beta\mathrm{d}\tau\sum_i\big[|\Omega_i| - \mathrm{i}A(\Omega_i)\cdot\partial_\tau\Omega_i - \mathcal{M}_{\mu\nu}(\Omega_i)\partial_\tau\Omega_i^\mu\partial_\tau\Omega_i^\nu + \cdots\big]. \tag{3}$$

Here $\boldsymbol{\Omega}_i = \sum_j J_{ij}\boldsymbol{\sigma}_j$ is the fluctuating 'molecular field' and the dots stand for higher-order terms in the 'fictitious time' derivative expansion. Also, A is Dirac's magnetic monopole potential ($\epsilon^{\mu\nu\lambda}\partial_{\Omega_\lambda}A_\nu(\Omega) = \Omega_\mu/|\Omega|^3$), associated with Berry's phase

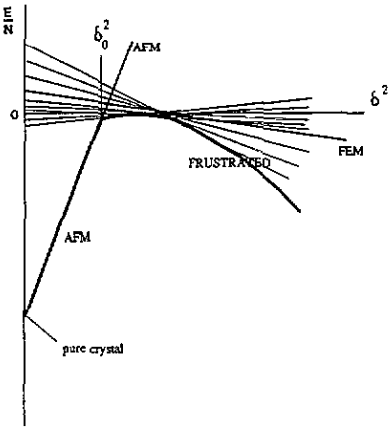

Figure 1. Ground-state energy plot versus doping for the Ising version of Hamiltonian (1) and (2). AFM and FEM refer to the antiferromagnetic and ferrimagnetic ordering, while the intermediate curves should correspond to finite concentrations of frustration vortices and antivortices.

and possibly giving rise to a topological term in the continuum limit action, while $\mathcal{M}_{\mu\nu}(\Omega) = (1/2|\Omega|^3)(\delta_{\mu\nu} - \Omega_\mu\Omega_\nu/|\Omega|^2)$. In order to work with a smooth spatially varying order-parameter field $\boldsymbol{n}_i(\tau)$, one can fix the arbitrary θ phase, chirality and plane of the spiral [9, 10] and make use of the transformation $\boldsymbol{\sigma} = s\mathcal{R}\boldsymbol{n}$, with

$$\mathcal{R}_i(\tau) = \begin{pmatrix} \cos\big((i_x + i_y)(\pi + \Delta a)\big) & -\sin\big((i_x + i_y)(\pi + \Delta a)\big) & 0 \\ \sin\big((i_x + i_y)(\pi + \Delta a)\big) & \cos\big((i_x + i_y)(\pi + \Delta a)\big) & 0 \\ 0 & 0 & \mathcal{R}_i^{33}(\tau) \end{pmatrix}. \tag{4}$$

For $\boldsymbol{n} = (n^1, n^2, 0)$ uniform (with $|\boldsymbol{n}| = 1$) the above matrix reproduces the classical spiral ground state, so the in-plane fluctuations can all be described by the dynamics of $\boldsymbol{n}_i^{\|}(\tau)$. But the off-plane spin fluctuations are not imposed by the ground state and need not necessarily be of the staggered form characterizing the $\delta = 0$ system.

