Doped Planar Quantum Antiferromagnets with Striped Phases

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We study the properties of the striped phases that have been proposed for the doped cuprate planar quantum antiferromagnets. We invoke an effective, spatially anisotropic, nonlinear sigma model in two space dimensions. Out theoretical predictions are in *quantitative* agreement with recent experiments. We focus on (i) the staggered magnetization at $T = 0$ and (ii) the Néel temperature as functions of doping; these have been measured recently in $La_{2-x}Sr_xCuO_4$ with $0 \leq x \leq 0.018$. Good agreement with experiment is obtained using parameters determined previously and independently for this system. These results support the proposal that the low doping (antiferromagnetic) phase of the cuprates has a striped configuration.

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Our understanding of the *undoped* planar cuprates related to high temperature superconductors has been informed largely by the insights of Chakravarty, Halperin, and Nelson [1] (hereafter, CHN). It is now widely accepted that the antiferromagnetic phase of these materials can be well described by an effective nonlinear sigma model. However, the situation is not so clear when we turn to the behavior of doped systems, as the antiferromagnetic moves toward a superconducting instability. It has long been recognized [2,3] that there is a tendency for the holes to phase separate in these strongly correlated insulators. Experimental observations [4] support this scenario for some of the La cuprates at high concentrations of dopants. In addition, recent nuclear quadrupole resonance (NQR) and muon spin resonance (μSR) experiments [5] in $La_{2-x}Sr_xCuO_4$, with $0 \leq x \leq 0.018$, have been interpreted within a picture where holes are segregated into a set of parallel stripes. It is the primary goal of this Letter, in fact, to do a more careful theoretical analysis of the consequences of that model and to compare the predictions to those experiments.

With the x-y coordinate axes chosen as the crystal axes in the CuO_2 plane, we take an array of equivalent uniformly spaced stripes parallel to the y axis. In this simplest of models we neglect both static and dynamic fluctuations (and domain formation). The situation is not very different if we consider diagonal stripes, such as the ones found in $La_2NiO_{4.125}$ and $La_{1.8}Sr_{0.2}NiO_4$ [6]. But here we will treat only the horizontal stripe geometry suggested for $La_{2-x}Sr_xCuO_4$ by the experimental data [7]. In the regions between the stripes, the Cu spin correlations are presumed to remain antiferromagnetic.

As in the CHN analysis [1] of the pure case, we will argue that the underlying symmetries suggest an appropriate nonlinear sigma model to describe the long wavelength behavior which determines the phase diagram. We start from a microscopic model with the spins interacting via Heisenberg antiferromagnetic exchange in the regions between stripes, and by a weaker such exchange across each stripe. Conceptually, we use real space renormalization in the x direction to integrate out the short distance dynamics, starting with blocks the size of the region between stripes. This is continued to a scale of the correlation length, much larger throughout the region of interest to us than the interstripe spacing. The expected leading result for the low frequency dynamics in which we are interested is a spatially anisotropic nearest neighbor Heisenberg exchange model,

$$H = J_y \sum_{n,\langle m,m'\rangle} \vec{S}(n,m) \cdot \vec{S}(n,m') + J_x \sum_{m,\langle n,n'\rangle} \vec{S}(n,m) \cdot \vec{S}(n',m), \qquad (1)$$

where n and m label the sites in the x and y directions, respectively. J_x and J_y are the effective spin exchange strengths in the two directions. In general they depend on the doping x, but the exact form of that dependence relies, of course, on microscopic details.

The destruction of long-range order at zero temperature and the suppression of the staggered magnetization with increased hole then come about from the dimensional crossover from two- to one-dimensional behavior with the increasing anisotropy of the system (in our effective σ model the critical coupling constant g_c, which separates ordered from disordered behavior at $T = 0$, decreases with doping). At the same time, the renormalized spin stiffness decreases as the density of holes grows. As $g_c(x)$ decreases it equals at some critical concentration x_c the coupling constant of the undoped system, and antiferromagnetism disappears.

