Spin Gaps and Bilayer Coupling
in YBa$_2$Cu$_3$O$_{7-\delta}$ and YBa$_2$Cu$_4$O$_8$

A. J. Millis$^{(a)}$ and H. Monien$^{(b)c}$

$^{(a)}$AT&T Bell Laboratories, 600 Mountain Avenue, Murray Hill, NJ 07974
$^{(b)}$Institute for Theoretical Physics, University of California, Santa Barbara, CA 93106

(March 23, 2022)

Abstract

We investigate the relevance to the physics of underdoped YBa$_2$Cu$_3$O$_{6+x}$ and YBa$_2$Cu$_4$O$_8$ of the quantum critical point which occurs in a model of two antiferromagnetically coupled planes of antiferromagnetically correlated spins. We use a Schwinger boson mean field theory and a scaling analysis to obtain the phase diagram of the model and the temperature and frequency dependence of various susceptibilities and relaxation rates. We distinguish between a low $\omega$, $T$ coupled-planes regime in which the optic spin excitations are frozen out and a high $\omega$, $T$ decoupled-planes regime in which the two planes fluctuate independently. In the coupled-planes regime the yttrium nuclear relaxation rate at low temperatures is larger relative to the copper and oxygen rates than would be naively expected in a model of uncorrelated planes. Available data suggest that in YBa$_2$Cu$_4$O$_8$ the crossover from the coupled to the decoupled planes regime occurs at $T\approx 700K$ or $T\approx 200K$. The predicted correlation length is of order 6 lattice constants at $T = 200K$. Experimental data related to the antiferromagnetic susceptibility of YBa$_2$Cu$_4$O$_8$ may be made consistent with the theory, but available data for the uniform susceptibility
are inconsistent with the theory.
I. INTRODUCTION

In this paper we investigate the relevance to the physics of underdoped YBa$_2$Cu$_3$O$_{6+x}$ and YBa$_2$Cu$_4$O$_8$ of a $T = 0$ order-disorder transition which occurs in a model of two antiferromagnetically coupled planes of antiferromagnetically correlated spins. This transition might be relevant because: (a) in these compounds the basic structural unit is a pair of CuO$_2$ planes separated from each other by the relatively inert CuO chains [1], (b) there is evidence for strong antiferromagnetic correlations within a CuO$_2$ plane [2–4], (c) neutron scattering experiments find that for all $\omega$ and $T$ studied a spin in one plane is perfectly anticorrelated with the nearest neighbor spin on the nearest-neighbor plane [5–7], (d) for $T < 150$ K both the static uniform susceptibility and the various NMR relaxation rates drop rapidly as $T$ decreases [8] suggesting [9–11] that the system is evolving as $T$ is decreased towards a quantum disordered ground state with a gap to spin excitations and (e) the spin physics of La$_{2-x}$Sr$_x$CuO$_4$, in which the CuO$_2$ planes are very weakly coupled, is apparently rather different [12], suggesting that the behavior of YBa$_2$Cu$_3$O$_{6+x}$ may be due at least in part to a coupling between planes. A preliminary version of this work was published previously [13].

The model we consider is a Heisenberg model of spins sitting on sites of the lattice depicted in fig. 1 and has two coupling constants, both taken to be antiferromagnetic. One, $J_1$, couples nearest neighbor spins in the same plane. The other, $J_2$, couples a spin in one plane to the nearest spin in the other plane. The Hamiltonian is

$$H = J_1 \sum_{\langle i,j \rangle,a} \vec{S}^{(a)}_i \cdot \vec{S}^{(a)}_j + J_2 \sum_i \vec{S}^{(1)}_i \cdot \vec{S}^{(2)}_i \tag{1.1}$$

Here $i$ labels sites in a given plane, $i$ and $j$ are nearest neighbors in the same plane, and $a = 1, 2$ labels two planes. There are two dimensionless parameters: $J_2/J_1$ and $S$, the magnitude of the spin. At temperature $T = 0$ eq. (1.1) has two phases. One is antiferromagnetically ordered; the other is a singlet phase with a gap to excitations and no long range order. Varying $J_2/J_1$ and $S$ produces transitions between the phases. In a physical
Heisenberg model $S$ would take only half-integer or integer values $1/2, 1, 3/2, \ldots$. However, it is interesting to consider values $S < 1/2$ because the singlet phases occurring for small $S$ in this model may be useful representations of the “spin gap” behavior occurring in the underdoped YBa$_2$Cu$_3$O$_{6+x}$. We shall determine the phase diagram and discuss the physical properties at the transition and on the disordered side. The $T = 0$ transition is in the universality class of the 2+1 dimensional Heisenberg model and some universal properties have been determined \[10,11\]. Here, we pay particular attention to the effects of the inter-plane coupling, $J_2$. We show that one must distinguish between a low $\omega, T$ “coupled planes” regime and a high $\omega, T$ “decoupled planes regime”. In the coupled-planes regime, one linear combination (essentially the optic mode of the spin excitation spectrum) is frozen out and the low energy physics is determined by acoustic spin fluctuations in which moments in the two planes fluctuate coherently. In the decoupled planes regime the two planes fluctuate essentially independently. One important feature of the quantum critical point considered here is the close relationship between the susceptibility at small $q$ and at a $q$ near the ordering wavevector \[11\]. We show that this, when combined with interplanar coupling, has a surprising implication for the yttrium relaxation rate: in the coupled-planes regime it is larger, relative to the other rates, than one would expect from a model of uncoupled planes.

We emphasize that eq. \[(1.1)\] is not a completely realistic model of YBa$_2$Cu$_3$O$_{6.6}$ or YBa$_2$Cu$_4$O$_8$ because it omits the itinerant carriers which make these materials metallic and indeed superconducting. The itinerant carriers also strongly affect the magnetism. In all of the hole-doped CuO$_2$ compounds, long-range magnetic order disappears essentially at the metal-insulator transition \[12\]. It therefore seems likely that the itinerant carriers substantially weaken the in-plane magnetic correlations. Itinerant carriers also presumably give rise to a particle-hole continuum of incoherent spin excitations which may strongly affect the physics and which in appropriate circumstances may change the universality class of the transition \[13,14\]. It has however recently been argued that there is some evidence that the behavior of YBa$_2$Cu$_3$O$_{6.6}$ and YBa$_2$Cu$_4$O$_8$ is in the universality class of eq. \[(1.1)\] \[9\].

The rest of the paper is organized as follows. In section II we solve eq. \[(1.1)\] via the
Schwinger-boson mean field theory. In section III we give the results of the Schwinger boson mean field theory for the phase diagram and the physical susceptibilities relevant to NMR and neutron scattering experiments. In section IV we combine selected results of the mean field theory with other arguments to map the problem onto a recently constructed scaling theory of the transition [11] and give the relevant results of the scaling analysis. Section V is a conclusion in which we discuss the results and their relation to experiments on YBa$_2$Cu$_3$O$_{6.6}$ and YBa$_2$Cu$_4$O$_8$. It may be read independently of the previous sections by readers uninterested in the derivations of the results. Appendices present details of various calculations.

II. MEAN FIELD SOLUTION

We first study eq. (1.1) by the Schwinger-boson mean-field method [13]. In this method one introduces bose operators $b_{i\alpha}^{\dagger}$ which create a state of spin $\alpha$ on site $i$ of plane $a$. One restricts oneself to the subspace in which each site on each plane has $2S$ bosons, corresponding to spin $S$; thus we enforce the constraint

$$\sum_{\alpha} b_{i\alpha}^{\dagger} b_{i\alpha}^{(a)} = 1 + 2S \quad (2.1)$$

A spin operator is written

$$\vec{S}_i^{(a)} = \sum_{\alpha\beta} b_{i\alpha}^{\dagger} \vec{\sigma}_{\alpha\beta} b_{i\beta}^{(a)} \quad (2.2)$$

We now substitute eq. (2.2) into eq. (1.1). Then on the even sublattice of plane 1 and the odd sublattice of plane 2 we make the time reversal transformation which in the $S = 1/2$ case is:

$$b_{\uparrow} \rightarrow -b_{\downarrow}^{\dagger}$$

$$b_{\downarrow}^{\dagger} \rightarrow b_{\uparrow}^{\dagger} \quad (2.3)$$

Rearranging and using eq. (2.1) leads to
\[ H' = -\frac{1}{2} J_1 \sum_{<i,j>\alpha\beta} \left( b_{i,\alpha}^\dagger b_{j,\alpha}^\dagger \right) \left( b_{i,\beta} b_{j,\beta}^\dagger \right) - \frac{1}{2} J_2 \sum_{i\alpha\beta} \left( b_{i,\alpha}^{(1)} b_{i,\alpha}^{(1)} \right) \left( b_{i,\beta}^{(2)} b_{i,\beta}^{(2)} \right) \] (2.4)

To proceed with the approximate mean-field treatment one introduces a Lagrange multiplier \( \mu \) to enforce the constraint, and an in-plane bond field \( Q \) and a between-planes bond-field \( \Delta \) to decouple the quartic interactions in eq. (1.1). In the mean-field approximation \( \mu, \Delta \) and \( Q \) are taken to be constant in space and time. The resulting theory may be diagonalized. The manipulations are standard and are given in Appendix A. The result is a model of two species of bosons (\( s \), for symmetric under interchange of planes and \( a \), for antisymmetric under interchange of planes) governed by the Lagrangian

\[ \mathcal{L}'_B = \sum_{k\alpha} s_{k\alpha}^\dagger [\partial_\tau + \omega_k] s_{k\alpha} + a_{k\alpha}^\dagger [\partial_\tau + \omega_{k+P}] a_{k\alpha} \] (2.5)

with

\[ \omega_k = \sqrt{\mu^2 - (Q\gamma_k + \Delta)^2}, \] (2.6)

\[ \gamma_k = \frac{1}{2} (\cos k_x + \cos k_y) \] (2.7)

and

\[ P = (\pi, \pi). \] (2.8)

Note that \( \gamma_{k+P} = -\gamma_k \). The parameters \( \mu, Q \) and \( \Delta \) are determined by the mean-field equations

\[ \int \frac{d^2 k}{(2\pi)^2} \frac{\mu}{\omega_k} \coth \frac{\omega_k}{2T} = 1 + 2S, \] (2.9a)

\[ \int \frac{d^2 k}{(2\pi)^2} \frac{(Q\gamma_k + \Delta)\gamma_k}{\omega_k} \coth \frac{\omega_k}{2T} = Q/2J_1, \] (2.9b)

\[ \int \frac{d^2 k}{(2\pi)^2} \frac{Q\gamma_k + \Delta}{\omega_k} \coth \frac{\omega_k}{2T} = 2\Delta/J_2. \] (2.9c)

These equations are derived in Appendix A and imply \( Q, \Delta, \mu \) are real, and \( \Delta, \mu > 0 \). Further, one may change the sign of \( Q \) by shifting the origin of reciprocal space to \( k = P \) and interchanging the labels \( s \) and \( a \). Thus we take \( Q > 0 \) with no loss of generality.
The integrals in eqs. (2.9) depend on \( k \) only via \( \gamma_k \); one may therefore recast them as

\[
\int \frac{d^k}{(2\pi)^2} \rightarrow \int d\gamma N(\gamma)
\]

where \( N(\gamma) \) is a density of states which is constant near the band edges \( \gamma = \pm 1 \) and logarithmically divergent at the band center \( \gamma = 0 \). To obtain an analytically tractable model we replace \( N(\gamma) \) by \( 1/2 \). The resulting equations are solved in Appendix B.