To understand which type of off-plane mode presents the lowest excitation energy, consider the Ising ground-state problem associated with Hamiltonian (1), (2). As $\delta \to 0$ one expects the standard staggered AFM arrangement to hold, but for sufficiently high δ a uniformly frustrated configuration such as the ferrimagnetic (FEM) will set in, as shown in figure 1. Also in this figure, energy curves for more complicated Ising ground states characterized by non-uniform frustration field configurations [9] are reported for this model; each curve might correspond to a different density of the frustration vortices depicted in figure 2 (a),(b). Back to the full quantal Heisenberg Hamiltonian, one can imagine that the off-plane fluctuations of σ_i^3 will follow the standard AFM arrangement with $\mathcal{R}_i^{33} = (-1)^{i_x+i_y}$ up to the threshold δ_0 in doping where the frustration field $\boldsymbol{w}$ will set in (figure 1). For $\delta > \delta_0$ the off-plane fluctuations will be organized by the fluctuating field $\boldsymbol{w}_i(\tau)$ through $\mathcal{R}^{33} = (-1)^{\phi[\boldsymbol{w}]}$, where ϕ is an appropriate mod(2) integer mapping out the $\boldsymbol{w}$-field configuration. All the discontinuous lattice variations of $\boldsymbol{\sigma}_i$ are now absorbed in the O(3) matrix $\mathcal{R}$, while the (highly singular) $\delta = 0$ limit form $\mathcal{R}_i = (-1\!\!1)^{i_x+i_y}$ is recovered. Since $\boldsymbol{n}_i(\tau)$ is slowly varying, one can now expand over several neighbour shells in this field to obtain the continuum-limit action from (3) to lowest suitable order in δ.

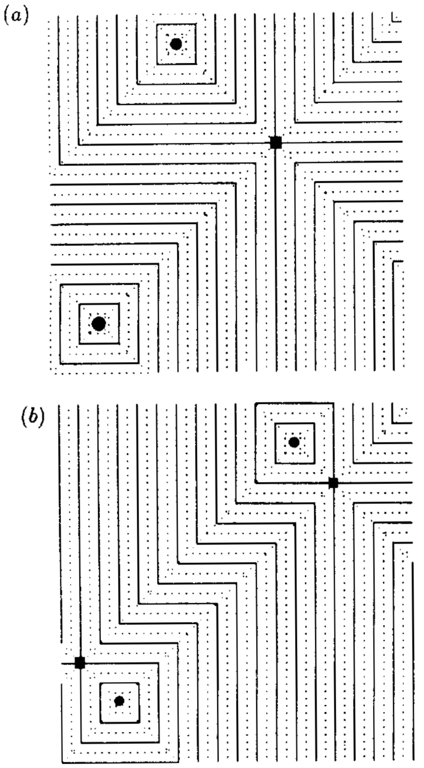

Figure 2. w-field vortex configurations. (a) low doping; (b) higher doping ($\delta > \delta_s$), with the formation of vortex–antivortex lattice pairs. $\mathcal{R}^{33}$ is (say) +1 on full and −1 on broken lines.

Drastically different non-linear-σ-model actions are obtained (the constraint $|\boldsymbol{n}(x,y,\tau)| = 1$ is always recovered) according to whether $\delta - \delta_0 < 0$ or $\delta - \delta_0 > 0$. For $\delta < \delta_0$ (no off-plane frustration) there is no topological term and the effective action is

$$\mathcal{S}_<[\boldsymbol{n}] = \frac{1}{2g_0}\int_0^\beta \mathrm{d}\tau \int \mathrm{d}^2\boldsymbol{r}\left((\nabla\boldsymbol{n})^2 + \frac{1}{c^2}(\partial_\tau\boldsymbol{n})^2 + m_0^2(\boldsymbol{n}^{\parallel})^2\right) \tag{5}$$

with the following doping dependence of the parameters:

$$\begin{aligned} g_0^{-1} &= s^2|J|\cos(\Delta a)\left(1 - \frac{1}{|\ln\delta|^3} + \cdots\right) \\ c &= 2as|J|\cos(\Delta a)\left(1 - \frac{1}{2|\ln\delta|^3} + \cdots\right) \\ m_0^2 &= 4a^{-2}(1-\cos(\Delta a))(1+\cdots) \simeq 2\Delta^2 \end{aligned} \tag{6}$$

and the quantities in brackets arising from the long-range part of the Hamiltonian. A dependence $\Lambda(\delta) \sim \delta^{-2/3}/|\ln\delta|$ for the $\mathcal{J}$ interaction range has been taken in deriving the above forms. Many important observations should be drawn from (5) and (6). First, doping generates a uniaxial anisotropy such that at distances greater than a crossover length of the order of the spiral's pitch, $\lambda \sim \Delta^{-1} \gg a$, the spin ordering is dominated by an Ising fixed point. Hence, the incommensurate spiral of [3] is destroyed by quantum and thermal fluctuations; this is probably why incommensurate order has not been observed at low doping in real oxides. Moreover, there is softening of the spin-wave motion with increasing δ while the true dimensionless coupling constant $u_0(\delta)$ increases rapidly by the effect of long-range tail corrections:

$$u_0(\delta)a = g_0 c = \frac{2a}{s}\left(1 + \frac{1}{2|\ln\delta|^3} + \cdots\right). \tag{7}$$

