Nearly antiferromagnetic Fermi-liquid description of magnetic scaling and spin-gap behavior

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We present a Fermi-liquid description of magnetic scaling and spin-gap behavior in strongly correlated electron systems. We show that a gap in the spin-excitation spectrum is a natural consequence of the existence of a second energy scale of magnetic origin, in systems of itinerant, but nearly localized electron spins, such as are found in the cuprate superconductors and heavy-electron systems. A second energy scale leads to a frequency-dependent restoring force $f^a(\mathbf{q},\omega)$ that becomes stronger as the frequency increases. A spin gap at $\mathbf{Q}=(\pi/a,\pi/a)$ is a consequence of these frequency-dependent vertex corrections; it takes on a constant value when the antiferromagnetic correlation length becomes a constant. We show that the spin-spin response function reduces to that recently introduced by Barzykin to describe the damping by particle-hole excitations of the spin-wave spectrum found in the $N=\infty$ quantum nonlinear σ model. We discuss fully doped and underdoped cuprate superconductors, the appearance of a pseudogap of magnetic origin in the quasiparticle density of states in the underdoped system, and the constraints nuclear magnetic resonance and neutron-scattering experiments impose on the magnitude and temperature dependence of the Fermi-liquid parameters.

I. INTRODUCTION

A unified magnetic phase diagram of the cuprate superconductors has recently been proposed by Sokol and Pines[1] (hereafter SP). They have shown how straightforward scaling arguments applied to the interpretation of measurements of the spin-echo decay rate $1/T_{2G}$ and spin-lattice relaxation rate $1/T_1$ demonstrate the remarkable universality of the low-frequency magnetic behavior at high temperatures. A feature of this phase diagram is a broad intermediate-doping region of quantum-critical (QC) behavior with dynamical exponent $z=1$, characterized by a temperature-independent ratio T_1T/T_{2G} and linear in T behavior for the product T_1T. As the temperature decreases there is a crossover to the quantum-disordered (QD), $z=1$, regime characterized by a temperature-independent correlation length ξ. A gap Δ in the spin excitation spectrum at $\mathbf{Q}=(\pi/a,\pi/a)$ in these underdoped materials is related to the suppression of the spectral weight for frequencies smaller than $\Delta=c/\xi$. The Gaussian or quantum-critical regime with dynamic exponent $z=2$, characterized by a temperature-independent ratio T_1T/T_{2G}^2, occurs only in the fully doped materials.

It is striking that the scaling arguments originally motivated by the study of the spin-$\frac{1}{2}$ Heisenberg model work well for such a wide range of hole doping. It is likely that the physical origin of this success is the proximity of the antiferromagnetic instability even in the fully doped materials. To demonstrate this, consider, for example $YBa_2Cu_3O_7$, where $\chi_\mathbf{Q}\approx 75$ states/eV just above T_c. If one writes

$$\chi_\mathbf{Q}=\frac{\tilde{\chi}_\mathbf{Q}}{1-F_\mathbf{Q}^a}\ , \tag{1}$$

this implies $F_\mathbf{Q}^a\geq +0.975$ when taking the value of $\tilde{\chi}_\mathbf{Q}\approx 1.7$ states/eV for the irreducible particle-hole susceptibility calculated by Monthoux and Pines[2] (hereafter MP). The detailed calculations of MP show that it is reasonable to regard $YBa_2Cu_3O_7$ as a nearly antiferromagnetic Fermi liquid (NAFL), which obeys Gaussian $z=2$ scaling.