At \( T = 0 \) we find the phase diagram shown in fig. 2. At \( J_2 = 0 \) we have two decoupled planes. As is well known [10,11,15,16] a single plane has a transition at \( S = S_c \sim (\pi/2 - 1)/2 \approx 0.28 \) (the numerical expression for \( S_c \) is obtained from the mean-field calculation) between a large-\( S \) ordered state and a small-\( S \) singlet state with a gap to all spin excitations. If one increases \( J_2 \) in the ordered \( (S > S_c) \) phase of the one-plane model, one reaches at a \( J_2 \sim J_1 \) another transition line, at which the ordered phase is destroyed in favor of singlets which are principally between planes. At \( S = 1/2 \) the Schwinger boson mean field method yields a second order transition at \( J_2 \approx 4.48 J_1 \). A previous series expansion study of eq. (1.1) by Hida [17] yielded a second-order transition at \( J_2 \approx 2.56 J_1 \) and a very recent Monte-Carlo study by Sandvik [18] found a second order transition at \( J_2 \approx (2.7 \pm 0.2) J_1 \).

Interestingly, for \( S < S_c \), we find that increasing \( J_2 \) from \( J_2 = 0 \) initially reduces the gap in the singlet phase, thus moving the system closer to order. For \( S^* < S < S_c \) (with \( S^* \approx 0.19 \) in the mean field calculation) the phase diagram is reentrant. We believe that the physics behind the reentrance is that a small \( J_2 \) splits the spectrum into acoustic and optic sectors, and because the optic sector involves a coupled motion of the spins in the two planes the effective spin of the model describing the low energy fluctuations is increased, promoting order, whereas at large \( J_2 \) the between-planes interaction produced singlets, favoring destruction of order.

In the disordered phase, \( \mu > (Q + \Delta) \) and the excitation spectrum has a gap at all wavevectors. Two gaps that will be particularly important in what follows are \( \omega_+ \) and \( \omega_- \), given by

\[
\omega_+ = \sqrt{\mu^2 - (Q + \Delta)^2}
\]  

and

\[
\omega_- = \sqrt{\mu^2 - (Q - \Delta)^2}
\]  

(2.10)
\[ \omega_- = \sqrt{\mu^2 - (Q - \Delta)^2}. \] (2.11)

For the s-bosons \( \omega_+ \) is the gap at \( k = 0 \) and \( \omega_- \) is the gap at \( k = P \); for the a-bosons 0 and P are interchanged. We shall see that the matrix elements coupling the bosons to externally applied fields have a strong \( k \)-dependence, so that measurable susceptibilities near \( k = 0 \) differ dramatically from those near \( k = P \). Both gap parameters are temperature dependent.

At the \( T = 0 \) phase transition, \( \omega_+ \) vanishes while \( \omega_- > 0 \). Near the large \( J_2 \) boundary of the ordered phase, we have \( \Delta \sim Q \) and \( \omega_- \sim J_1 \gg \omega_+ \). The s-boson mode has one low energy branch, centered at \( k = 0 \),

\[ \omega_+(k)^2 = \omega_+^2 + 2\mu^2(1 - \gamma_k) = \omega_+^2 + \nu^2 k^2 \] (2.12)

Here we have expanded \( \gamma_k = 1 - k^2/4 \), set \( Q + \Delta = \mu \) and defined \( \nu^2 = \mu^2/2 \).

In the lower, reentrant branch of the phase diagram, i.e. at \( T = 0, S^* < S < S_c, J_2 \ll J_1 \) we find from eqs. (B7) that the phase boundary is given by

\[ \frac{J_2^*}{J_1} = \pi(S_c - S) + (\pi^2 - 8)(S - S_c)^2 \] (2.13)

On the phase boundary,

\[ \omega_- = J_2 + ... \] (2.14)

Here the ellipsis denotes terms of order \( (S_c - S)^3 \), \( (J_2/J_1)^3 \) and higher. If we tune through the phase transition by varying \( J_2 \) we find that sufficiently deep in the ordered phase \( \omega_- \) increases as \( (J_2 J_1)^{1/2} \) as expected from spin-wave theory \[4\], while \( \omega_- \) approaches \( \omega_+ \) very rapidly as \( J_2 \) is decreased into the disordered phase. Indeed, within mean field theory we find find that for \( J_2/J_1 \leq \pi(S_c - S) - (8 - \pi^2/2)(S_c - S)^2 \) a solution with \( \omega_+ \neq \omega_- \) is not possible. The sharp transition from a solution with \( \omega_- \omega_+ \) to one with \( \omega_- = \omega_+ \) is an artifact of mean field theory, but the qualitative result, that \( (\omega_- - \omega_+)/\omega_- \) drops rapidly as one moves into the disordered phase, is likely to be correct for this model. The argument is that the ground state of the one plane model in the disordered phase is a singlet with a
gap of order $J_1 (S_c - S)$; for $J_2$ less than this value the interplane coupling can only slightly perturb the singlets.

For $S = S_c$ and $J_2 \ll J_1$ the $s$-boson has two low energy branches, one centered at $k = 0$ with dispersion given by eq. (2.12) and one given by

$$\omega_-(k)^2 = \omega_+^2 + 2\mu^2 (1 + \gamma_k) = \omega_+^2 + v^2 (k - P)^2 \tag{2.15}$$

Here $v = \mu/2 + ...$ and the ellipsis indicates terms of order $(J_2/J_1)^2$.

We now consider $T > 0$. In a realistic model there are no phase transitions, however different regimes of behavior exist. In the mean field theory, crossovers between different regimes sometimes appear as unphysical phase transitions. We are interested in properties in the disordered regime near the critical line. At the $T = 0$ phase transition, $\omega_+$ vanishes; close to it $\omega_+$ is much smaller than $J_1$. For $T < \omega_+(T = 0)$ the number of thermal excitations is negligible; the physics is of a singlet ground-state with a $q$-dependent gap to excitations. In the literature this is referred to as a "quantum disordered" regime. In this regime the low energy spectrum only involves one linear combination of the spin excitations in the two different planes; the antisymmetric one for $k$ near $P$ and the symmetric one for $k$ near 0. For $\omega_+(T = 0) < T < \omega_-(T = 0)$ this one linear combination becomes thermally excited. We refer to this as the "coupled-planes quantum critical regime". It only exists if $\omega_-(T = 0) - \omega_+(T = 0)$ is large enough. In the coupled-planes critical regime $\omega_+(T) \sim T$, but $\omega_-(T)$ takes its zero temperature value. The crossover from the quantum disordered regime to this quantum critical regime is identical to that occurring in a one-plane model. Finally, as $T$ is increased through $\omega_-(T = 0)$ the other linear combination of spin excitations also becomes excited and the two planes begin to fluctuate more or less independently. If $\omega_-(T = 0) \ll J_1$ then we find in the mean field theory that the behavior in this regime will be controlled by the $T = 0$ critical point of a single plane. We refer to this regime as the "decoupled-planes critical regime". In the mean field theory the change from the coupled-planes to the decoupled-planes regime occurs via a second order phase transition. We expect fluctuations not included in the mean field theory will convert this into a smooth
crossover. In the decoupled-planes regime, both $\omega_+$ and $\omega_-$ are proportional to $T$ with the same coefficient. Fig. 3 shows the $T$-dependence of $\omega_+$ and $\omega_-$ for parameters chosen so that $\omega_+(T = 0) = 0$, and indicates the different regimes.

III. PHYSICAL QUANTITIES

To obtain the magnetic susceptibilities we compute the linear response of the system to an externally applied magnetic field $\vec{H}_i^{(a)}$. The details are given in Appendix C. We find it convenient to decompose the externally applied field into parts symmetric and antisymmetric under interchange of planes, and compute the linear response to

$$\Delta H = \sum_q \frac{h_q^{(1)} - h_q^{(2)}}{2} O^a_q + \frac{h_q^{(1)} + h_q^{(2)}}{2} O^s_q$$  \hspace{1cm} (3.1)

Here $O^s$ and $O^a$ are operators creating spin fluctuations symmetric and antisymmetric under interchange of planes respectively. The only non-zero susceptibilities are

$$\chi^{aa}_q(\omega) = \int_0^\infty dt e^{i(\omega+i\epsilon)t} <[O^a_q(t), O^a_{-q}(0)]>$$  \hspace{1cm} (3.2a)

and

$$\chi^{ss}_q(\omega) = \int_0^\infty dt e^{i(\omega+i\epsilon)t} <[O^s_q(t), O^s_{-q}(0)]>$$  \hspace{1cm} (3.2b)

The uniform susceptibility (written as a susceptibility per spin and not as a susceptibility per unit cell) is

$$\chi(T) = \lim_{q \to 0} \chi^{ss}_q(\omega = 0) = \frac{1}{4T} \sum_k \sinh^{-2} \left( \frac{\omega_k}{2T} \right)$$  \hspace{1cm} (3.3)

We note that in the approximation of section II and the Appendices, namely,

$$\frac{k dk}{2\pi} = N(\gamma) d\gamma = \frac{\omega d\omega}{2}$$  \hspace{1cm} (3.4)

eq (3.3) becomes

$$\chi(T) = 2T \left[ \int_{\omega_-/2T}^{\infty} \frac{dxx}{\sinh^2(x)} + \int_{\omega_+/2T}^{\infty} \frac{dxx}{\sinh^2(x)} \right]$$  \hspace{1cm} (3.5)
From eq. (3.5) we see that in the coupled-plane quantum disordered regime \((\omega_+(T = 0) \gg T)\), \(\chi(T) \sim \omega_+ e^{-\omega_+ / T}\); this is a factor of two smaller than would be found for a single plane in the disordered regime with the same gap. In the coupled-plane critical regime \(\omega_+(T = 0) \ll T \ll \omega_-(T = 0)\), \(\chi(T) \sim T\) and in the decoupled-plane critical regime \(T \ll \omega_-(T = 0)\), we also have \(\chi(T) \sim T\) but with a coefficient larger by a factor of two. This behavior is easy to understand: in the coupled-plane regime one of the two spin degrees of freedom per unit cell is frozen out; in the decoupled-plane region both are free to fluctuate.

Next we consider \(\chi''(q, \omega)\) for \(q = P\). From the results of eq. (3.2a, 3.2b) we find, for \(\omega_0\)

\[
\chi_{aa}''(P, \omega, T) = \frac{\pi}{\omega} \coth(\omega/4T) \left[ \Theta(\omega - 2\omega_-) + \Theta(\omega - 2\omega_+) \right] 
\]

\[
\chi_{ss}''(P, \omega, T) = \frac{2\pi}{\omega} \left[ \Theta(\omega - (\omega_+ + \omega_-)) \left[ 1 + b((\omega^2 - \omega_+^2 + \omega_-^2)/2\omega) + b((\omega^2 + \omega_+^2 - \omega_-^2)/2\omega) \right] 
+ \Theta(\omega_- - \omega_+ - \omega) \left[ b((\omega_-^2 - \omega_+^2 - \omega^2)/2\omega) - b((\omega_-^2 - \omega_+^2 + \omega^2)/2\omega) \right] \right] 
\]

These formulae are plotted in fig. 5 for the parameters used to construct fig. 3. The sharp onset at \(T = 0\) is an unphysical feature of the dynamics in the mean field theory, which is removed when fluctuations are included [11,19]. A related peculiarity of the mean field theory is that \(\chi'(q, \omega = 0)\) decays as \(1/q\) for \(q\) near \(P\). We believe that despite the obvious artificialities the mean field expressions give some reliable information about the spin excitations of the model, as in the case of the one-plane Heisenberg model [13]. In particular, we believe that the location of the peaks and their relative magnitudes and temperature dependences give a reasonable representation of the location, relative magnitude and temperature dependence of the peaks in the appropriate susceptibilities of the model. We see that from eqs. (3.6) and (3.7) and fig. 5 that at low \(T\) the important energy scale for \(\chi_{aa}''\) is \(2\omega_+\) while for \(\chi_{ss}''\) it is \(\omega_+ + \omega_-\). Everywhere in the disordered phase the difference between these energies is less than \(J_2\). It is also clear that until the temperature becomes comparable to the scale \(T^*\) at which the crossover from the coupled-planes to the decoupled-planes critical regime occurs, \(\chi_{aa}'' \gg \chi_{ss}''\), and that \(\chi_{ss}''\) is confined mostly to high frequencies, of order \(2J_2\). For this reason we suspect that the neutrons scattering data,
which have not observed any \( \chi^{s\prime\prime}_{s} \) component for \( \omega < 40 \text{ meV} \), do not set a stringent limit on \( J_2 \), although they suggest that it is greater than 20 meV.