To simplify the study of the long wavelength physics, it is convenient to take the continuum limit of (1). We use the usual spin coherent state representation [8] and we find that the effective action (in Euclidean time) in the

partition function can be written as

$$S_{\rm eff} = \frac{1}{2}\int_0^{\beta\hbar} d\tau \int dx \int dy \Big\{ S^2[J_y(\partial_y \hat{n})^2 + J_x(\partial_x \hat{n})^2] + \frac{\hbar^2}{2a^2(J_x + J_y)}(\partial_\tau \hat{n})^2 \Big\}, \tag{2}$$

where $\hat{n}$ is a unit vector and a is the sublattice constant. This gives spin wave velocities $c_y^2 = 2S^2a^2J_y(J_x + J_y)/\hbar^2$ and $c_x^2 = 2S^2a^2J_x(J_x + J_y)/\hbar^2$, which agree with a simple (noninteracting) spin wave calculation based on (1). This action was studied numerically in a different context a few years ago [9].

It is useful to rewrite (2) more symmetrically by a dimensionless rescaling of the variables: $x' = (J_y/J_x)^{1/4}x\Lambda$, $y' = (J_x/J_y)^{1/4}y\Lambda$ (Λ is a momentum cutoff), and $\tau' = \sqrt{2(J_x + J_y)\sqrt{J_xJ_y}}\, Sa\tau/\hbar$. Then the effective action (2) becomes

$$S_{\rm eff} = \frac{\hbar}{(2g_0)}\int_0^{\hbar\Lambda\beta c_0} d\tau' \int dx' \int dy' \,(\partial_\mu \hat{n})^2, \tag{3}$$

where μ takes the values x', y', τ', $g_0 = \hbar c_0\Lambda/\rho_s^0 = [2(J_x + J_y)/\sqrt{J_xJ_y}\,]^{1/2}a\Lambda/S$ is the bare coupling constant, $c_0 = [2(J_x + J_y)/\sqrt{J_xJ_y}\,]^{1/2}aS/\hbar$ the spin wave velocity, and $\rho_s^0 = \sqrt{J_xJ_y}\,S^2$ the classical spin stiffness of the rescaled model. The original anisotropy is now hidden in the limits. We started with a problem with a finite bandwidth, a lower bound on length which requires us to impose a cutoff in the original continuum formulation. The change of variables introduces an anisotropy in the cutoffs.

The σ model action, and the spin correlations it implies, can be studied in the large N limit (N is the number of components of $\hat{n}$), where a saddle point approximation becomes exact [10,11]. The staggered spin-spin correlation function is given by $\Xi(\vec{k}, \omega_n) = g_0/(k^2 + \omega_n^2 + m^2)$, where m is defined by the self-consistent condition, $\sum_n \sum_{\vec{k}} \Xi(\vec{k}, \omega_n; m) = 1$, and sets the scale for the correlations in the system. The self-consistency equation can also be written, after the sum over Matsubara frequencies, as

$$\frac{g_0}{2}\int \frac{d^2k}{(2\pi)^2}\,\frac{\coth(\sqrt{k^2 + m^2}\,\beta c_0\Lambda/2)}{\sqrt{k^2 + m^2}} = 1. \tag{4}$$

Formally, this integral has a logarithmic ultraviolet divergence. If we choose an isotropic cutoff $\pi/\Lambda a$ for the Fourier transform of the original problem (2), then $|k_x| < \pi\alpha^{1/4}/\Lambda a$ and $|k_y| < \pi\alpha^{-1/4}/\Lambda a$, where

$$\alpha = J_x/J_y \tag{5}$$

is the anisotropy parameter (as usual, we take $\Lambda a = 2\sqrt{\pi}$ to preserve the area of the magnetic Brillouin zone). By the definition above, the coupling constant $g_0(\alpha) = g_0(1)\sqrt{(1 + \alpha)/2\sqrt{\alpha}}$. In what follows we will choose $g_0(1)$ renormalized to give the *interacting* spin wave velocity of Oguchi [12], rather than the simple spin wave value above. Because the effective exchange J_x in the x direction is weakened by the stripes, we have $0 \le \alpha \le 1$.