However, in the case of the underdoped materials with QC $z=1$, the straightforward mean-field theory for itinerant magnets, which always yields $z=2$, does not apply. There are two possibilities to describe these systems. The first approach, as proposed by Chubukov and Sachdev[3] and discussed by SP (Ref. 1) and recently by Sachdev,[4] is that of the nonlinear σ model with holes, which is a kind of two-component system. The main advantage of this point of view is that the magnetic scaling and spin-gap behavior follow from the properties of the nonlinear σ model. In this paper we wish to explore the second possibility, which is that of a one-component fermion-only model. There are certain virtues to the fermion-only approach. We know from experiment that one has a one-component system, in that the magnetic properties change at the transition to the superconducting state. This is most clearly seen in $YBa_2Cu_3O_7$, where one finds a sharp drop in both the Knight shift and the copper spin-lattice relaxation rate below T_c, a result which must arise from the feedback of superconductivity on the spin-excitation spectrum. These changes are less apparent in the underdoped systems because they are masked by effects associated with a pseudogap in the quasiparticle density of states. Thus for $YBa_2Cu_3O_{6.63}$, where the one-component nature of the spin description is established by Knight shift experiments on ^{63}Cu and ^{17}O nuclei[5] in the normal state, there is no abrupt drop in the Knight shift below T_c; rather one sees at T_c an

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inflection point, with a temperature-dependent Knight shift which as T increases is concave (as pairing theory requires) below T_c, and convex (because of the quasiparticle pseudogap) above T_c. The one-component approach thus explains naturally the change of the magnetic properties at T_c. However, the origin of the magnetic scaling is not transparent.

We demonstrate below that the appearance of a gap in the spin-excitation spectrum behavior found in the QD $z=1$ regime can be understood as a consequence of a second energy scale ω_J, which leads to a frequency-, wave-vector-, and temperature-dependent spin-antisymmetric mean field $f^a(\mathbf{q},\omega,T)$, which is a generalization of the constant long-wavelength mean field f_0^a that describes the magnetic interaction between quasiparticles in Landau's Fermi-liquid theory. We show that for a nearly antiferromagnetic system, in both $z=1$ and $z=2$ systems, one then finds two distinct low-energy scales; $\omega_{\rm SF}$, the relaxational mode introduced independently by Millis, Monien, and Pines[6] (hereafter MMP) and Moriya, Takahashi, and Ueda[7] which is related to low-energy quasiparticle behavior, and Δ, the spin gap. We show that scaling tells us what must be the temperature dependence of the product of $f_{\rm Q}^a$ and the irreducible particle-hole susceptibility $\tilde{\chi}_{\rm Q}(\omega,T)$. We find that the spin gap can be described as a consequence of frequency-dependent vertex corrections; it takes on a constant value in the QD regime because the antiferromagnetic correlation length becomes constant. We discuss how, in the underdoped systems, the temperature dependence of $\omega_{\rm SF}$ reflects the pseudogap in the quasiparticle density of states, and argue that this pseudogap is of magnetic origin.

We find that for a physically reasonable choice of ω_J ($\sim 3J$) the values we deduce for the spin gap Δ are so high that the high-frequency spin waves in the vicinity of $\mathbf{Q}$ are strongly overdamped by the particle-hole excitations in both the fully doped and underdoped cuprate superconductors. As a result the high-frequency dynamical behavior of both systems is dominated by the relaxational mode at $\omega_{\rm SF}$, and is not far from that calculated using MMP theory. The principal experimental constraints on the Fermi-liquid parameters then come from the low-frequency behavior as measured in NMR experiments, and we consider these in some detail.

Of course the cuprates are not the only strongly correlated electron system which exhibits nearly antiferromagnetic or ferromagnetic behavior, since similar behavior is found in a wide variety of heavy-electron systems.[8] We therefore anticipate that a nearly antiferromagnetic Fermi liquid description might be useful as well for many of the latter systems, including the antiferromagnetic metals, the superconductors, and the Kondo insulators.

In Sec. II, we develop the nearly antiferromagnetic Fermi liquid description, and show that it leads to the spin-gap behavior proposed by Barzykin[9] for $z=1$ systems. We consider the application of NAFL theory to the overdoped, QC $z=2$, system, $YBa_2Cu_3O_7$ and the constraints placed on NAFL parameters by experiments on the underdoped, QC $z=1$ materials such as $YBa_2Cu_3O_{6.63}$ in Sec. III, and discuss some open questions and present our conclusions in Sec. IV.