We now turn to the relaxation rates. Details of the computations may be found in Appendix C. We begin with that of Yttrium, \( 1/YT_1 T \), which is found to be

\[
\frac{1}{Y T_1 T} = 2\pi D^2 \lim_{\omega \to 0} \frac{1}{\omega} \sum_q |g(q)|^2 \chi^{s\prime\prime}_{s}(\omega)
\] (3.8)

The form factor \( g \) is equal to 4 for \( q \) near 0 and to \((q - P)^2\) for \( q \) near \( P \); a more precise formula is given in eq. (C15).

Using eqs. (3.4) and (C13) we find

\[
\frac{1}{Y T_1 T} = 8\pi D^2 T^2 \left[ \int_{\omega_+(T)/2T}^{\infty} \frac{dxx^2}{\sinh^2(x)} + \int_{\omega_-(T)/2T}^{\infty} \frac{dxx^2}{\sinh^2(x)} \right]
\] (3.9)

In the mean field approximation to both the coupled planes and the decoupled planes critical regimes, the yttrium rate \( 1/YT_1 T \sim T^2 \), so it vanishes faster than the static susceptibility, while in the low \( T \) limit \( 1/YT_1 T \sim e^{-\omega_+/T} \) is proportional to the uniform susceptibility. Note that the ratio of \( 1/YT_1 T \) to \( \chi^2 \) is the same in the coupled-plane critical regime as it is in the decoupled-plane critical regime. There are two compensating effects at work: in the coupled-plane regime there is only one spin mode at small \( q \) (instead of the two that occur in a model of two uncoupled planes) but in this mode the 8 spins add coherently to the yttrium relaxation rate, whereas in the decoupled-plane regime there are twice as many spin excitations (so one would naively expect the rate to be four times as large) but the two planes add incoherently (reducing the rate by a factor of two). \( 1/YT_1 T \) is plotted in fig. 4 for the parameters used to construct fig. 3.

We now consider the oxygen rate. This has one contribution from the small \( q \) fluctuations and one from fluctuations with \( q \) near \( P \). The latter is suppressed by a form factor because each oxygen sits symmetrically between copper sites, so a perfectly antiferromagnetic fluctuation would cancel on the oxygen site \([2]\). The result, derived in eq. (C17) is

\[
\frac{1}{O T_1 T} = \frac{C^2}{4} \lim_{\omega \to 0} \frac{1}{\omega} \sum_q |f(q)|^2 \left( \chi^{s\prime\prime}_{s}(\omega) + \chi^{aa\prime\prime}_{s}(\omega) \right)
\] (3.10)
This is precisely the usual result [2]. Again using the approximation of eq. (3.4), we get

\[
\frac{1}{\tau_1 T} = C^2 (2T)^2 \left[ \int_{\omega_-(T)/2T}^{\infty} dx \frac{2x^2 - (\omega_+/2T)^2}{\sinh^2(x)} + \int_{\omega_-(T)/2T}^{\infty} dx \frac{6x^2 - 2(\omega_+/2T)^2 - (\omega_+/2T)^2}{\sinh^2(x)} \right]
\]

(3.11)

In contrast to the yttrium, where the variation was by a factor of two, here the coefficient of the \( T^2 \) term varies by a factor of four between the coupled and decoupled-plane critical regimes.

In the mean field theory the oxygen rate varies as \( T^2 \) in the critical regime. We shall see in the next section that in the more physically reasonable scaling analysis the antiferromagnetic spin fluctuations lead to an oxygen relaxation rate proportional to \( T \) in the critical regime.

We now turn to the copper rate, which is given by

\[
\frac{1}{c u T_1 T} = \frac{1}{4} \lim_{\omega \to 0} \frac{1}{\omega} \sum_q (A - 4B\gamma(q))^2 (\chi^{ss''}(q, \omega) + \chi^{aa''}(q, \omega))
\]

(3.12)

Again this may be evaluated, giving

\[
\frac{1}{c u T_1 T} = \frac{(A - 4B)^2}{4} \left[ \int_{\omega_+(T)/2T}^{\infty} dx / \sinh^2(x) + 3 \int_{\omega_-(T)/2T}^{\infty} dx / \sinh^2(x) \right]
\]

(3.13)

This also is plotted in fig. 4 for the parameters used in fig. 3, and again there is a factor of four change from the coupled-planes critical regime to the decoupled-planes critical regime. Note that in the critical regime the Cu relaxation rate is \( T \)-independent. Again, this is due to the artificiality of the Schwinger-boson mean field theory. The scaling analysis predicts a \( 1/T \) behavior [11].

IV. SCALING ANALYSIS

The mean field analysis of the previous sections is known [11,19,20] to give incorrect results for dynamical susceptibilities for the single-plane Heisenberg model at finite spin degeneracy \( N \). A scaling theory which corrects these discrepancies has been developed [10,11]. In this section we extend the scaling theory to the coupled-plane system of interest here, and also construct a universal amplitude ratio for the NMR \( T_1 \) and \( T_2 \) relaxation times.
In the scaling theory of the one-plane model the important parameters for the physics on the disordered side of the phase boundary are the spin-wave velocity, $v$, the $T = 0$ gap to spin-1 excitations, $\Delta$, the quasiparticle residue of the lowest-lying $S=1$ excitation at $T = 0$, $A_{qp}$, and the temperature, $T$. Low energy physical quantities are universal functions of these parameters. Further, one must distinguish the "quantum disordered" $T \ll \Delta$ regime from the "quantum critical" $T \gg \Delta$ regime.

We now extend the theory to two coupled planes. We expect on general grounds, and showed explicitly using the mean field theory, that the between-planes coupling $J_2$ splits the spin excitation spectrum into acoustic and optic branches. The minimum gap to optic excitations, $\Delta_o$, is nonzero for $J_2 > 0$; the acoustic excitations acquire a gap $\Delta_a$ in the disordered phase. In the mean field treatment of the previous section, $\Delta_a = 2\omega_+$ while $\Delta_o = \omega_+ + \omega_-$. We found that on the phase boundary $\Delta_o \sim J_2$ while $\Delta_a = 0$. As one moves into the disordered phase, $\Delta_a$ rapidly approaches $\Delta_o$. Deep in the ordered phase, for small $J_2$, $\Delta_o \sim \sqrt{J_2 J_1}$ in agreement with spin-wave theory [4].

As we tune the system through the order-disorder transition, $\Delta_o$ remains nonzero, so the optic fluctuations are irrelevant in the renormalization group sense. Within the mean field approximation the transition is thus one in which the Heisenberg order vanishes and a single two-fold degenerate spin-wave mode of velocity $v_a$ acquires a gap $\Delta_a$. The usual universality arguments then imply that the transition is in the previously considered universality class, and that at $\omega, T \ll \Delta_o$ the physical quantities are given by the previously calculated universal functions [11] evaluated at arguments $v_a$ and $T/\Delta_a$. We refer to this $\omega, T \ll \Delta_o$ regime as the coupled-plane regime, and distinguish the $T \ll \Delta_o$ "coupled-plane disordered regime" from the $T \gg \Delta_o$ "coupled-plane critical regime". Of course, if $(\Delta_o - \Delta_a)/\Delta_o$ is too small the coupled-planes critical regime may not exist.

There is one subtlety in the analysis of the coupled-planes regime: the universal forms give susceptibilities in units of $\text{emu/area}$. A unit cell contains two Cu atoms (one in each plane); the susceptibilities are evenly divided between the two planes, thus the susceptibilities per Cu are one half of the one-plane values. Further, because the Cu and O nuclei of interest
for high-Tc NMR experiments sit in one CuO$_2$ plane, the hyperfine coupling of the Cu or O nucleus to the surviving spin-degree of freedom is half as large as in a single-plane model, so the Cu and O relaxation rates, which go as the square of the hyperfine coupling constant, will be one quarter of the usual size. The yttrium nucleus, however, sits between two planes and over the center of a plaquette of four Cu nuclei. In the coupled-planes regime the hyperfine coupling per moment is half the expected value, but the eight nearest neighbor spins add coherently, so the yttrium NMR rate is only one half of the expected value. These factors were explicitly derived in the mean field analysis of the previous section; we have given a qualitative argument here.

As one increases the temperature from zero in the disordered phase one passes first through the coupled planes disordered regime and then, if $(\Delta_o - \Delta_a)/\Delta_o$ is sufficiently large, through the coupled-planes critical regime. As one continues to increase the temperature it becomes comparable to the optic mode energy $\Delta_o$ and the bilayers become uncorrelated. If $\Delta_o$ is sufficiently small, i.e. if $J_2 \ll J_1$ then at $T\Delta_o$ the physics will still be controlled by a $T = 0$ critical point. We showed using the mean field theory that in this regime each plane fluctuates independently and is in the quantum critical regime of a one-plane model. We believe this conclusion survives beyond mean field theory. We refer to the regime $T\Delta_o$ as the “decoupled-planes critical regime”. It is probable that one could extend the calculation of reference [11] to incorporate fluctuations into our mean-field analysis of the crossover between the coupled and decoupled planes regimes, but we have not attempted this. Instead, we consider the uniform susceptibility and NMR in each plane separately. The scaling properties of the single-plane transition have recently been elegantly derived and discussed [11]. We summarize, as briefly as possible, the results we will need and their extension to the two-plane system.

The correlation length, $\xi$ is a universal function of $T$ and $\Delta$,

$$\xi = \frac{\hbar v}{k_B T} X(k_B T / \Delta)$$

(4.1)

with $X(y)$ a universal function which tends a number very nearly unity (1.03 in a large N
expansion with terms of order 1 and 1/N included and N set equal to 3) as $y$ tends to infinity (so $\xi \sim h v/k B T$ for $T \gg \Delta$) and to $y$ as $y$ tends to zero (so $\xi$ tends to $h v/\Delta$ for small $T$). Note that for $J_2 \ll J_1$, $v$ is essentially the same for acoustic and optic modes, so that this relation is valid in both coupled and decoupled-plane regimes.

