Theory of Spin Fluctuations in Striped Phases of Doped Antiferromagnetic Cuprates

Daniel Hone\textsuperscript{1} and A.H. Castro Neto\textsuperscript{2}

\textsuperscript{1} Institute for Theoretical Physics, University of California, Santa Barbara, California, 93106
\textsuperscript{2} Department of Physics, University of California, Riverside, California, 92521

(Received November 19, 2018)

We study the properties of generalized striped phases of doped cuprate planar quantum antiferromagnets. We invoke an effective, spatially anisotropic, non-linear sigma model in two space dimensions. Our theoretical predictions are in quantitative agreement with recent experiments in La\textsubscript{2−x}Sr\textsubscript{x}CuO\textsubscript{4} with 0 ≤ x ≤ 0.018. We focus on (i) the magnetic correlation length, (ii) the staggered magnetization at T = 0 and (iii) the Néel temperature, as functions of doping, 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.

KEY WORDS: Quantum antiferromagnets; doped cuprates; striped phases.

There is no direct evidence for periodically structured striped phases in doped antiferromagnetically ordered cuprates, such as La\textsubscript{2−x}Sr\textsubscript{x}CuO\textsubscript{4} (with x < 0.02). Indeed, recent neutron scattering measurements\textsuperscript{\textsuperscript{[1]}} show that the incommensurate magnetic peaks which are characteristic of dynamic stripe formation at higher hole concentrations x, seem to disappear below x of order 0.05, well above the antiferromagnetic regime. Yet the growing theoretical literature\textsuperscript{\textsuperscript{[2]}} supporting the tendency toward microscopic phase separation of holes in these strongly correlated quasi-two-dimensional materials, as well as the experimental observation\textsuperscript{\textsuperscript{[3,4]}} of stripe phenomena in many related systems, raises the strong possibility that the doped antiferromagnetic cuprates will also be characterized by such stripes. Moreover, there is indirect evidence of linear, or striped, features in the magnetic structure of these materials, including the finite size scaling properties\textsuperscript{\textsuperscript{[5]}} of the Néel temperature and uniform magnetic susceptibility, and the successful interpretation\textsuperscript{\textsuperscript{[6]}} of muon spin resonance (µSR) and nuclear quadrupole resonance (NQR) experiments within models that presume a striped structure.

Those latter theories are nominally based on a static periodic array of stripes, which separate antiferromagnetic slabs, or ladders, at most weakly coupled to one another across the stripes. Since such regular arrays are not observed in the neutron scattering experiments, we want to consider a broader class of striped structures. These may include arrays with varying separation between neighboring stripes, as suggested\textsuperscript{\textsuperscript{[7]}} by the neutron scattering lineshapes in the related doped nickelates, or dynamic behavior of the stripes, including amplitude fluctuations, rigid translations, or the meanderings proposed\textsuperscript{\textsuperscript{[8]}} by Zaanen and coworkers. We also note that a magnetic phase domain, rather than anti-phase boundary\textsuperscript{\textsuperscript{[5]}} , which locally only suppresses, rather than reverses the antiferromagnetic order parameter, would give at best only a weak incommensurate scattering, even for a periodic array. It is then our purpose here to develop a reliable effective field theory which will predict the experimentally observable behavior while making a minimum of assumptions about the details of the underlying structure, beyond the demand that it corresponds on average to periodic one-dimensional weakening of the antiferromagnetic exchange between spins.

Encouraged and guided by the remarkable success of Chakravarty, Halperin and Nelson\textsuperscript{\textsuperscript{[9]}} in describing undoped La\textsubscript{2}CuO\textsubscript{4} by just such an approach, we introduce a suitably anisotropic non-linear sigma model parametrized so as to reproduce the long wavelength behavior of the doped material in the antiferromagnetically ordered phase. Whatever the origin of the average periodic modulation of exchange, the corresponding long wavelength magnetic excitations from the antiferromagnetic ground state, which determine the thermodynamics, will have the same character as those of a static array of stripes with the same period. They are gapless (Goldstone modes, from spin rotational symmetry), with a dispersion relation for the frequency squared which is analytic in wave vector, giving a linear dispersion with anisotropic “spin wave” velocity, where the principal axes of the velocity tensor must be parallel and perpendicular to the stripes (which lie along a crystal axis\textsuperscript{\textsuperscript{[10]}}). Such behavior is described in the continuum limit by the action of an effective anisotropic non-linear sigma model,