II. A MEAN-FIELD DESCRIPTION OF A NEARLY ANTIFERROMAGNETIC FERMI LIQUID

We consider a system of strongly correlated electrons which is nearly antiferromagnetic, and which possesses a second energy scale ω_J of magnetic origin. We take as a starting point a generalized mean-field expression for the dynamical susceptibility $\chi(\mathbf{q},\omega)$:

$$\chi(\mathbf{q},\omega)=\frac{\tilde{\chi}(\mathbf{q},\omega)}{1-f^a(\mathbf{q},\omega)\tilde{\chi}(\mathbf{q},\omega)}\ , \tag{2}$$

where $\tilde{\chi}(\mathbf{q},\omega)$ is the irreducible particle-hole susceptibility, and $f^a(\mathbf{q},\omega)$ is a wave-vector-, frequency-, and temperature-dependent mean-field vertex correction. In using such an expression, we are *not* assuming that either f^a or $\tilde{\chi}$ takes on the values found in a weak-coupling random-phase approximation description, but rather that this form of the response function provides reasonable account of the actual strong-coupling situation. Support for this point of view comes from the work of Bulut and Scalapino who have found, in their Hubbard model calculations, that a generalized mean-field description does an excellent job of reproducing the result of their Monte Carlo calculations.[10] Moreover, both the high-temperature $z=1$ and $z=2$ regimes are very close to mean-field behavior. It therefore should be possible to construct a mean-field description of the crossover from $z=2$ to $z=1$ behavior.

We consider first the mean-field expression Eq. (2) at the antiferromagnetic wave vector $\mathbf{Q}$ and in the low-frequency limit. Expanding to order ω^2, we have

$$\tilde{\chi}(\mathbf{Q},\omega)=\chi_{\rm Q}\left[1+i\frac{\omega}{\tilde{\Gamma}}-\frac{\omega^2}{\tilde{\Gamma}^2}\right]\ , \tag{3}$$

$$f^a(\mathbf{Q},\omega)=f_{\rm Q}^a\left[1+\frac{\omega^2}{\omega_J^2}\right]\ , \tag{4}$$

where $\tilde{\Gamma}$ and ω_J (assumed to be less than $\tilde{\Gamma}$) provide a measure of the relevant frequency scales for $\tilde{\chi}(\mathbf{Q},\omega)$ and $f^a(\mathbf{Q},\omega)$, respectively. On substituting these expressions into Eq. (2) and keeping only the leading terms in ω we find

$$\chi(\mathbf{Q},\omega)=\frac{\tilde{\chi}_{\rm Q}(1+i\omega/\tilde{\Gamma}-\omega^2/\tilde{\Gamma}^2)}{1-F_{\rm Q}^a-F_{\rm Q}^a\omega^2/\omega_J^2-iF_{\rm Q}^a\omega/\tilde{\Gamma}+F_{\rm Q}^a\omega^2/\tilde{\Gamma}^2} \tag{5}$$

on introducing the dimensionless NAFL parameter

$$F_{\rm Q}^a=f_{\rm Q}^a\tilde{\chi}_{\rm Q}\ . \tag{6}$$

On making use of Eq. (1), Eq. (5) then takes the form

$$\chi(\mathbf{Q},\omega)=\frac{\chi_{\rm Q}}{1-\omega^2/\Delta^2-i\omega/\omega_{\rm SF}}\ , \tag{7}$$

where

$$\omega_{\rm SF}=\tilde{\Gamma}(1-F_{\rm Q}^a) \tag{8a}$$

represents the low-frequency relaxational mode introduced by MMP (Ref. 6) and Moriya, Takahashi, and Aeda[7] for the case of $z=2$ and $\tilde{\Gamma}=$const, and

$$\Delta=\omega_J\left[\frac{1-F^a_{\mathbf{Q}}}{F^a_{\mathbf{Q}}}\right]^{1/2} \tag{8b}$$

describes a second, distinct, low-energy scale. There are thus two independent energy scales, $\tilde{\Gamma}$ and ω_J; when combined with the antiferromagnetic enhancement coefficient, $1-F^a_Q$, these determine $\omega_{\rm SF}$ and Δ, respectively.