The divergent part of the order parameter susceptibility, $\chi_{AF}$, may be written

$$\chi_{AF}(q, \omega; T) = \chi_{AF} \xi^{2-\eta} \phi_{AF}(q \xi, \omega \xi/v; T/\Delta) \quad (4.2)$$

Here $\chi_{AF}$ contains the dimensions and $\phi_{AF}$ is a universal function. We have introduced the exponent $\eta$ for completeness even though for the transition in question it is very nearly zero [11,21]. In the coupled-planes regime we should interpret this as a susceptibility per unit area; in the decoupled-planes regime as a susceptibility per area per plane. Here $\chi_{AF}$ is a critical amplitude; its value is not universal but from it and other measurable quantities universal amplitude ratios may be constructed. In particular, $\chi_{AF} = A_{qp}/v^2$ where $A_{qp}$ is the quasiparticle residue of the lowest-lying $S=1$ excitation in the disordered phase at $T=0$ and we have made explicit the factors of the velocity which were set to unity in [11].

The uniform susceptibility has also a scaling form; here even the dimensional prefactor is known [11]. The susceptibility in units of emu per area is

$$\chi_u(q, \omega; T) = \frac{g^2 \mu_B^2}{h v \xi} \phi_u(k_B T/\Delta) \frac{(D_s/\xi)(q \xi)^2}{-i \omega \xi + D_s/\xi(q \xi)^2} \quad (4.3)$$

Here $g$ is the electron g-factor and $\mu_B$ is the Bohr magneton. Again this is a susceptibility per unit area in the coupled planes regime and a susceptibility per area per plane in the decoupled planes regime. $D_s$ is the spin diffusion coefficient; it has a dependence on $T$ and $q$ which we have suppressed here. $\phi_u$ is a universal function which tends to a constant as $y$ tends to infinity and vanishes rapidly as $y$ tends to zero. It is usually assumed that the quantity $g \mu_B$ may be taken to have the free electron values because in the nonlinear sigma model treatment of the critical point it is not renormalized from its bare value; however this assumption has not been proven for more general models.

We shall be most interested in applying this formula in the critical regime $T \gg \Delta$; we
therefore proceed to estimate $D_s$ in this regime. We argue that for the modes relevant to NMR experiments,

$$ D_s = D_s^0 v^2 \frac{\hbar \ln^{1/2}(1/q)}{k_B T} \quad (4.4) $$

Here $D_s^0$ is a number, presumably of order unity. The factor of $1/T$ arises as follows. For excitations of velocity $v$ and scattering rate $\Gamma$, $D_s \sim v^2/\Gamma$. Further, conventional dynamic scaling suggests that modes at scales shorter than the correlation length are weakly damped, while those at longer scales are overdamped, implying that the scattering rate for spin excitations is proportional to $T$. The factor of $\ln^{1/2}$ comes from the breakdown of hydrodynamics in two spatial dimensions [22].

We are now able to discuss relaxation rates. We begin with the yttrium rate. We saw in the previous section that the yttrium nucleus is coupled only to fluctuations of the uniform magnetization. By comparing the notations of this and the previous section we see that in the coupled-planes regime the coupling constant is $4Da^2/\mu_B g$ (recall that there are 8 Cu neighbors but that the spin density is evenly divided between the two planes). Calculating the relaxation rate in the usual way gives

$$ \frac{\hbar}{\sqrt{T_1 k_B T}} = \frac{16D^2a^4}{\hbar^3 D_s^0 v^2 \xi} \frac{k_B T}{\pi} \ln^{1/2}(1/qa) \quad (4.5) $$

Recall that $\phi_u$ refers to two planes; normalizing per plane restores the factor of 32 from [3.9]. A power of $\ln^1$ was obtained previously by Chakravarty and Orbach in a calculation of relaxation in an ordered magnet [20]; the different power comes because they did not consider the corrections to hydrodynamics. The logarithm will be cut off at some scale by a three dimensional coupling $J_{3D}$ and is presumably not important in practice. The important result is that in the quantum disordered regime both $D_s$ and $\xi$ go as $1/T$ so the yttrium relaxation rate in this model is proportional to $T^2$ up to logarithms, as was found in the mean field theory of the previous section. In the decoupled-planes critical regime the calculation is identical except that we must add two contributions, one from each plane. For each contribution the coupling constant is $4Da^2/\mu_B g$ and we must neglect interplanar
correlations. The result is a factor of two increase in the coefficient of the $T^2$ term, as was found in mean field theory.

We now consider the oxygen relaxation rate. This has one contribution from the small-$q$ fluctuations which may be evaluated as we did for yttrium and which will be seen to be sub-dominant, and another contribution from the antiferromagnetic fluctuations, which we evaluate. The coupling constant connecting the oxygen nucleus to an antiferromagnetic fluctuation in a given plane of wavevector $q$ (measured from $P$) may be written $C_{AF}a^2 f(qa)$ where $C_{AF}$ is a priori not the same as the coupling constant $C$ introduced before. Symmetry implies that $f(x) \sim x^2$ at small $x$. Combining this with eq. (4.2) for $\chi_{AF}$ gives, in the coupled planes regime:

$$\frac{\hbar}{c_{T_1}k_B T} = \frac{1}{4} \frac{C_{AF}^2 a^3 \chi_{AF}(\xi/a)^{(1+\eta)} \phi_0(T/\Delta_a)}{\hbar \nu \mu_B^2}$$

Here $\phi_0(z)$ is a universal function obtained by integrating $\lim_{y\to0} x^2 \phi''_{AF}(x, y; z)/y$ over $x$. We have assumed the integral converges; in the spin-only model this is reasonable because at momentum scales larger than the inverse correlation length the model goes over to spin-wave theory and the integrals there converge. In a more general model the issue of convergence is less clear. Thus the oxygen relaxation rate in this model scales at $T^{1+\eta}$ with a non-universal prefactor involving both the hyperfine coupling $C_{AF}$ and the amplitude $\chi_{AF}$. The oxygen relaxation rate scales differently from the yttrium because the oxygen is coupled (albeit weakly) to the antiferromagnetic fluctuations, while the yttrium is not. As we have previously argued, the constant $C_{AF}$ is larger by a factor of two in the decoupled-planes regime than it is in the coupled-planes regime, leading to a factor-of-four change in the relaxation rate.

We finally consider the copper. This is coupled to the spins by a matrix element $A_{AF}a^2/\mu_B$. The relaxation rate in the coupled-planes regime is

$$\frac{\hbar}{c_{T_1}k_B T} = \frac{A_{AF}^2 a^3 \chi_{AF}(\xi/a)^{1-\eta} \phi_{Cu}(T/\Delta)}{4\hbar \nu \mu_B^2}$$

Thus the Cu relaxation rate $1/T_1 T$ in this model scales at $T^{\eta-1}$ times a non-universal prefactor involving both the hyperfine coupling and the amplitude $\chi_{AF}$. The formula [4.7]
has been previously given [11]. The same factor of four change in the coefficient of the leading $T$-dependent term between the coupled-plane and decoupled-plane regimes that occurred for the oxygen relaxation rate occurs for the copper.

The $T_1$ relaxation rate is determined by the imaginary part of $\chi$. The $T_2$ rate measures the real part of $\chi$. Specifically, in circumstances relevant to experiments on high-$T_c$ materials [23]

\[ \left(\frac{1}{T_2}\right)^2 = n_m \sum_q \left[A_{AF} \chi'(q, \omega = 0)\right]^2 \]  

(4.8)

where $n_m$ is the density of NMR nuclei. Substituting the scaling ansatz and integrating gives

\[ \frac{\hbar}{T_2} = n_m^{1/2} \frac{A_{AF}^2 a^3 \chi_{AF}}{\mu_B^2} (\xi/a)^{1-n} \phi_{T2}(T/\Delta) \]  

(4.9)

By combining eqs. (4.7,4.9) we see that apart from the factor $n_m^{1/2}$ and the velocity $v$, the ratio of $T_2$ to $T_1T$ is universal, and indeed takes the same value in the coupled-planes and decoupled-planes critical regimes. Note however that in the coupled-planes regime the contribution of the optic excitations to $1/T_2$ will be large (of order $1/\Delta_o$). The contribution of the acoustic sector is of order $1/\Delta_a$. Thus $1/T_2$ will attain its universal value in the coupled-planes regime only if $(T, \Delta_a) \ll \Delta_o$.

Sokol and Pines [8] have previously made the interesting observation that the observed $T$-independence of $T_2/T_1T$ in YBa$_2$Cu$_3$O$_{6.6}$ for $T > 150$ K suggests that the magnetic dynamics in this material is controlled by the $z = 1$ critical point considered here. We see that the magnitude provides information about the velocity, $v$, and that this must be consistent with the uniform susceptibility.

V. CONCLUSION

We have studied some aspects of the $T = 0$ magnetic-non-magnetic transition occurring in a model of two antiferromagnetically coupled planes of antiferromagnetically correlated
spins. The model is defined in eq. (1.1) and depicted in fig. 1. The two dimensionless parameters are \( J_2/J_1 \) (the ratio of the between-planes coupling \( J_2 \) to the in-plane coupling \( J_1 \)) and \( S \), the magnitude of the spin in one plane. The important dimensional parameter is the spin wave velocity, \( v \). The phase diagram at \( T = 0 \) in the \( J_2/J_1 - S \) plane is shown in fig. 2. For a single plane (i.e. \( J_2 = 0 \)), decreasing \( S \) through a critical value \( S_c \) causes a phase transition between a magnetically ordered phase and a singlet phase with a gap to spin excitations. Some properties of this transition were determined by Chakravarty, Halperin and Nelson [10] and it was analyzed in detail by Sachdev, Chubukov and Ye[11].

For the coupled-plane system we found using a Schwinger-boson mean field theory that a large value of the interplanar coupling \( J_2 \) destroys the magnetism even for \( SS_c \) (because it favors binding of nearest neighbor spins on different planes into singlets), while a small \( J_2 \) promotes order by increasing the effective size of the spin in a unit cell. The interplay of these two different sorts of physics leads to the reentrant phase diagram shown in fig. 2. This phase diagram differs in an important respect from our previous interpretation of the data on spin susceptibilites of \( La_{2-x}Sr_xCuO_4 \) and \( YBa_2Cu_3O_{6.6} \) [7]. In both compounds it is clear that doping destroys the magnetism. In \( La_{2-x}Sr_xCuO_4 \) interplane coupling is negligible and at least the Cu relaxation rate and single crystal susceptibility data show no clear evidence of a singlet phase with a gap to excitations (although some susceptibility and Knight shift data have been so interpreted [9][11]). On the other hand, in \( YBa_2Cu_3O_{7-\delta} \) it is clear that the nearest-neighbor CuO_2 planes are coupled by an interaction at least of order 300 K, and ”spin-gap” effects are very easily observed in susceptibilities and relaxation rates for \( 0.1 < \delta < 0.5 \). Thus it appears that in the real materials a presumably modest between-planes coupling promotes ”spin-gap” behavior, and therefore that the spin-only model is missing some essential feature of the physics, most likely related to the presence of mobile holes.