\begin{equation}
S_{\text{eff}} = \frac{1}{2} \int_0^{\beta} d\tau \int dx \int dy \left\{ S^2 \left[ J_y (\partial_y \tilde{n})^2 + J_x (\partial_x \tilde{n})^2 \right] + \frac{\hbar^2}{2a^2(J_x + J_y)} (\partial_x \tilde{n})^2 \right\},
\end{equation}

where \( \tilde{n} \) is a unit vector field. The symbols have been chosen to suggest the continuum limit of an underlying effective integer spin\textsuperscript{\textsuperscript{[11]}} Heisenberg hamiltonian on a square lattice with lattice constant a, and with nearest neighbor exchanges \( J_x \) and \( J_y \). In terms of these parameters the principal spin wave velocities are

\begin{align}
\alpha_y^2 &= 2S^2a^2 J_y(J_x + J_y) \\
\alpha_x^2 &= 2S^2a^2 J_x(J_x + J_y).
\end{align}

The fundamental underlying anisotropy parameter is
then equivalently the ratio of the two exchange constants or of the two velocities,
\[ \alpha = J_x / J_y. \]  

(3)

Its value characterizes the theory, but just how it decreases with increasing doping concentration \( x \) will have to be set later.

We note that in restricting the subsequent analysis to these longest wavelength excitations we ignore both the non-linear dispersion of these acoustic modes and all optical branches associated with the (average) superlattice in the \( \tau \)-direction. As an estimate of the lowest lying optical mode energies we can take the location of the lowest gap introduced by a stripe superlattice in the hole-free antiferromagnetic host, which occurs approximately at \( J_\pi \sqrt{2}/N_0 \) for a superlattice of period \( N_0 \) lattice constants in the host with exchange constant \( J \). Coulomb energy costs would seem to prevent values of \( N_0 \) much greater than 20 to 30, giving a lowest optical mode energy greater than about 250 - 350 K. These energies lie above the temperatures of interest, and the neglect seems reasonable.

From this point on we make use of well established techniques to analyze the behavior of the field theory described by the action \((\bar{1})\) so as to make predictions for the physical properties of the system of interest. First it is useful to rewrite \((\bar{1})\) more symmetrically by a dimensionless rescaling of the variables: \( x' = (\alpha)^{-1/4} x \Lambda, \ y' = (\alpha)^{1/4} y \Lambda (\Lambda \sim 1/\alpha \) is a momentum cut-off), and \( \tau' = \sqrt{2(J_x + J_y)} \sqrt{J_x J_y} \text{Sar} \tau / \hbar \). Then the effective action \((\bar{1})\) becomes

\[ S_{\text{eff}} = \frac{\hbar}{2g_0} \int_0^{\hbar \Lambda \beta_0} d\tau' \int dx' \int dy' (\partial_{\mu} \hat{n})^2, \]  

(4)

where \( \mu \) takes the values \( x', y', \tau' \),

\[ g_0(\alpha) = \hbar c_0 \Lambda / \rho_0 = \left[ 2(1 + \alpha) / \sqrt{\alpha} \right]^{1/2} (a \Lambda) / S \]  

(5)

is the bare coupling constant, \( c_0 = [2(J_x + J_y) \sqrt{J_x J_y}]^{1/2} (a \Lambda) / \hbar \) the spin wave velocity and \( \rho_0 = \sqrt{J_x J_y} \text{S}^2 \) 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 \( \sigma \)-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 \([\bar{13}]\). In the antiferromagnetically disordered phase the staggered-spin static correlation function is given \([15]\) by

\[ \langle \sigma(x, y) \sigma(0, 0) \rangle = \frac{g_0(\alpha)}{r_s} e^{-mr}, \]  

(6)

where \( \sigma \) is the component of \( \hat{n} \) in the ordering direction, \( r_s \) is the scaled length, \( r_s^2 = x^2/\sqrt{\alpha} + \sqrt{\alpha} y^2 \), and \( m \) is the inverse correlation length, given formally by imposing the condition that the magnitude of the field \( \hat{n} \) is unity at each point. At zero temperature this condition becomes

\[ 1 = \frac{2g_0(\alpha)}{g_0(1)} \int_0^{\alpha^{-1/4}} \frac{dk_y}{2\pi} \int_0^{\alpha^{1/4}} \frac{dk_x}{2\pi} \frac{1}{\sqrt{k^2 + m^2}}. \]  

(7)

We find that \( m < \alpha^{1/4} \) over the full range of parameters of interest, in which case \((\bar{6})\) gives

\[ m(\alpha) = 8\pi \left( \frac{\sqrt{\alpha}}{1 + \alpha} \right)^{1/2} \left[ \frac{1}{g_c(\alpha)} - \frac{1}{g_0(1)} \right], \]  