Hence, as shown in figure 3(*a*), where the large-distance phase diagram for $\mathcal{S}_<$ is sketched, there will be rapid disordering of the spin layer with increased doping and a corresponding rapid drop of both the two- and three-dimensional Néel temperature $T_N(\delta)$, as observed in real systems. The prediction here is that, bearing in mind the crossover, T_N is an Ising AFM critical point.

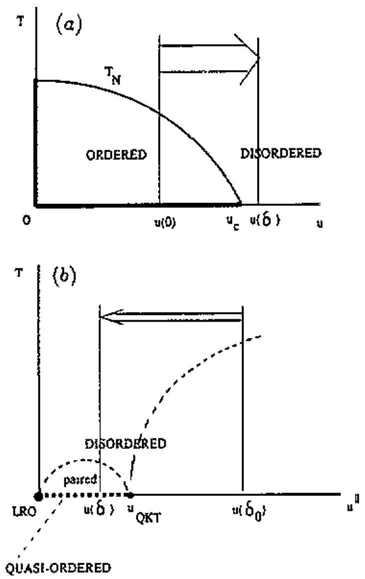

Figure 3. Large-scale fixed point phase diagrams. (*a*) the $\mathcal{S}_<$ case, where the rapid growth of $u(\delta)$ destroys (Ising) antiferromagnetism. (*b*) the $\mathcal{S}_>$ case, where the slow drop of $u(\delta)$ recovers pair formation within a latent XY magnetic structure.

For $\delta > \delta_0$ (when real frustration sets in) there are non-trivial topological terms and the effective action, within a dilute frustration vortex approximation, is

$$\mathcal{S}_>[\boldsymbol{n}, \boldsymbol{w}] = \frac{1}{2g_0^{\|}} \int_0^{\beta} \mathrm{d}\tau \int \mathrm{d}^2 r \left[(\nabla \boldsymbol{n}^{\|})^2 + \frac{g_0^{\|}}{g_0^{\perp}} \left(-(\partial_w n^{\perp})^2 + (\partial_v n^{\perp})^2 \right) + m_0^2 (n^{\perp})^2 + \frac{1}{c^2} (\partial_\tau \boldsymbol{n})^2 \right] + \mathrm{i}\mathcal{S}_B[\boldsymbol{n}, \boldsymbol{w}] \tag{8}$$

with the following doping dependence of the parameters:

$$g_0^{\perp\,-1} = s^2 |J|$$

$$g_0^{\|-1} = 2A\delta^2 s^2|J|(1 + K\delta^{4/3} + \cdots)$$
$$c = \sqrt{8}A\delta^2 sa|J|(1 + \tfrac{1}{2}K\delta^{4/3} + \cdots) \tag{9}$$
$$m_0^2 = 2a^{-2}(1 - K\delta^{4/3} + \cdots)$$