Although it is not completely realistic, the coupled-plane model might capture some aspects of the physics of \( YBa_2Cu_3O_{6.6} \) and \( YBa_2Cu_4O_8 \). We therefore calculated the predictions of the model for the temperature and frequency dependence of the susceptibilities.
measured in NMR and neutron scattering using the Schwinger boson mean field method and a scaling analysis. We studied parameters such that the model has no long range order at $T = 0$. The behavior in the disordered phase of a single plane of Heisenberg spins is understood [11-13]. In the single-plane case, the important parameter is the $T = 0$ gap to spin one excitations, $\Delta$. The spin-one excitations are essentially spin waves with a gap. There are several regimes of temperature. For $T \ll \Delta$ the number of thermal spin excitations is negligible; the static spin susceptibility at $q = 0$ and the dissipative part of the dynamic susceptibility at all $q$ and at $\omega \ll \Delta$ have an activated temperature dependence $\sim e^{-\Delta/T}$. This regime is referred to as the ”quantum disordered regime”. If the microscopic exchange constant $J \gg \Delta$ then for $\Delta \ll T \ll J$ another regime exists in which the physics is dominated by the $T = 0$ critical point but the gap is not important. In this regime the static uniform susceptibility is proportional to $T$ and the antiferromagnetic correlation length grows as $1/T$. The regime is referred to as the ”quantum critical regime”.

In the two plane model of interest here the between-planes coupling $J_2$ splits the spin excitation spectrum into acoustic and optic modes. There are two important scales: $\Delta_a$, the $T = 0$ gap to acoustic excitations and $\Delta_o$, the $T = 0$ gap to optic excitations. Both gaps are nonzero in the disordered phase. At the antiferromagnetic-singlet transition $\Delta_a$ vanishes while $\Delta_o$ remains non-zero. At the transition we found from the mean field theory that $\Delta_o = J_2$. As one moves deeper into the disordered phase, $(\Delta_o - \Delta_a)/\Delta_o$ decreases rapidly. If one is sufficiently close to the phase boundary, so that $0 < \Delta_a \ll \Delta_o \ll J_1$, there are three regimes. These are depicted in fig. 6. For $(T, \omega) \ll \Delta_o$ the optic mode of the two plane system is frozen out and the physics is dominated by the acoustic mode of the two plane system. We refer to this as the ”coupled-planes” regime. For $(T, \omega) \ll \Delta_a$ even the acoustic mode is frozen out. This is the ”coupled-planes disordered regime”. For $\Delta_a \ll T \ll \Delta_o$ the acoustic mode is thermally activated and the system is in the ”coupled-planes quantum critical regime”. Finally, for $\Delta_o \ll T$ the coupling between the planes become negligible and the planes fluctuate independently. This is the ”decoupled planes” regime. If $\Delta_o \ll T \ll J_1$ then we argued that the spin dynamics in each plane is separately
given by the quantum critical behavior of a one-plane model. Of course if \((\Delta_o - \Delta_a)/\Delta_o\) is too small, the coupled-plane critical regime does not exist, while if \(\Delta_o/J_1\) is too large, the physics in the decoupled-planes regime will not be controlled by a \(T = 0\) critical point.

We now summarize the results we obtained in sections III and IV for the temperature and frequency dependence of the NMR rates and susceptibilities. We found that the difference, \(\Delta_o - \Delta_a < J_2\) everywhere in the disordered phase, and that the contribution from the optic modes near the antiferromagnetic point was rather small and only weakly temperature dependent if \(\Delta_o \gg \Delta_a\). The uniform susceptibility, \(\chi(T)\), is activated in the coupled planes disordered regime; in the coupled-planes critical regime \(\chi(T) = 0.5ET\) (here \(E\) is a number) and in the decoupled-planes critical regime \(\chi(T) = ET\). The factor of two change in the coefficient of \(T\) between the coupled and decoupled planes regimes was derived explicitly from the Schwinger boson mean field theory. The physical origin, we believe, is that in the coupled-plane regime one of the two spin modes at each \(k\) (namely, the optic mode) is frozen out and does not contribute to \(\chi\), whereas in the decoupled-planes regime both modes contribute.

The \(T\)-dependences of the nuclear relaxation rates are more subtle. They are summarized in fig 6. We consider first the copper and oxygen rates. In the quantum disordered regime all rates are activated. In the coupled-planes critical regime the Cu rate \(1/T_1 T = 0.25A/T\) while the oxygen rate is given by \(0.25CT\) Here we have set the exponent \(\eta\), which is in practice very small [21] to zero. \(A\) and \(C\) are constants. In the decoupled planes critical regime the formulae are the same except that the number 0.25 becomes 1. The factor of four change in the coefficient of the leading \(T\)-dependence of the Cu and O rates between the coupled-planes and decoupled-planes critical regimes was derived from the mean field theory. We believe that the physical origin is that in the coupled-planes regime only the acoustic mode contributes to relaxation rates. In this mode the spin fluctuation is even divided between the two planes; the hyperfine coupling constant connecting a Cu or O nucleus in a given plane to the spin fluctuation is thus half of what it would be in a one-plane theory, and the rate goes as the square of the hyperfine coupling. The factor of four variation has an
interesting implication for estimates of the relative strengths of the antiferromagnetic spin fluctuations in different materials. Authors (including us) who had considered the question previously argued that because the Cu relaxation rate in $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ was smaller than in $\text{La}_{2-x}\text{Sr}_x\text{CuO}_4$, while the hyperfine couplings were approximately the same, the spin fluctuations must be weaker in the former material. We see now that until one knows whether $\text{YBa}_2\text{Cu}_3\text{O}_{7-\delta}$ is in the coupled-planes or decoupled-planes regime one cannot meaningfully compare the magnitudes of the relaxation rates to those of $\text{La}_2\text{CuO}_4$.

The yttrium relaxation rate behaves slightly differently, because the yttrium nucleus is coupled to a symmetric combination of Cu nuclei in the two planes. In the disordered regime the yttrium rate is activated, in the coupled-planes critical regime it goes as $0.5DT^2$ and in the decoupled-planes critical regime it goes as $DT^2$. The yttrium rate changes only by a factor of two between the coupled-planes and decoupled-planes critical regimes because in the coupled-planes regime the spins in different planes move coherently while in the decoupled-planes regime the spins move incoherently. The difference between coherent and incoherent addition of spin fluctuations produces a factor of two which partially compensates for the factor of four discussed previously.

We now consider the implications of our results for experiments on $\text{YBa}_2\text{Cu}_3\text{O}_{6.6}$ and $\text{YBa}_2\text{Cu}_4\text{O}_8$. Below $T = T^* \sim 150$ K all of the relaxation rates including the Cu $1/T_1T$ drop as $T$ is decreased. We believe that this can only occur if the physics below $T \sim 150$ K is dominated by thermal excitations above a $T = 0$ singlet state with a gap to spin excitations. In a spin-only model such as that considered here one would model this by choosing a value of spin $S$ such that the system was near to, but on the disordered side of, the phase boundary in fig. 2. Further, the value of $T^*$ implies that $\Delta_0 \sim 150$ K. We must next consider the value of the interplanar coupling $J_2$. The experimental evidence is not conclusive. Only the acoustic excitation of the two-plane system has been observed via neutron scattering in any member of the YBa$_2$ family of high-$T_c$ materials [4,5]. The main effort has been at energies less than 40 meV and temperatures less than 150 K. This would suggest that in the metallic YBa materials, $\Delta_0 \geq 40$ meV. NMR measurements on $\text{YBa}_2\text{Cu}_4\text{O}_8$ provide more
information. The Cu $T_1$ has been found to obey very well the Curie law $1/T_1 T \sim 1/T$ for $200 \text{ K} < T < 700 \text{ K}$ \cite{24}. This implies that the temperature scale at which the bilayers become decoupled in this material is less than 200 K or greater than 700 K. We believe a bilayer coupling greater than 700 K would be very hard to justify on theoretical grounds. The argument is that the in-plane $J \sim 1500 \text{ K}$, while $J_2 \ll J_1$ because band structure \cite{25} and photoemission \cite{26} results imply that the between-planes hybridization is much less than the in-plane hybridization, and the exchange energy scales as a high power of the hybridization. However, a bilayer coupling much less than 200 K may not be consistent with the neutron data. From the mean field theory we found $\Delta_o \leq J_2 + \Delta_a$; our estimate $\Delta_a \sim 150 \text{ K}$ then implies $\Delta_o \leq 350 \text{ K}$ if $J_2 < 200 \text{ K}$. Thus presently available data provide somewhat contradictory answers to the question whether YBa$_2$Cu$_4$O$_8$ is in the coupled-planes or decoupled-planes regime for $200 \text{ K} \leq T \leq 700 \text{ K}$. In what follows we consider both possibilities.

We now turn to a more quantitative discussion. Sokol and Pines have proposed that the magnetic dynamics of underdoped high-$T_c$ materials are determined by the critical point discussed here, and their discussion has been amplified and extended by Barzykin, Pines, Sokol and Thelen \cite{9}. They do not consider the bilayer coupling. They propose that these materials are in the quantum critical regime for $T \geq 150 \text{ K}$ and in the quantum disordered regime for $T \leq 150 \text{ K}$. The essential piece of evidence they cite in favor of their proposal is the observed approximate $T$-independence of the ratio $T_1 T/T_2$ for $150 \text{ K} \leq T \leq 300 \text{ K}$. The observed \cite{27} magnitude of this ratio is approximately one-half of the value observed \cite{28} in La$_2$CuO$_4$ and calculated \cite{29} for the $S = 1/2$ Heisenberg model with $J = 0.13 \text{ eV}$. The density $n_m$ of $^{63}\text{Cu}$ NMR ions is the same in the La-Sr and YBa materials, so we conclude from eq. (1.9) that if the magnetic dynamics of YBa$_2$Cu$_3$O$_{6.6}$ and YBa$_2$Cu$_4$O$_8$ are well described by the universal scaling forms in either the coupled-planes or the decoupled-planes regimes, then the appropriate spin-wave velocity $v$ is about one half of the 0.8 eV Å appropriate for La$_2$CuO$_4$ \cite{30}, i.e.
The value of \( v \) makes a prediction for the magnitude of the correlation length. From eq. (4.1) we find \( \xi/a = 4 \) at \( T = 300K \) and \( \xi/a = 6 \) at \( T = 200K \); below this temperature the crossover to the quantum disordered regime presumably means that the \( T \) dependence of the correlation length becomes much weaker. These lengths are rather larger than observed in neutron scattering experiments [34].

These considerations also have an implication for the Cu \( T_1 \) relaxation rate. In the quantum critical regime, the theoretical result for the Cu relaxation rate is \( 1/T_1T = A/T \). The coefficient \( A \sim A_{qp}/v^2 \) [11] where \( A_{qp} \) is the quasiparticle residue of the lowest lying \( S=1 \) state above the gap at \( T = 0 \). It may in principle be determined from neutron scattering measurements at low \( T \). The coefficient \( A \) also depends on hyperfine couplings (which have been claimed to be the same in \( La_2CuO_4 \) as in \( YBa_2Cu_3O_{6.6} \) and \( YBa_2Cu_4O_8 \) [23]) and on whether the material is in the coupled-planes or decoupled-planes regimes. In the absence of a measurement of \( A_{qp} \) one cannot definitively calculate the Cu relaxation rate; however, it is interesting to attempt to estimate it. We first argue as follows: \( La_2CuO_4 \) has been claimed to be in the quantum critical regime for \( T > 600K \) [9,11,28]; further, at these temperatures the Cu \( T_1 \) has only a weak doping dependence, implying that the combination \( A_{qp}/v^2 \) depends only weakly on doping. If this is correct, then we would expect that if \( YBa_2Cu_3O_{6.6} \) and \( YBa_2Cu_4O_8 \) were in the decoupled planes regime, \( A \) would be well approximated by the value \( A = 3300 \text{ sec}^{-1} \) [31] appropriate to \( La_2CuO_4 \), while if it were in the coupled plane regime we would expect \( A = 800 \text{ sec}^{-1} \). (In fact, the values might be slightly larger since the \( J \) for \( YBa_2Cu_3O_{6.0} \) is smaller than the \( J \) for \( La_2CuO_4 \) [33]). In fact, in \( YBa_2Cu_4O_8 \), \( A = 1600 \text{ sec}^{-1} \) [24] compatible with neither estimate. An alternative argument would be to say that \( A_{qp} \) has the dimension of energy, and the characteristic energy scale is given by dividing the velocity, \( v \), by the lattice constant, \( a \), implying \( A \sim 1/v \) so from eq (5.1) we would expect that in the coupled-planes regime the value of the Cu \( T_1 \) would come out about right. A third possibility is that for some unknown reason \( A_{qp} \) could
drop by a factor of 8 upon going from $La_{2-x}Sr_xCuO_4$ to YBa$_2$Cu$_4$O$_8$, so that the data for $T > 150K$ would be consistent with the decoupled planes regime. Of course a fourth possibility is that the theory is not applicable. Neutron measurements of absolute scattering intensities on underdoped YBa materials would be very helpful in resolving this issue.