At high anisotropy ($\alpha \to 0$) the spin chains become disconnected and we find one-dimensional behavior. In this limit $m \gg \alpha^{1/4}$, and we find at zero temperature from (4), $m(\alpha) \approx 4\alpha^{-1/4}/\sqrt{\pi}\,\exp[-4\pi^{3/2}/\alpha^{1/4}g_0(\alpha)]$, which is just the Haldane gap [13]. We came to this result because the nonlinear σ model without a topological term describes the behavior of an *integer* spin chain [14]. In the opposite limit, $m \ll \alpha^{1/4}$, the system is fully two-dimensional, and Eq. (4) at zero temperature leads to $m(\alpha) \approx 4\sqrt{2}\,\pi\alpha^{1/4}/\sqrt{1 + \alpha}\,[1/g_c(\alpha) - 1/g_0(1)]$, where

$$g_c(\alpha) = 8\pi^{3/2}\sqrt{\alpha/(1 + \alpha)}\,\{\ln(\sqrt{\alpha} + \sqrt{1 + \alpha}\,) + \sqrt{\alpha}\,\ln[1 + \sqrt{1 + \alpha}\,/\sqrt{\alpha}\,]\}^{-1} \tag{6}$$

is the critical coupling constant of the theory. It is easy to see that g_c decreases monotonically to zero as the system becomes more anisotropic and the increasing quantum fluctuations again make magnetic order less stable. Dimensional crossover occurs when the correlation length in the x direction becomes of the order of the lattice spacing, that is, $m(\alpha_t) \approx \alpha_t^{1/4}$, and a numerical estimate gives $\alpha_t \approx 0.001$.

To understand the corrections to the classical limit, we employ a renormalization group (RG) calculation up to second order in the coupling constant. Proceeding as in [1], we find within a one-loop approximation the renormalized spin stiffness

$$\rho_s(\alpha) \approx \rho_s^0(\alpha)[1 - g_0(1)/g_c(\alpha)], \tag{7}$$

reduced from its classical value ρ_s^0 for fixed α. As a first consequence we see that the stiffness will vanish for some critical value, $\alpha = \alpha_c$, which can be calculated numerically. Oguchi's spin wave theory [1,12] gives $g_0(1) \approx 9.536$. Then (7) gives $\alpha_c \approx 0.047$, much greater than α_t, so the transition from classical to quantum regimes (ordered to disordered ground state) occurs well before the potential crossover from two- to one-dimensional behavior [15].

We turn to the finite temperature behavior. Again, we can use the inequality $m \ll \alpha^{1/4}$ in estimating the correlation length $\xi \propto 1/m$ from Eq. (4). However, we know from studies of the undoped system that the one-loop calculation does not give a very good results for the prefactor of the temperature dependent exponential expression for ξ, and the same will surely be true for $\alpha < 1$. Here we use an interpolation formula between the exact result of Hasenfratz and Niedermayer [16] for

the nonlinear sigma model, which is valid close to the ordered phase, and the result for the renormalized critical regime where $\xi \propto T^{-1}$:

$$\xi(T,\alpha) \approx \frac{e}{8}\,\frac{\hbar c_0}{2\pi\rho_s(\alpha)}\,\frac{e^{2\pi\rho_s(\alpha)/k_BT}}{1 + k_BT/4\pi\rho_s(\alpha)}. \quad (8)$$

This gives excellent agreement [1] with experiment in the pure case, $x = 0$.