According to Eq. (3), since

$$\frac{\tilde{\chi}''(\mathbf{Q},\omega)}{\omega}=\frac{\tilde{\chi}_{\mathbf{Q}}}{\tilde{\Gamma}}, \tag{9}$$

it is $\tilde{\chi}_{\mathbf{Q}}/\tilde{\Gamma}$ which measures the slope of $\tilde{\chi}''(\mathbf{Q},\omega)$ at low ω, and hence characterizes the low-frequency irreducible quasiparticle response. It may be expected to reflect the "spin-pseudogap" behavior of the quasiparticles in the underdoped systems. We have seen that $f^a(\mathbf{Q},\omega)=f^a_{\mathbf{Q}}(1+\omega^2/\omega_J^2)$. It is tempting to conjecture that this expression is the low-frequency expansion of the expression

$$f^a(\mathbf{Q},\omega)=\frac{f^a_{\mathbf{Q}}\omega_J^2}{\omega_J^2-\omega^2},$$

a form which suggests that the frequency dependence of $f^a(\mathbf{q},\omega)$ arises via the exchange of excitations with energy ω_J. It is important to note from the expression for $f^a(\mathbf{q},\omega)$ that, contrary to normal Fermi liquids which possess a single energy scale E_F as long as $\omega<\omega_J$, this effective interaction increases as ω increases.

If we write

$$\chi_{\mathbf{Q}}=\alpha\xi^2, \tag{10a}$$

where ξ is the antiferromagnetic correlation length and α a constant, it follows that

$$\tilde{\chi}_{\mathbf{Q}}=\alpha\tilde{\xi}^2 \tag{10b}$$

with

$$\xi^2=\frac{\tilde{\xi}^2}{1-F^a_{\mathbf{Q}}}. \tag{10c}$$

In this form it is clear that to the extent that $\tilde{\xi}$ is weakly temperature dependent (we shall present arguments later which suggest this is the case) the temperature dependence, and scaling behavior, of ξ arise primarily from that of $F^a_{\mathbf{Q}}$. From Eq. (2) it follows that $f^a_{\mathbf{Q}}$ and $F^a_{\mathbf{Q}}$ take the form

$$f^a_{\mathbf{Q}}=\frac{1}{\tilde{\chi}_{\mathbf{Q}}}-\frac{1}{\alpha\xi^2}=\frac{1}{\alpha\tilde{\xi}^2}-\frac{1}{\alpha\xi^2}, \tag{11a}$$

$$F^a_{\mathbf{Q}}=1-\frac{\tilde{\chi}_{\mathbf{Q}}}{\alpha\xi^2}=1-\frac{\tilde{\xi}^2}{\xi^2}. \tag{11b}$$

The form Eq. (11b) makes it evident that $F^a_{\mathbf{Q}}\lesssim 1$ in the long-correlation-length, nearly antiferromagnetic limit. It is also evident that the spin gap takes the spin-wave form

$$\Delta=\frac{\omega_J\tilde{\xi}}{(1-\tilde{\xi}^2/\xi^2)^{1/2}}=\frac{c}{\xi} \tag{12}$$

with

$$c=\frac{\omega_J\tilde{\xi}}{(1-\tilde{\xi}^2/\xi^2)^{1/2}}\cong\omega_J\tilde{\xi} \tag{13}$$

becoming temperature independent when $\xi\gg\tilde{\xi}$. In the limiting case of a temperature-independent correlation length ξ_0 the spin gap Δ becomes a constant, $\Delta_0=c/\xi_0$.

It is straightforward to extend these considerations to wave vectors $\mathbf{q}$ in the vicinity of $\mathbf{Q}$. In place of Eqs. (3) and (4), we have, on expanding to lowest nonvanishing order in $\mathbf{q}-\mathbf{Q}$,

$$\tilde{\chi}(\mathbf{q},\omega)=\tilde{\chi}_{\mathbf{Q}}\left[1+\xi_\chi^2(\mathbf{q}-\mathbf{Q})^2+i\frac{\omega}{\tilde{\Gamma}}-\frac{\omega^2}{\tilde{\Gamma}^2}\right], \tag{14}$$