Our discussion so far has emphasized properties related to the antiferromagnetic fluctuations. These are in a sense robust and relatively model-independent, depending as they do primarily on the existence of a growing correlation length, a weak $J_2$ and a spin-gap at low $T$. We now consider small-$q$ properties. In the Heisenberg model, the behavior of the small-$q$ susceptibility is very closely tied to the behavior of the large-$q$ susceptibility [11,32]. In a more fermi-liquid-like model this need not be true, and therefore the bilayer coupling, which strongly affects the behavior near the antiferromagnetic point, need not in a more realistic model also strongly affect the susceptibility near $q = 0$. It is also clear that the spin-only model is not, by itself, a reasonable description of the small-$q$ spin dynamics of $YBa_2Cu_3O_{7-\delta}$ or $YBa_2Cu_4O_8$. For example, the observed yttrium nuclear relaxation rate does not vary as $T^2$ but is more nearly proportional to the static susceptibility [6]. Also, our calculated oxygen nuclear relaxation rate is too small by about a factor of 16 to explain the data [34]. Thus, we must invoke an extra contribution to $\chi''$ existing at least at small $q$. It is natural to suppose that this is due to the mobile carriers and that therefore the contribution to $\chi''$ is of more or less the fermi-liquid form. However, the fermi-liquid like contribution cannot be appreciable near the antiferromagnetic point or it would overdamp the spin waves and change the universality class of the magnetic fluctuations [13,14]. It has very recently been argued [35] that in the Shraiman-Siggia model of doped antiferromagnets [?] precisely the required behavior occurs, with the fermions making an additive contribution to the small $q$ but not the large $q$ susceptibilities. A similar conclusion was drawn from high temperature series expansions [29]. In the resulting two-component picture $\chi = \chi_{spin} + \chi_{qp}$, with the fermi-liquid like piece $\chi_{qp}$ providing the yttrium and oxygen relaxation and the $\chi_{spin}$ given by the theory we have discussed and providing the nontrivial temperature dependence of the uniform susceptibility and the Cu relaxation rate. Sokol
and co-workers have made a similar argument on phenomenological grounds, claiming that
the temperature dependence of $\chi$ in YBa$_2$Cu$_4$O$_8$ for $200 \, K \leq T \leq 700 \, K$ is consistent
with the behavior of the spin-only model in the quantum critical regime [9]. Now whether
one supposes the material to be in the coupled-planes or decoupled-planes critical regime,
the theory implies $\chi(T) = a + bT$. We ignore the value of $a$, on the grounds that it is
dominated by the fermions which are beyond the scope of the theory, and consider the
value of $b$, which is given by eq. (1.3). From eq. (??) assuming $g\mu_B$ takes the same value
as in La$_2$CuO$_4$ we find $b = 5 \times 10^{-3}$ states/eV − Cu − K for the decoupled-planes regime
and $b = 2.5 \times 10^{-3}$ states/eV − Cu − K for the coupled-planes regime. The data say that
$b \sim 1.6 \times 10^{-3}$ states/eV − Cu − K [37]. This too weak $T$ dependence of $\chi$ in the critical
regime suggests to us that the straightforward two-component approach is not applicable to
YBa$_2$Cu$_4$O$_8$, and that the presence of carriers modifies the magnetic behavior more dramat-
ically. We note, however, that two results which seem to be qualitatively consistent with
the calculations presented here are: (a) although the difference is not dramatic, the yttrium
rate seems to drop faster than the oxygen rate as $T$ is lowered and (b) the magnitude of the
yttrium rate is larger than expected from a model in which the planes are uncoupled [38].

Whatever is the correct theory, the distinction we have drawn between the coupled-planes
and the decoupled-planes regimes will still be important. Further, if the NMR and neutron
data on underdoped YBa superconductors are both taken at face value, then the crossover
between the coupled-planes and decoupled-planes regimes occurs either at $T > 700K$ or at
$T \sim 200K$. The larger value seems to us to require an implausibly large between-planes
coupling; the smaller value would imply that the crossover to the quantum disordered regime
is complicated by a simultaneous freezing out of the optic mode of the bilayer system.

ACKNOWLEDGMENTS

H. M. was supported in part by the NSF under Grant No. PHY89-04035. We thank D.
Pines and A. V. Sokol for helpful discussions and for preprints of their work. A. J. M. thanks
P. C. Hohenberg for a helpful discussion concerning amplitude ratios and R. E. Walstedt for a critical reading of the manuscript. The authors thank the Correlated Electron Theory Program at Los Alamos National Laboratory for hospitality while part of the manuscript was written.

APPENDIX A: DERIVATION OF MEAN FIELD EQUATIONS

We begin from eq. (1.1). We write the model as a functional integral, introduce a field $Q^{(a)}_{<i,j>}$ to decouple the $J_1$ interaction, a field $\Delta_i$ to decouple the $J_2$ interaction and a field $\mu$ to enforce the constraint. We find for the partition function, $Z$,

$$Z = \int \mathcal{D}\Delta \mathcal{D}Q^+ \mathcal{D}b^\dagger b^\dagger \mathcal{D}\mu \exp \left( - \int_0^\beta d\tau \mathcal{L}' \right)$$  \hspace{1cm} (A1)

with

$$\mathcal{L}' = \sum_{i\alpha} b^\dagger_{i\alpha} \left[ \partial_\tau + \mu^{(a)}_i \right] b^{(a)}_{i\alpha} + \frac{1}{4} \sum_{<i,j>,\alpha} b^\dagger_{i\alpha} b^{(a)}_{j\alpha} Q^{(a)}_{<i,j>} + h.c.$$

$$+ \sum_{i\alpha} b^\dagger_{i\alpha} b^{(2)}_{i\alpha} \Delta_i + h.c.$$

$$+ \sum_{<i,j>,\alpha} \frac{|Q^{(c)}_{<i,j>}|^2}{8J_1} + \sum_i \frac{2|\Delta_i|^2}{J_2}$$  \hspace{1cm} (A2)

The different normalizations of $Q$ and $\Delta$ have been introduced, so that the final expression for the boson energy, eq. (A9), has no numerical factors. We next introduce symmetric (s) and antisymmetric (a) bose fields via

$$b^{(1)}_{k\alpha} = \frac{1}{\sqrt{2}} (s'_{k\alpha} + a'_{k\alpha})$$  \hspace{1cm} (A3a)

$$b^{(2)}_{k\alpha} = \frac{1}{\sqrt{2}} (s'_{k\alpha} - a'_{k\alpha})$$  \hspace{1cm} (A3b)

We make the mean field approximation of space and time independent $Q, \Delta, \mu$, Fourier transform the boson operators and obtain

$$\mathcal{L}_B = \sum_{k\alpha} s^\dagger_{k\alpha} [\partial_\tau + \mu] s_{k\alpha} + \frac{1}{2} (Q_k + \Delta) s^\dagger_{k\alpha} s^\dagger_{-k\alpha} + h.c.$$

28
\[ + \sum_{k\alpha} a_{k\alpha}^\dagger [\partial_r + \mu] a_{k\alpha}^\prime + \left[ \frac{1}{2}(Q\gamma_k - \Delta) a_{k\alpha}^\dagger a_{-k\alpha}^\dagger \right] + h.c. \]  

(A4)

with

\[ \gamma_k = \frac{1}{2}(\cos k_x + \cos k_y) \]  

(A5)

The boson part of this equation may be decoupled by a Bogoliubov transformation. The resulting quasiparticles \( s \) and \( a \) are defined by

\[ s_{k\alpha}^\dagger = \cosh \theta_k s_{k\alpha}^\dagger - \sinh \theta_k s_{-k\alpha} \]
\[ a_{k\alpha}^\dagger = \cosh \theta_{k\alpha} a_{k\alpha}^\dagger + \sinh \theta_{k\alpha} a_{-k\alpha} \]  

(A6)

with

\[ \tanh 2\theta_k = [Q\gamma_k + \Delta]/\mu \]  

(A7)

and

\[ P = (\pi, \pi) \]  

(A8)

The energy of the \( s \)-bosons is

\[ \omega_k = \sqrt{\mu^2 - (Q\gamma_k + \Delta)^2} \]  

(A9)

The energy of an \( a \)-boson at a wavevector \( k \) is \( \omega_{k+p} \).

The free energy \( F \) may be computed in the standard way and is

\[ F = 4NT \sum_k \ln[2 \sinh(\omega_k/2T)] + NQ^2/2J_1 + 2N\Delta^2/J_2 - 2N(1 + 2S)\mu \]  

(A10)

The mean field equations, eqs. (2.9), follow from differentiating this equation with respect to \( \mu \), \( Q \) and \( \Delta \).

**APPENDIX B: APPROXIMATE SOLUTION OF MEAN FIELD EQUATIONS**

We begin with eqs. (2.9). We recast them as \( \int \frac{\rho_k}{(2\pi)^2} \to \int d\gamma N(\gamma) \), we replace
\( N(\gamma) \) by 1/2, we normalize \( Q \) and \( \Delta \) by \( \mu \) and integrate, obtaining at \( T = 0 \)

\[
\frac{\sin^{-1}(\Delta + Q) - \sin^{-1}(\Delta - Q)}{2Q} = \frac{1}{2} \sin^{-1}(\Delta + Q) - \frac{(\Delta - Q)\sqrt{1 - (\Delta + Q)^2} - (\Delta + Q)\sqrt{1 - (\Delta - Q)^2}}{4Q^2} = \frac{Q\mu}{2J_1} \tag{B1a}
\]

\[
\frac{\sqrt{1 - (\Delta - Q)^2} - \sqrt{1 - (\Delta + Q)^2}}{2Q} = \frac{2\Delta\mu}{J_2} \tag{B1b}
\]

\[
\frac{\sqrt{1 - (\Delta + Q)^2} - \sqrt{1 - (\Delta - Q)^2}}{2Q} = \frac{2\Delta\mu}{J_2} \tag{B1c}
\]

These three equations may be reduced to one by taking the sine of eq. (B1a) and substituting into eq. (B1b) to obtain an equation for \( \mu(Q) \), solving eq. (B1c) to obtain an equation for \( \Delta(Q) \) and then substituting the results into eq. (B1b). However, for our purposes a simpler approach suffices. We first locate the critical point at which the minimum boson energy vanishes. In the notation of this appendix this implies \( \Delta^* + Q^* = 1 \) (we denote by \( * \) the values of the quantities at the critical point). Then eq. (B1a) may be solved for \( Q^* \). For \( S > S_c = (\pi/2 - 1)/2 \) this has only one solution; e.g. at \( S = 1/2 \)

\[
Q^* \approx 0.277 \tag{B2}
\]

For \( S^* < S < S_c \), with \( S^* \approx 0.19 \) there are two solutions, one at \( Q \) near 1 which is the lower energy solution for \( J_1 \gg J_2 \) and one at \( Q \) near 1/2 which is the lower energy solution for \( J_1 \) near \( J_2/4 \). For \( S < S^* \) there are no solutions.