In general the staggered magnetization depends on the short, as well as on the long wavelength physics of the problem. As in [1], instead of using the nonlinear sigma model directly, we observe that the equal time staggered spin-spin correlation function at large distances becomes proportional to the square of the staggered magnetization, $\lim_{x\to\infty,y\to\infty} \Xi(x,y) = (M_s/M_0)^2$, where M_0 is the staggered magnetization for the classical problem (the fully aligned Néel state, without quantum fluctuations). At zero temperature, in the ordered phase, the correlation length is infinite. The only scale left is the Josephson length, $\xi_J = \hbar c_0/\rho_s$. On one hand, the asymptotic (large distance) limit of the correlation function has been established at this scale. On the other hand, this is the maximum scale at which the long wavelength dominated theory we have developed can be trusted. Therefore, we equate the correlation function at this (scaled) length to the square of the relative zero point magnetization, and using the RG result (7), we find

$$\frac{M_s(\alpha)}{M_s(1)} = \sqrt{\frac{1 - g_0(1)/g_c(\alpha)}{1 - g_0(1)/g_c(1)}}. \quad (9)$$

As expected, $M_s(\alpha_c) = 0$, and close to α_c we find $M_s(\alpha) \approx (\alpha/\alpha_c - 1)^{1/2}$, which has the mean field exponent of $1/2$.

To have true long-range order at $T > 0$, we need to invoke the weak coupling between planes, $J_\perp$. Because $J_\perp/J \approx 5 \times 10^{-5}$ [17] is so small, long-range correlations have built up in the plane well above the ordering temperature T_N. Spin fluctuations then involve large correlated regions, and it is a good approximation to treat $J_\perp$ within a mean field theory. To determine the dependence of the Néel temperature on anisotropy, one needs to know the connection between the classical spin stiffness and α. Here we assume as a simple model that the classical stiffness is approximately independent of α over the region of interest, equal to the undoped value $\rho_s^0(\alpha = 1)$, so $\sqrt{J_x J_y} = J$.

Magnetic order is destroyed by thermal fluctuations, at a temperature T_N, when the energy k_BT_N becomes sufficient to flip the spins in a region of linear dimension of the order of the coherence length ξ. Since the number of spins in this region is proportional to $(\xi/a)^2$, and the relative staggered magnetization in the region is given by M_s/M_0, we estimate

$$k_BT_N(\alpha) \approx J_\perp\left(\frac{\xi(T_N,\alpha)}{a}\,\frac{M_s}{M_0}\right)^2. \quad (10)$$

This expression has been used previously [1] to estimate $J_\perp/k_B \approx 0.01$ K from the experimental T_N of the pure material. Since $M_s/M_0 < 1$, this gives $\xi/a > 10$ for $T_N > 1$ K, suggesting that this mean field theory is reasonable for T_N greater than a few kelvin. We now substitute the expression (8) for ξ in the quantum critical regime into (10) to find $T_N(\alpha) \approx (\alpha/\alpha_c - 1)^{1/3}$, defining a critical exponent of $1/3$.

In order to compare our results with the experiments, we need the relationship between the anisotropy parameter (5) and the doping concentration x. Explicit calculation of that is complicated, depending intrinsically on the chemistry of the material; it goes beyond our previous analysis. Instead, we propose a simple parametrization,

$$\alpha(x) = e^{-x/x_0}, \quad (11)$$

with x_0, the single (nonuniversal) parameter characterizing the behavior, dependent in an unknown way on the microscopic details of the system. We fix the value of x_0 from experiment. We stress that this is the *only* free parameter in our theory. All others are obtained independently for the undoped material, and they are well known.