$$f^a(\mathbf{q},\omega)=f^a_{\mathbf{Q}}\left[1-\xi_f^2(\mathbf{q}-\mathbf{Q})^2+\frac{\omega^2}{\omega_J^2}\right], \tag{15}$$

where ξ_f and ξ_χ describe the dispersion of $f^a(\mathbf{q},\omega)$ and $\tilde{\chi}(\mathbf{q},\omega)$ in the vicinity of the antiferromagnetic wave vector $\mathbf{Q}$. Note that, for the Fermi surfaces relevant to the cuprates, the irreducible particle-hole susceptibility has a local *minimum* at $\mathbf{Q}$ and the commensurate peak in $\chi(\mathbf{q},\omega\to 0)$ is actually due to the momentum dependence of $f^a(\mathbf{q},\omega\to 0)$ which has a local *maximum* at $\mathbf{Q}$. On substituting these expressions into Eq. (2), and keeping only terms of order $(\mathbf{q}-\mathbf{Q})^2$ and ω^2, one obtains, using $\chi_{\mathbf{Q}}=\tilde{\chi}_{\mathbf{Q}}/(1-f^a_{\mathbf{Q}}\tilde{\chi}_{\mathbf{Q}})$,

$$\frac{\tilde{\chi}(\mathbf{q},\omega)}{1-f^a(\mathbf{q},\omega)\tilde{\chi}(\mathbf{q},\omega)}=\chi_{\mathbf{Q}}\left[1-(\xi_f^2f^a_{\mathbf{Q}}\chi_{\mathbf{Q}}-\xi_\chi^2\tilde{\chi}_{\mathbf{Q}}^{-1}\chi_{\mathbf{Q}})(\mathbf{q}-\mathbf{Q})^2+\frac{\omega^2}{\omega_J^2}f^a_{\mathbf{Q}}\chi_{\mathbf{Q}}-\frac{\omega^2\chi^2_{\mathbf{Q}}}{\tilde{\Gamma}^2\tilde{\chi}^2_{\mathbf{Q}}}+i\frac{\omega\chi_{\mathbf{Q}}}{\tilde{\Gamma}\tilde{\chi}_{\mathbf{Q}}}\right]. \tag{16}$$

We now compare this with the phenomenological expression for $\chi(\mathbf{q},\omega)$ introduced by Barzykin, which describes the damping by particle-hole excitations of the spin-wave spectrum, $\omega^2=\Delta^2+c^2(\mathbf{q}-\mathbf{Q})^2$, found starting with the $N=\infty$ quantum nonlinear σ model[9]

$$\chi_B(\mathbf{q},\omega)=\frac{\chi_{\mathbf{Q}}}{1+\xi^2(\mathbf{q}-\mathbf{Q})^2-\omega^2/\Delta^2-i\omega/\omega_{\rm SF}}; \tag{17}$$

in the limit $\Delta\gg\omega_{\rm SF}$ and $\omega\ll\Delta$, this reduces to the expression introduced by Millis, Monien, and Pines.[6] On expanding Eq. (17) to the same order in $\mathbf{q}-\mathbf{Q}$ and ω, we obtain

$$\chi_B(\mathbf{q},\omega)=\chi_{\mathbf{Q}}\left[1-\xi^2(\mathbf{q}-\mathbf{Q})^2+\frac{\omega^2}{\Delta^2}-\frac{\omega^2}{\omega^2_{\rm SF}}+i\frac{\omega}{\omega_{\rm SF}}\right]. \tag{18}$$

On making the identification

$$\xi^2=\chi_Q\left[\xi_f^2 f_Q^a-\frac{\xi_\chi^2}{\tilde{\chi}_Q}\right]\cong\frac{\xi_f^2-\xi_\chi^2}{1-F_Q^a}\ , \tag{19a}$$

$$\omega_{SF}=\frac{\tilde{\Gamma}\tilde{\chi}_Q}{\chi_Q}=\tilde{\Gamma}(1-F_Q^a)=\tilde{\Gamma}\frac{\tilde{\xi}^2}{\xi^2}\ , \tag{19b}$$

$$\Delta=\frac{\omega_J}{(f_Q^a\chi_Q)^{1/2}}=\omega_J\left[\frac{1-F_Q^a}{F_Q^a}\right]^{1/2}\ , \tag{19c}$$

we see that the two expressions are identical. We see that our NAFL description leads naturally to spin waves whose dispersion relation is that of the $N=\infty$ quantum nonlinear σ model and whose damping arises solely from the particle-hole excitations whose characteristic energy is specified by Γ.