Once a solution for \( Q^* \) is found, eq. (B1c) implies

\[
\frac{\mu^*}{J_2} = \frac{1}{2\sqrt{Q^*(1 - Q^*)}} \tag{B3}
\]

and eq. (B1b) implies

\[
\frac{J_2^*}{J_1^*} = \frac{2(1 + 2S)\sqrt{Q^*(1 - Q^*)} - 1 + Q^*}{Q^*} \tag{B4}
\]

Solving eq. (B1b) and then using the solution in eq. (B4) yields the phase diagram given in fig. 2.

We now consider the \( T_0 \) behavior. We are most interested in the regime near the phase boundary, and in small \( J_2 \). We therefore solve the equations perturbatively in the small
parameters $S_c - S$, $J_2/J_1$ and $T$. We neglect terms of third order and higher in these small parameters. To this order the $T$ dependent terms may be evaluated exactly. The equations are conveniently expressed in terms of the variables $\omega_+$, $\omega_-$ and $\mu$ and are (note we need $\mu$ only to first order in the small parameters)

$$\frac{\pi - \omega_+ / \mu - \omega_- / \mu + (2T / \mu)(f(\omega_+/T) + f(\omega_-/T))}{2(1 - \omega_+^2/(4\mu^2) - \omega_-^2/(4\mu^2))} = 1 + 2S \tag{B5a}$$

$$\frac{\pi - \omega_- / \mu - \omega_+ / \mu + (2T / \mu)(f(\omega_+/T) + f(\omega_-/T))}{4} = \frac{\mu}{2J_1} \tag{B5b}$$

$$\omega_- - \omega_+ + 2T(f(\omega_+/T) - f(\omega_-/T)) = \frac{\omega_-^2 - \omega_+^2}{J_2} \tag{B5c}$$

Here the function $f$ is defined by

$$f(x) = -\ln[1 - e^{-x}] \tag{B6}$$

We use eq. (B5b) to solve for $\mu$. Substituting and rearranging gives

$$\omega_+ + \omega_- - 2T(f(\omega_+/T) + f(\omega_-/T)) - \frac{\omega_+^2 + \omega_-^2}{j} = \epsilon \tag{B7a}$$

$$\omega_- - \omega_+ - 2T(f(\omega_+/T) - f(\omega_-/T)) = \frac{\omega_-^2 - \omega_+^2}{J_2} \tag{B7b}$$

with

$$j = 2J_1(1 + 8(S_c - S)/\pi) \tag{B8}$$

and

$$\epsilon = \frac{2\pi J_1(S_c - S)}{1 + 8(S_c - S)/\pi} \tag{B9}$$

These two equations may be easily solved numerically for $\omega_+$ and $\omega_-$ by adding the two equations to obtain an expression for $\omega_+$ in terms of $\omega_-$ and $T$, and then substituting that into one of the two equations to get a single equation for $\omega_-$. At low $T$ and sufficiently close to the phase boundary the equations have two solutions, one with $\omega_+ < \omega_-$ and one with $\omega_+ = \omega_-$. Above a critical temperature the two solutions merge. By substituting the results in to eq. (A9) we have verified that where the solution with $\omega_+ < \omega_-$ exists it has a lower energy than the solution with $\omega_+ = \omega_-$. The results displayed in fig. 3 were obtained in this manner.
APPENDIX C: SUSCEPTIBILITIES AND RELAXATION RATES

We begin with the dynamic susceptibilities, which we obtain by computing the linear response of the system to an externally applied magnetic field \( \vec{h}(a) \). The Schwinger boson formalism is rotationally invariant. We therefore compute only the response to a field in the \( z \)-direction. Thus we add to the Hamiltonian a term

\[
\Delta H = \sum_i \hat{h}_i^{z(\text{cc})} \cdot S_i^{(a)}
\]

(C1)

After using eq. (2.2), eq. (2.3), and eq. (A3) this becomes

\[
\Delta H = \sum_q \frac{h_q^{(1)} - h_q^{(2)}}{2} O_q^a + \frac{h_q^{(1)} + h_q^{(2)}}{2} O_q^s
\]

(C2)

with

\[
O_q^a = \sum_{k\alpha\beta} \cosh(\theta_{k+q+P} + \theta_k) (s_{k+q+P\alpha}^\dagger \sigma^z_{\alpha\beta} s_{k+q+P\beta} + a_{k+q+P\alpha}^\dagger \sigma^z_{\alpha\beta} a_{k+q+P\beta})
\]

\[+ \sinh(\theta_{k+q+P} + \theta_k) (s_{k+q+P\alpha}^\dagger \sigma_{\alpha\beta}^{**} s_{k+q+P\beta}^\dagger + \text{h.c.} + a \rightarrow s)\]  

(C3a)

\[
O_q^s = \sum_{k\alpha\beta} \cosh(\theta_{k+q} - \theta_k) (s_{k+q\alpha}^\dagger \sigma_{\alpha\beta}^z a_{k-P\beta} + a_{k+q\alpha}^\dagger \sigma_{\alpha\beta}^z s_{k-P\beta} + \text{h.c.})
\]

\[+ \sinh(\theta_{k+q} - \theta_k) (s_{k+q\alpha}^\dagger \sigma_{\alpha\beta}^{**} a_{k-P\beta}^\dagger + a_{k+q\alpha}^\dagger \sigma_{\alpha\beta}^{**} s_{k-P\beta}^\dagger + \text{h.c.})\]  

(C3b)

The only non-zero correlation functions are

\[
\chi_{a\alpha}^{aa}(\omega) = \int_0^\infty dt e^{i(\omega+i\epsilon)t} <[O_q^a(t), O_{-q}^a(0)]>
\]

\[= 4 \sum_k \cosh^2(\theta_{k+q+P} + \theta_k) \frac{b(\omega_k) - b(\omega_{k+q+P})}{\omega - \omega_k + \omega_{k+q+P} + i\epsilon}
\]

\[+ 4 \sum_k \sinh^2(\theta_{k+q+P} + \theta_k) \frac{[1 + b(\omega_k) + b(\omega_{k+q+P})](\omega_k + \omega_{k+q+P})}{(\omega_k + \omega_{k+q+P})^2 - (\omega + i\epsilon)^2}\]  

(C4a)

and

\[
\chi_{a\alpha}^{ss}(\omega) = \int_0^\infty dt e^{i(\omega+i\epsilon)t} <[O_q^s(t), O_{-q}^s(0)]>
\]

\[= 4 \sum_k \cosh^2(\theta_{k+q} - \theta_k) \frac{b(\omega_k) - b(\omega_{k+q})}{\omega - \omega_k + \omega_{k+q} - i\epsilon}
\]

\[+ 4 \sum_k \sinh^2(\theta_{k+q} - \theta_k) \frac{[1 + b(\omega_k) + b(\omega_{k+q})](\omega_k + \omega_{k+q})}{(\omega_k + \omega_{k+q})^2 - (\omega + i\epsilon)^2}\]  

(C4b)
We are interested in low energy phenomena; this implies that \( k \) and \( k + q + P \) are near 0 or \( P \). In this case we may approximate:

\[
\cosh(\theta_k) = (\mu/2\omega_k)^{1/2}(1 + \omega_k/2\mu)
\]

\[
\sinh(\theta_k) = sgn(\gamma_k)(\mu/2\omega_k)^{1/2}(1 - \omega_k/2\mu)
\]

Then near \( q = 0 \) we have

\[
\chi_{q}^{ss}(\omega) = \sum_{k} \frac{(\omega_k + \omega_{k+q})^2}{\omega_k \omega_{k+q}} \frac{b(\omega_k) - b(\omega_{k+q})}{\omega - \omega_k + \omega_{k+q} - i\epsilon} + \sum_{k} \frac{(\omega_k - \omega_{k+q})^2}{\omega_k \omega_{k+q}} \frac{(1 + b(\omega_k) + b(\omega_{k+q}))(\omega_k + \omega_{k+q})}{(\omega_k + \omega_{k+q})^2 - (\omega + i\epsilon)^2}
\]

while near \( q = P \)

\[
\chi_{q}^{ss}(\omega) = 4 \sum_{k} \frac{\mu^2}{\omega_k \omega_{k+q}} \left[ \frac{b(\omega_k) - b(\omega_{k+q})}{\omega - \omega_k + \omega_{k+q} - i\epsilon} + \frac{(1 + b(\omega_k) + b(\omega_{k+q}))(\omega_k + \omega_{k+q})}{(\omega_k + \omega_{k+q})^2 - (\omega + i\epsilon)^2} \right]
\]

\[
\chi_{q}^{aa}(\omega) = 4 \sum_{k} \frac{\mu^2}{\omega_k \omega_{k+q} + P} \left[ \frac{b(\omega_k) - b(\omega_{k+q} + P)}{\omega - \omega_k + \omega_{k+q} + P - i\epsilon} + \frac{(1 + b(\omega_k) + b(\omega_{k+q} + P))(\omega_k + \omega_{k+q} + P)}{(\omega_k + \omega_{k+q} + P)^2 - (\omega + i\epsilon)^2} \right]
\]

In all of these formulae there are important contributions from \( k \) near 0 and \( k \) near \( P \).

We now consider NMR. To derive nuclear relaxation rates we take the standard \(^2\) hyperfine Hamiltonians describing how nuclei are coupled to the electronic spins, write the spins in terms of bosons, and then compute the appropriate boson correlation functions. We assume throughout that \( T \ll J_1 \).