(8)

where

\[ g_c(\alpha) = \sqrt{\pi}^2 \sqrt{\alpha/(1 + \alpha)} \left\{ \ln \left( \sqrt{\alpha} + \sqrt{1 + \alpha} \right) + \sqrt{\alpha} \ln((1 + \sqrt{1 + \alpha})/\sqrt{\alpha}) \right\}^{-1}, \]  

(9)

is the critical coupling constant of the theory: the ground state is disordered \([\bar{14}]\) if \( m(\alpha) > 0 \), or \( g_0(1) < g_c(\alpha). \) It decreases monotonically with increasing anisotropy \( 1/\alpha \), as the hole doping concentration \( x \) grows. Thus the system remains disordered at \( T = 0 \) for \( \alpha < \alpha_c \), where \( \alpha_c \), the critical anisotropy, is defined by the condition \( g_c(\alpha_c) = g_0(1) \). We will see below, as this suggests, that as \( \alpha \) approaches \( \alpha_c \) from above with increasing doping, this is also the value where the spin stiffness — and the three dimensional Néel temperature — vanishes. Numerically, \( \alpha_c \approx 0.047 \).

For sufficiently weak anisotropy \((1 > \alpha > \alpha_c)\) the system orders magnetically at zero temperature, we can take advantage of the power of renormalization group techniques for systems with diverging correlation lengths, to understand the corrections to the classical limit above. As always, we introduce an explicit length scale, \( a \rightarrow \Lambda a = e^{-\xi} \), where \( a \) is the original lattice parameter. Then the normalization condition on the field \( \hat{n} \) at \( T = 0 \) becomes

\[ \bar{\sigma}^2 = 1 - \frac{2g_0(\alpha)}{\Lambda} \int_0^{\alpha^{-1/4} \Lambda} \frac{dk_y}{2\pi} \int_0^{\alpha^{1/4} \Lambda} \frac{dk_x}{2\pi} \frac{1}{k}, \]  

(10)

where \( \bar{\sigma} \) is the average value of the order parameter (staggered magnetization), and the second term on the right hand side represents the spin flip fluctuations away from perfect Néel order. The RG procedure can be carried out in various ways, including (see, e.g., \([\bar{13}]\)) explicit integration over large momentum values and suitable rescaling to restore Eq. \((\bar{\bar{1}})\) to its original form. Instead we introduce \([\bar{13}]\) the explicit re-scaling function \( Z(\Lambda) \): \( \sigma = Z(\Lambda) M \), and \( g_0(\alpha) = Z(\Lambda) g_R(\alpha) \), which renders \((\bar{\bar{1}})\) renormalizable, with the renormalization equation,

\[ \frac{dg_R}{dt} \approx -g_R + \frac{g_0(1)}{g_0(\alpha) g_c(\alpha)} \sigma^2 R, \]  

(11)
which can be integrated from the bare value \( g_R(\alpha) \) at \( \ell = 0 \) to the fully renormalized value at \( \ell \to \infty \). The stable fixed point is at \( g_R = 0 \), justifying keeping only the lowest two powers of \( g_R \) in the equation \((13)\), a one-loop approximation. The result then gives for the renormalized spin stiffness,

\[
\rho_s(\alpha) \to \left[ \frac{\hbar c}{ae^g g_R(\ell, \alpha)} \right]_{\ell \to \infty} = \rho_s^0(\alpha) \left[ 1 - \frac{g_R(1)}{g_s(\alpha)} \right].
\]

reduced from its classical value \( \rho_s^0(\alpha) \) for fixed anisotropy \( \alpha \) in such a way that it vanishes, as foreseen above, at the critical value \( \alpha = \alpha_c \).

Now we turn to prediction of and comparison with experimental quantities, including correlation length \( \xi(\alpha, T) \), zero point magnetization \( M_s(\alpha) \), and Néel temperature \( T_N(\alpha) \). We know from studies of the undoped system that while the one-loop calculation accurately predicts the leading exponential dependence on inverse temperature of \( \xi(T) \), its results are not very good for the prefactor of that exponential or the algebraic temperature dependent corrections, and the same will surely be true for the doped system, with \( \alpha < 1 \). Therefore we use an interpolation formula between the exact result of Hasenfratz and Niedermayer \((19)\) for the nonlinear sigma model in the neighborhood of magnetic order, and the result for the quantum critical regime, where \( \xi \propto T^{-1} \):

\[
\xi(T, \alpha) \approx \left( \frac{\hbar c g_0}{4} \right) e^{\frac{2\pi g_s(\alpha)}{4\pi g_s(\alpha) + k_B T}}. \tag{13}
\]