An alternative form of the Barzykin response function Eq. (17) is useful for comparing with NMR experiments on the cuprate superconductors. On making use of Eqs. (9), (10), and (13), we find the Barzykin response function can then be written as

$$\chi_B(\mathbf{q},\omega)=\frac{\alpha c^2}{c^2/\xi^2+c^2(\mathbf{q}-\mathbf{Q})^2-\omega^2-i\alpha c^2\omega/\chi_Q\omega_{SF}}\ , \tag{20}$$

where, apart from ξ, the quantities which determine $\chi(\mathbf{q},\omega)$, are the two constants $\alpha\equiv\chi_Q/\xi^2$ and the spin-wave velocity $c\equiv\omega_J\tilde{\xi}$, and the product $\chi_Q\omega_{SF}$. The latter may be determined from NMR measurements of the ^{63}Cu spin-lattice relaxation rate and spin-echo decay rate. In the limit of long correlation lengths, Thelen and Pines[11] have shown these may be written as

$$\frac{1}{^{63}T_1T}\sim\frac{\chi_Q}{\omega_{SF}\xi^2}\sim\frac{\alpha}{\omega_{SF}}\ , \tag{21a}$$

$$\frac{1}{^{63}T_{2G}}\sim\frac{\chi_Q}{\xi}\sim\alpha\xi\ . \tag{21b}$$

Hence

$$\frac{^{63}T_1T}{^{63}T_{2G}^2}=C\chi_Q\omega_{SF}=C\tilde{\chi}_Q\tilde{\Gamma}\ , \tag{22}$$

where the constant of proportionality, C, depends only on the choice of hyperfine coupling constants in the Mila-Rice Hamiltonian for these systems. The same NMR measurements together with the spin-wave velocity determine the damping γ_Q of the spin waves near Q, which is given by the ratio of the spin gap Δ to the characteristic frequency for the relaxational mode, ω_{SF}. Thus

$$\gamma_Q=\frac{\Delta_Q}{\omega_{SF}}=\left[\frac{c}{\alpha\xi}\right]\left[\frac{\alpha}{\omega_{SF}}\right]=Dc\left[\frac{^{63}T_{2G}}{^{63}T_1T}\right]\ , \tag{23}$$

where the constant of proportionality, D, is specified by the choice of hyperfine coupling constants in the Mila-Rice Hamiltonian.

III. APPLICATION TO THE CUPRATE SUPERCONDUCTORS

A NAFL with two distinct energy scales cannot, in general, exhibit pure scaling behavior, since the latter requires that there be only one characteristic frequency, $\bar{\omega}\sim\xi^z$, where z denotes the scaling regime. Still, as we shall demonstrate for the cuprates, for some regimes of hole doping and temperature, the predicted magnetic behavior is consistent with the scaling behavior obtained by SP. When written in the form Eq. (20), it is evident that the possible scaling regimes of interest for the nearly antiferromagnetic Fermi liquid will be specified by the temperature dependence of ξ and $\chi_Q\omega_{SF}$. We now consider separately the fully (and overdoped) regimes and the underdoped regimes, and the constraints these impose on the parameters f_Q^a, $\tilde{\chi}_Q$, and $\tilde{\Gamma}$ which determine ω_{SF} and Δ in the more familiar form, Eq. (17), of the Barzykin response function.