We begin with the yttrium. An yttrium nucleus sits halfway between two nearest-neighbor CuO₂ planes and above the center of a plaquette formed by four Cu atoms. We
denote the hyperfine coupling to one spin by $D$. Thus we write the hyperfine Hamiltonian for yttrium,

$$H_{hf}^Y = D \sum_{a,i=1..4} \vec{S}_i^{(a)}$$ (C11)

After performing the transformations of section II and Appendix A and retaining only those terms capable of giving dissipation at NMR frequencies we have

$$H_{hf}^Y = D \sum_{k_1,q,\alpha,\beta} g(q) \cosh(\theta_{k+q} - \theta_k) (s_{k+q \alpha}^{\dagger} \sigma_{\alpha \beta} a_{k+\beta} + h.c.)$$ (C12)

with

$$|g(q)| = 4 \cos(q_x/2) \cos(q_y/2)$$ (C13)

Here we have omitted an unimportant phase factor in $g$. We now calculate the relaxation rate in the usual way, from

$$\lim_{\omega \to 0} \frac{1}{T_1} = \frac{2\pi D^2}{T} \sum_{k,q} |g(q)|^2 \cosh^2(\theta_k - \theta_{k+q}) \delta(\omega_k - \omega_{k+q}) \frac{\sinh^2(\omega_k/2T)}{\sinh^2(\omega_{k+q}/2T)} = 2\pi D^2 \lim_{\omega \to 0} \frac{1}{\omega} \sum_q |g(q)|^2 \chi_{ss''}^{ss'}(q,\omega)$$ (C15)

We now consider the planar oxygen. Each oxygen is located in a CuO$_2$ plane and is in the center of a bond connecting two Cu sites. Thus

$$H_{hf}^O = C \sum_{i=1,2} \vec{S}_i^{(a)}$$ (C16)

Expressing the spins in terms of bosons as was done for yttrium gives:

$$H_{hf}^O = \frac{C}{2} \sum_{k,q} f(q)(\cosh(\theta_k + \theta_{k+q} + p) (s_{k \alpha}^{\dagger} \sigma_{\alpha \beta} s_{k+q+P \beta} + a_{k+P \alpha}^{\dagger} \sigma_{\alpha \beta} a_{k+q+P \beta} + h.c.) + \cosh(\theta_k - \theta_{k+q}) s_{k \alpha}^{\dagger} \sigma_{\alpha \beta} a_{k+q+P \beta} + h.c.)$$ (C17)

with
\[ |f(k)| = 2 \cos \left( \frac{q_x}{2} \right) \]

Proceeding as we did with yttrium yields eq. (3.10) of the text. To evaluate this it is convenient to consider \( q \) near 0 and \( q \) near \( P \) separately. The case of \( q \) near 0 goes through just as for yttrium, except that the square of the form factor is 4, not 16, and one must add \( \chi^{aa''} \). For \( q \) near \( P \) it is convenient to write \( q = P + k_2 - k_1 \) and to sum over \( k_1 \) and \( k_2 \). The integrals have contributions from \( k_1, k_2 \) near 0 and \( P \). The form factor becomes

\[ |f(k_1 - k_2)|^2 = (k_1^2 - k_2^2)^2 = (k_1^2 + k_2^2)/2 \] (C18)

where in the second equality we have done the angular integral and \( k \) stands for either \( k \) or \( (k - P) \) as appropriate. Now we have, from eqs. (A9) and (2.7),

\[ k^2 = 4(1 - \gamma_k) = 2(\omega_k^2 - \omega_+ - \omega_-)/\mu^2 \] (C19)

where the gap is \( \omega_+ \) for \( k \) near 0 and \( \omega_- \) for \( k \) near \( P \). Putting this into eq. (3.10) yields eq. (3.11). Finally, we consider the Cu relaxation rate. A Cu nuclear moment is believed to be coupled to the spin on the same site, via a hyperfine coupling \( A \), and to the spins on the four nearest neighbor sites in the same plane, via a hyperfine coupling \( B \). Thus

\[ H_{hf}^{Cu} = A S_0^{(1)} + B \sum_{i=1,4} S_i^{(1)} \] (C20)

After transforming to the boson representation we have

\[ H_{hf}^{Cu} = \frac{1}{2} \sum_{kq} [A - 4B\gamma(q)] \left( \cosh(\theta_k + \theta_{k+q+p}) (s_{k\alpha}^{\dagger} \sigma_{\alpha\beta} s_{k+q+p\beta} + a_{k\alpha}^{\dagger} \sigma_{\alpha\beta} a_{k+q+p\beta}) \right. \\
\left. + \cosh(\theta_k - \theta_{k+q+P}) s_{k+q\alpha}^{\dagger} \sigma_{\alpha\beta} a_{k+q+P\beta} + h.c. \right) \] (C21)

Again we may construct the relaxation rate. It is given by eq. (3.12) and may be simply evaluated because the dominant contribution is at \( q \) near \( P \).
REFERENCES

(c) Address from September 1st 1993 on: Theoretische Physik, ETH Höngherberg, CH-8093 Zürich, Switzerland

1 T. Siegrist, S. Sunshine, D. W. Murphy, R. J. Cava and S. M. Zahurak, Phys. Rev B35, 7137 (1989).

2 A. J. Millis, H. Monien and D. Pines, Phys. Rev. B42, 996 (1991), H. Monien, D. Pines and M. Takigawa, Phys. Rev. 43, 258 (1991)

3 J. Rossad-Mignod, L. P. Regnault, C. Vettier, P. Bourges, P. Burlet, J. Bossy, J. Y. Henry and G. Lapertot, Physica C185-189, 86 (1991).

4 J. M. Tranquada, P. M. Gehring, G. Shirane, S. Shamoto and M. Sato, Phys. Rev. B46, 5561, (1992).

5 H. A. Mook, M. Yethiraj, G. Aeppli and T. Mason, Phys. Rev. Lett. 70, 3490 (1993).

6 M. Takigawa et. al. Phys. Rev B42, 243 (1991).

7 A. J. Millis and H. Monien, Phys. Rev. Lett. 70, 2810 (1993)

8 T. M. Rice in the Proceedings of the ISSP Symposium on the Physics and Chemistry of Oxide Superconductors, Tokyo (1991), Springer Verlag (1991).

9 A. Sokol and D. Pines, Phys. Rev. Lett. 71 2813, (1993), and V. Barzykin, D. Pines, A. V. Sokol and D. Thelen, unpublished.

10 S.Chakravarty, B. I. Halperin and D. R. Nelson, Phys. Rev. Lett. 60, 1057 (1988) and S. Chakravarty, B. I. Halperin and D. R. Nelson, Phys. Rev B39, 7443 (1988).

11 S. Sachdev and J. Ye, Phys. Rev. Lett. 69, 2411 (1992) and A. V. Chubukov and S. Sachdev Phys. Rev. Lett. 71, 169 (1993).

12 N. W. Preyer, R. J. Birgeneau, C. Y. Chen, D. Gabbe, H. P. Jensen, M. A. Kastner, P.
J. Picone and T. Thio, Phys. Rev. B42, 11563 (1989).

13 J. A. Hertz, Phys. Rev. B14, 1165, (1976).

14 A. J. Millis, Phys. Rev. B48 7183 (1993).

15 D. Arovas and A Auerbach, Phys. Rev. B38, 316 (1988).

16 S. Sachdev and N. Read, Int. J. Mod. Phys. B5, 219 (1991).

17 K. Hida, J. Phys. Soc. Jpn. 61, 1013 (1992).

18 A. Sandvik, private communication

19 A. V. Chubukov, Phys. Rev. B44, 12318 (1991).

20 S. Chakravarty, in High Temperature Superconductivity: Proceedings, K. Bedell, D. Coffey, D. E. Meltzer, D. Pines and J. R. Schrieffer, eds. (Addison Wesley: Redwood City, CA), 179 (1990) and S. Chakravarty and R. Orbach, Phys. Rev. Lett. 64, 224 (1990).

21 P. Peczak, A. M. Ferrenberg and D. P. Landau, Phys. Rev. B43, 6087 (1991).

22 D. Forster, D. R. Nelson and M. Stephen, Phys. Rev. A16, 732 (1977).

23 C. H. Pennington and C. P. Slichter, Phys. Rev. Lett. 66, 381 (1991).

24 T. Machi I. Tomeno, T. Miyatake, N. Koshizuka, S. Tanaka, T. Imai and H. Yasuoka, Physica C173, 32 (1991).

25 W. E. Pickett, Rev. Mod. Phys. 61, 433 (1991), see especially section IV-D and fig. 30.

26 R. Liu, B. W. Veal, A. P. Paulikas, J. W. Downey, P. J. Kostic, S. Fleshler, U. Welp, C. G. Olson, X. Wu, A. J. Arko and J. Joyce, Phys. Rev. B46, 11056 (1992).

27 For $T_2$, M. Takigawa et. al., unpublished; for $T_1$ see ref. [6].

28 T. Imai, C. P. Slichter, K. Yoshimura, M. Katoh and K. Kosuge, Phys. Rev. Lett. 71, 1254 (1993).
29. R. Glenister, R. R. P. Singh and A. Sokol, unpublished.

30. S. Hayden, G. Aeppli, R. Osborn, A. D. Taylor, T. G. Perring, S. W. Cheong and Z. Fisk, Phys. Rev. Lett. 67, 3622 (1991).

31. T. Imai, C. P. Slichter, K. Yoshimura and K. Kosuge, Phys. Rev. Lett. 70, 1002 (1993).

32. D. Forster *Hydrodynamic Fluctuations, Broken Symmetry and Correlation Functions*, (Benjamin Cummings: Reading, PA) 1975.

33. There is some disagreement in the literature about the value of J appropriate to $YBa_2Cu_3O_6$. The estimate $0.1eV < J < 0.12eV$ is given in sec 2.3 of a recent review (D. C. Johnston, J. M. M. M. 100, p. 218 (1991)). The J value for $La_2CuO_4$ is 0.13eV.

34. A. J. Millis and H. Monien, Phys. Rev. B45, 3059 (1992). Hyperfine couplings are given in a convenient dimensionless form in Table 1 of this work, and the observed ratio of Cu to O relaxation rates in $YBa_2Cu_3O_{6.6}$ at $T = 300K$ is quoted to be 16; we assume the ratio is similar in $YBa_2Cu_4O_8$. The quantity defined here as $A_{AF}$ is related to B in Table 1 of the cited work via $A_{AF} = 4B(1 - \alpha)/(1 + \alpha)$. The bounds $0.2 < \alpha < 0.3$ were obtained from data in this work also. The quantity defined here as $C_{AF}$ is actually a tensor with different principal axes along and perpendicular to the Cu-O bond. For the estimates used here we set $C_{AF} = C$ and took the value for fields along the Cu-O bond (as appropriate for relaxation with fields in the c-direction). The ratio $A_{AF}/C_{AF}$ then turns out to be 4 so at $T = 300K$ where the predicted $\xi = 4$ the predicted ratio is about 256.

35. S. Sachdev and A. V. Chubukov, Phys. Rev. Lett. in press (1993).

36. B. I. Shraiman and E. D. Siggia, Phys. Rev. B42 2485 (1990).

37. H. Zimmermann, M. Mali, M. Bankay and D. Brinkmann, Physica C 185-189, 1145 (1991). The relevant data are in fig. 3. To convert Knight shifts to susceptibilities we used the hyperfine couplings given in ref. [34] for $YBa_2Cu_3O_7$ with the quantity $\chi_0/\mu_B^2$ of ref [34] taken to be $2.7\text{states/eV} - Cu$. 

38.
38 M. Takigawa, J. L. Smith and W. Hults, unpublished.
FIGURES

FIG. 1. Model system considered in this paper: two square arrays of spins with in-plane coupling $J_1$ and between-plane coupling $J_2$.

FIG. 2. $T = 0$ Phase diagram of eq. (1.1) as described in Appendix B from the Schwinger boson mean field theory.

FIG. 3. Temperature dependence (in units of $J_2$) of the Schwinger boson gaps $\omega_+$ and $\omega_-$ defined in eqs. (2.10) and (2.11) and computed as described in Appendix B, for parameters such that at $T = 0$ the model is at the phase boundary for small $J_2$ and $S_c - S$. The temperature $T^* \sim J_2$ separates the low-$T$ coupled planes regime from a high-$T$ decoupled planes regime; in the mean field theory there is a second order phase transition at $T^*$; we believe fluctuations would convert this to a smooth crossover.

FIG. 4. Temperature dependence of uniform susceptibility and copper, oxygen and yttrium relaxation rates calculated from mean field theory for parameters used in constructing fig. 3. The temperature $T^*$ at which the model crosses over from the decoupled-planes to the coupled-planes critical regimes is indicated.

FIG. 5. Frequency dependence of antisymmetric and symmetric susceptibilities calculated from mean field theory for several different temperatures.

FIG. 6. Different regimes of behavior of scaling theory and temperature dependence of relaxation rates in each regime.