where $K \simeq C^{2/3}$ and $A \ll 1$ is a virtually doping-independent positive constant. Since $g_0^{\|}/g_0^{\perp} > 0$, the above action is exactly of the type found for the triangular-lattice Heisenberg AFM [9]; w and v are cartesian coordinates attached to the local $\boldsymbol{w}$-field direction. Doping for $\delta > \delta_0$ results in completely novel structures (though the large-distance behaviour of (8) is lamentably not completely understood). First, an easy-plane anisotropy is generated such that at distances greater than a short crossover length $\lambda \sim a(1 + \frac{1}{2}K\delta^{4/3})$ the spin ordering is dominated by an XY fixed point. The incommensurate spiral is now stable to quantum and thermal fluctuations and could be observed in a scattering experiment [1]. However, there is simultaneously a crossover to reduced (1+1) dimensionality owing to strong high-momentum fluctuations of $\boldsymbol{n}$ in the direction of the frustration field $\boldsymbol{w}$ which thus gets renormalized away. The true large-distance fixed point is the (1+1)-dimensional XY, and the associated phase diagram for $\mathcal{S}_>$ is sketched in figure 3(*b*). Moreover, there is a re-stiffening of the in-plane spin-wave motion with increased δ while the dimensionless coupling constant $u_0(\delta)$ changes to show a slow decrease

$$u_0(\delta)a = g_0^{\|}c = \frac{\sqrt{2}a}{s}(1 - \tfrac{1}{2}K\delta^{4/3} + \cdots). \tag{10}$$

Depending on the details of the model, the following scenario may occur, as shown in figure 3(*b*). At first the ground state is a disordered spin liquid with free magnetic and frustration vortices, the latter, like in figure 2(*a*), living apart on the physical layer. But above a second $T = 0$ threshold δ_s (corresponding to a 'quantum' Kosterlitz–Thouless transition) $u_0(\delta)$ enters a region characterized by a power-law correlated spin liquid with the formation of pairs of both magnetic and frustration vortices, the latter associated in pairs like in figure 2(*b*). Vortex pairs exist below a crossover curve in the u–T phase diagram, which the coupling between CuO_2 layers will transform in a true transition curve. Although there are no charge degrees of freedom in this model as such, one could show that the $T = 0$ concentration of vortices is given exactly by δ. In addition, each vortex, be it magnetic or frustration in type (the two go together), carries a topologically generated spin $\pm\frac{1}{2}$ for half-integer spin s. This because the topological term $\mathcal{S}_B$ in (8) generates one (1+1)-dimensional Pontryagin density term [8] for each frustration vortex of a $\boldsymbol{w}$-configuration like in figure 2. This is in line with the effective large-scale (1+1)-dimensional nature of the fixed-point behaviour. Hence, it is tempting to associate a hole with each frustration vortex living in the AFM background, which can now be thought of as the perturbation in the Cu^{++} spins 'dug out' by a mobile vacancy [11]. The crossover curve of figure 3(*b*) then becomes the transition for 'Cooper pair' formation, and its doping dependence looks qualitatively right for real oxides. The attraction between holes is magnetic and is mediated by the quantum of the frustration field $\boldsymbol{w}$ (the 'frustron'). The coherence length ξ will be of the order of the average separation between vortex centres; it is clear from figure 2(*b*) that pair motion will be highly correlated.

In conclusion, on the basis of the analysis above, I would expect the δ–T phase diagram shown in figure 4. With suitable inclusion of disorder (e.g. a random spatial distribution of δ), a small RKKY-type interaction such as (2) should generate a

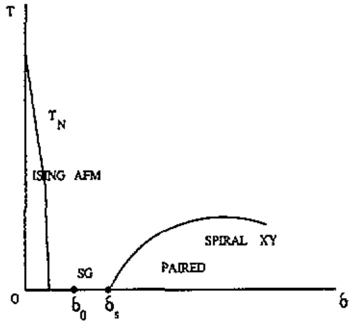

Figure 4. Qualitative phase diagram proposed for the present model.

low-temperature spin-glass phase. Figure 4 is in complete qualitative agreement with experimental findings for the $La_{2-x}Sr_xCuO_4$ family of oxide superconductors [2], particularly where magnetism is concerned [1]. Further quantitative understanding of the present approach is within reach, although a proper treatment and quantization of the field w is yet to be developed. The form (2) for the long-range spin interaction is clearly too naive to quantitatively account for the properties of real systems. Further work is in progress and will be reported in due course, together with the details of the present calculations adapted for a realistic model of the cuprate superconductors.

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