This gives excellent agreement \((11)\) with experiment in the pure case, \( x = 0 \). The experimental data \((21)\) for \( \xi^{-1}(x, T) \) have been interpreted phenomenologically, not according to \((13)\), but as the sum of the pure system function plus a constant depending only on doping concentration \( x \): \( \xi^{-1}(x, T) = \xi^{-1}(0, T) + \xi^{-1}(x, 0) \). But only the pure \( (x = 0) \) experimental results are reliably in the antiferromagnetic region we treat here. The other curves, with nominal values of \( x = 0.02, 0.03 \) and 0.04, correspond most likely to the cluster spin glass phase. Of course, to make a direct comparison with the experiments, yet to be done, in the region \( x < 0.02 \), we need the connection between the anisotropy parameter \( \alpha \) and the hole concentration \( x \). We can do this indirectly, by comparing experimental properties, for example, as a function of Néel temperature, as we will do below for the zero point staggered magnetization. One additional parameter is still required, though, for comparison with \((13)\). The spin stiffness \((12)\) depends through \( \rho_s^0 \) on the product \( J_x J_y \), as well as the ratio \( \alpha \). If we take that product, for example, to be independent of \( x \), or \( \alpha \), then the curves for \( \xi^{-1}(T) \) for doped and undoped systems will be found to cross, as seems to be suggested by the experiments \((21)\) for \( x = 0 \) and 0.02.

In general, the staggered magnetization \( M_s \) depends on the short, as well as the long wavelength physics of the problem, so we can’t use the results at \( T = 0 \) of the long distance nonlinear sigma model theory directly. Instead, as in \((14)\), we use the asymptotic long distance behavior of the equal time spin-spin correlation function: \( \langle \sigma(x, y) \sigma(0, 0) \rangle \to (M_s/M_0)^2 \) as \( x, y \to \infty \), where \( M_0 \) represents perfect Néel spin alignment. To do this we evaluate \((6)\) at the point where the scaled length \( r_s \) is equal to the Josephson correlation length \( \xi_J = \hbar c/\rho_s \), which separates long from short wavelength scales. On the one hand, this is large enough for the correlation function to have reached its desired asymptotic behavior, but it is still short enough that the (exponential) decay due to the long wavelength fluctuations at \( T = 0^+ \) where \((6)\) holds has not yet become effective. Thus we find,

\[
\frac{M_s(\alpha)}{M_s(1)} = \sqrt{\frac{1 - g_0(1)/g_s(\alpha)}{1 - g_0(1)/g_s(1)}}. \tag{14}
\]

As usual \((21)\) for quasi-two-dimensional systems, we make use of the long range order parameter correlations that have developed in the plane above the ordering temperature \( T_N \), to call on the validity of mean field theory for the weak exchange \( J_\perp \) in the third dimension in establishing 3-d magnetic order at a finite temperature. A simple physical interpretation of the result is that \( T_N \) is the temperature at which the energy of thermal fluctuations, \( k_B T_N \), becomes sufficient to flip the spins in a region of linear dimension of the order of the 2-d correlation length, \( \xi(T_N) \). Since the number of spins in this region is proportional to \( (\xi/\alpha)^2 \), and the relative staggered magnetization in the region is given by \( M_s/M_0 \), we estimate

\[
k_B T_N(\alpha) \approx J_\perp \left( \frac{\xi(T_N, \alpha)}{\alpha} \right)^2. \tag{15}
\]

This expression has been used previously \((11)\) 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 \( (\xi/\alpha) > 10 \) for \( T_N > 1 \) K, suggesting that this mean field theory is reasonable for \( T_N \) greater than a few kelvin.

Though the predicted staggered magnetization \((14)\) and the Néel temperature \((15)\) both depend on the anisotropy parameter \( \alpha \), whose explicit dependence on doping \( x \) is not established by the model, we can eliminate this dependence between the two relations, plotting \( M_s \) \textit{versus} \( T_N \), each normalized to the corresponding undoped \( (x = 0) \) value, as is done in Fig. 1. The experimental values are those of Ref. \((6)\). We note, in particular, that the zero point magnetizations are extrapolated values. As is explained in \((1)\), there is a change of behavior around \( T = 30 \) K for all values of doping. The authors have interpreted this as some sort of freezing of the holes, which may be binding to the donor impurities, establishing static charge density waves within the stripes, or some other change in behavior. In any case, the reported values of \( M_s \) are those extrapolated from the observed magnetization curves at temperatures above this “freezing”. We emphasize that the comparison in Fig. 1 has
no adjustable theoretical parameters, and the agreement with experiment is excellent. This, and the further comparisons made in [7], then supports a generalized stripe picture of the antiferromagnetic doped cuprates.