Experimentally the staggered magnetization and the Néel temperature vanish at a critical doping $x_c \approx 0.02$–0.023 [5]. This value of x_c must correspond in our model to the point at which the spin wave stiffness vanishes, that is, to the critical value $\alpha_c \approx 0.047$. Then (11) gives $x_0 \approx 0.007$. Depending on the density of holes in the stripes, this corresponds to a stripe spacing of order 10 lattice constants or so, a reasonable scale on which to expect substantial changes to occur. Substituting (11) into (9), we find the staggered magnetization as a function of doping. In Fig. 1 we show the theoretical prediction (full line) and the experimental values (dots) from Ref. [5]. In view of the approximations used in the theory above, the agreement is impressive.

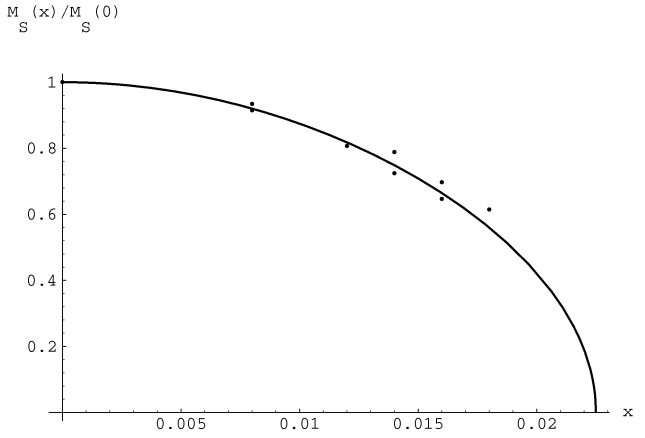

FIG. 1. Staggered magnetization (normalized relative to the undoped case) as a function of doping (line) and experiment (dots).

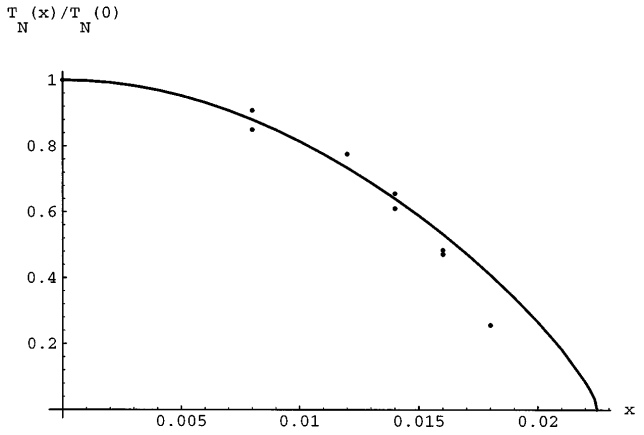

FIG. 2. Néel temperature (normalized relative to the undoped case) as a function of doping. Theory (continuous line) and experiment (dots).

The calculation of the Néel temperature from (10) brings in new parameters, including the interplanar exchange $J_\perp$, but they are all set by those of the undoped material. We need no additional assumptions; we simply use the same parameters taken [1] by CHN to fit experiment: $\rho_s(1)/k_B \approx 187$ K and $\hbar c_0(1) \approx 7.7 \times 10^3$ Å K. Using Eqs. (8) and (10), we obtain the full curve in Fig. 2. The agreement between theory and experiment is very good except for the smallest value of T_N, and can be improved by small adjustments of the parameters [18]. Our conclusion is, therefore, that our theory is fully consistent with the recent experiments on $La_{2-x}Sr_xCuO_4$.

In summary, we have developed an effective field theory for magnetic correlations in doped antiferromagnets that are anisotropic due to the stripe correlations expected from microscopic phase segregation of holes. We suggest that the long wavelength spin fluctuations are described by a spatially anisotropic nonlinear sigma model. The experimental parameter, the doping concentration x, is reflected in the theory by the magnetic exchange anisotropy α, taken to depend exponentially on x (introducing the only free parameter of the theory, the decay rate x_0). We further assume that the classical spin stiffness is not affected by doping. We believe that the good agreement between this theory and experiment gives new support to the picture of stripe correlations of holes in $La_{2-x}Sr_xCuO_4$ for $0 \leq x \leq 0.018$.

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