![Graph](image)

FIG. 1. Neel temperature versus staggered magnetization normalized to the undoped values. Line: theory; diamonds: experiment.

We are indebted to S.A. Kivelson for introducing us to this problem and for his illuminating comments and suggestions throughout the work. We thank A. Balatsky, S. Chakravarty, C. Di Castro, and C. Castellani for valuable comments, and F. Borsa for discussion of his and other experiments. We also acknowledge support by NSF Grant PHY 94-07194.

[1] K. Yamada, et al., preprint, and this volume.
[2] V. Hizhnyakov and E. Sigmund, Physica C 156, 655 (1988); H.J. Schulz, J. Phys. France 50, 2833 (1989); J. Zaanen and J. Gunnarson, Phys. Rev. B 40, 7391 (1989); V.J. Emery, S.A. Kivelson and H.-Q. Lin, Phys. Rev. Lett. 64, 475 (1990); M. Grilli, et al., Phys. Rev. Lett. 67, 259 (1991); J.A. Vergés et al., Phys. Rev. B 43, 6099 (1991); V.J. Emery and S.A. Kivelson, Physica C 209, 597 (1993); S. Haas et al., Phys. Rev. B 51, 5989 (1995).
[3] J.M. Tranquada, et al., Nature, 375, 561, (1995).
[4] S-W. Cheong, et al., Phys. Rev. Lett. 67, 1791 (1991); E.D. Isaacs et al., Phys. Rev. Lett. 72, 3421 (1994); T.E. Mason et al., Physica B 199, 284 (1994).
[5] J.H. Cho, et al. Phys. Rev. Lett. 70, 222 (1993).
[6] F. Borsa, et al., Phys. Rev. B 52, 7334 (1995).
[7] A.H. Castro Neto and D. Hone, Phys. Rev. Lett. 76, 2165 (1996).
[8] J.M. Tranquada, et al., Phys. Rev. Lett. 73, 1003 (1994); cond-mat 9612007.
[9] H. Eshke, R. Grimberg, W. van Saarloos and J. Zaanen, Phys. Rev. B 54, R724 (1996), and this volume.
[10] A.H. Castro Neto, cond-mat 9611144.
[11] S. Chakravarty, B.I. Halperin and D.R. Nelson, Phys. Rev. Lett. 60, 1057 (1988); Phys. Rev. B 39, 2344, (1989).
[12] This might be appropriate for an even number of spins between stripes (see S.R. White, R.M. Noack and D.J. Scalapino, Phys. Rev. Lett. 73, 886 (1994); N. Hatano and Y. Nishiyama, J. Phys. A 28, 3911 (1995), or for spin Peierls dimerized chains (Z. Wang, cond-mat 9611129). The topological term may be important, and the physics different, for coupled ladders with odd numbers N of legs (gapless spectrum for the individual isolated ladder). It seems that $T_N > 0$ for arbitrarily weak anisotropy when $N = 1$, for example: I. Affleck, M.P. Gelfand and R.R.P. Singh, J. Phys. A 27, 7313 (1994).
[13] S. Sachdev, in Low dimensional quantum field theories for condensed matter physicists, Proc. of the Trieste Summer School (World Scientific, Singapore, 1992).
[14] D. P. Arovas and A. Auerbach, Phys. Rev. B 38, 316 (1988); Phys. Rev. Lett. 61, 617 (1988).
[15] A.H. Castro Neto and D. Hone, in preparation.
[16] Note that the condition is expressed relative to the fixed undoped coupling constant $g_0(1)$, given by Oguchi’s renormalized spin wave theory [17,18] as $g_0(1) \approx 9.54$. By using Eq. (5), which gives $g_0(\alpha)/g_0(1)$ we could readily write this directly as an inequality for the actual coupling constant of the anisotropic system for each value of $\alpha$, a more obvious condition physically, but it is algebraically simpler to do it in terms of $g_0(1)$.
[17] T. Oguchi, Phys. Rev. 117, 117 (1960).
[18] A.H. Castro Neto and E. Fradkin, Nucl. Phys. B400, 525 (1993).
[19] P. Hasenfratz and F. Niedermayer, Phys. Lett. B 268, 231 (1991).
[20] S.M. Hayden et al., Phys. Rev. Lett. 66, 821 (1991); B. Keimer et al., Phys. Rev. B 46, 14034 (1992); T. Imai, et al., Phys. Rev. Lett. 70, 10002 (1993).
[21] See, e.g., D.J. Scalapino, Y. Imry, and P. Pincus, Phys Rev. B 11, 2042 (1975).