Fully and overdoped systems

For $YBa_2Cu_2O_{7-x}$, with $x\lesssim 0.1$, and for the overdoped bismuth- and thallium-based superconductors, one finds an essentially temperature-independent $\chi_0(T)$ and a monotonic behavior for $^{63}T_1T$, which decreases as T decreases. In this regime we expect that $\tilde{\Gamma}$, which is inversely proportional to an effective quasiparticle density of states, will be of order of the Fermi energy and independent of temperature. Hence for these systems, which are those considered by MMP (Ref. 6) and Moriya, Takahashi, and Ueda,[7] one is in the Gaussian $z=2$ magnetic scaling regime, with

$$\omega_{SF}\sim\frac{1}{\xi^2}\sim a+bT$$

as is observed for $YBa_2Cu_3O_7$. From Eqs. (9) and (10a), $\chi_Q\omega_{SF}=$const and $\tilde{\chi}_Q\sim\tilde{\xi}^2=$const. More precisely, $\tilde{\Gamma}\tilde{\chi}_Q$ must be constant to get $z=2$ scaling. From Eq. (11a), one finds that f_Q^a is weakly temperature dependent,

$$f_Q^a=\frac{1}{\tilde{\chi}_Q}-\frac{1}{\alpha\xi^2}=\frac{1}{\alpha}\left[\frac{1}{\tilde{\xi}^2}-\frac{1}{\xi^2}\right]\sim a-bT\ ,$$

where a and b are positive constants, and we have used the fact that in this regime $\xi^{-2}=$const$+bT$.

An interesting consequence of our ansatz that f_Q^a possesses a characteristic frequency dependence arising from the exchange of excitations of energy $\omega\simeq\omega_J$ is that, even though, as we shall see, the spin-wave excitations are overdamped in this regime, these still may influence the Barzykin response function, Eq. (17) or Eq. (20), at high energies through its dependence on $\Delta=c/\xi$. The quantities c,ξ which enter Eq. (20) can be determined for a given system by combining the results of microscopic calculations of $\tilde{\xi}$ with an analysis of NMR experiments on T_1 and T_{2G}.

The only $z=2$ system for which these results are available is $YBa_2Cu_3O_7$, and we consider that briefly. We take $\alpha\cong 15$ states/eV, following Thelen and Pines,[11] and, at 100 K, take $\tilde{\chi}_Q=\alpha\tilde{\xi}^2=1.67$ states/eV, close to the value 1.7 states/eV calculated by MP; we then have for the temperature-independent quantities which characterize this system

$$\tilde{\xi}=0.33 \ ,$$

$$c\equiv\omega_J\tilde{\xi}=44 \text{ meV}\,(\omega_J/J)\cong 132\text{ meV} \ ,$$

$$\tilde{\Gamma}=\frac{(\chi_{\mathbf{Q}}\omega_{\mathrm{SF}})_{\mathrm{expt}}}{\tilde{\chi}_{\mathbf{Q}}}\cong\frac{1}{\tilde{\chi}_{\mathbf{Q}}}=600 \text{ meV} \ ,$$

on making use of the result $\chi_{\mathbf{Q}}\omega_{\mathrm{SF}}\cong 1$, independent of temperature, obtained by Thelen and Pines[11] from the T_1 and T_{2G} measurements of Imai and Slichter[12] and taking $\omega_J\sim 3J$, the energy per spin required to interchange two nearest-neighbor spins, as measured in two-magnon Raman scattering,[13] with $J=0.132$ eV.

The other quantities which characterize the spin-fluctuation spectrum of $YBa_2Cu_3O_7$ are all temperature dependent, and can be determined directly from the measured values of $T_1T\sim\omega_{\mathrm{SF}}/\alpha$. With $\alpha=15$ states/eV, one finds, for example, at $T=100$ K,

$$\chi_{\mathbf{Q}}(100\text{ K})=70 \text{ states/eV} \ ,$$

$$\omega_{\mathrm{SF}}(100\text{ K})=14.2 \text{ meV} \ ,$$

$$F^a_{\mathbf{Q}}(100\text{ K})=0.976 \ ,$$

$$\xi(100\text{ K})=2.16 \ .$$

We further note that in our strong-coupling calculations for this system, reported in Ref. 2, we found a weak temperature dependence for $\tilde{\xi}_Q$; as T decreases, ξ_Q increases, because the lifetime of the quasiparticles responsible for $\tilde{\xi}_Q$ has increased. The net increase in $\tilde{\xi}_Q$ between 200 and 100 K we found was some 3%.

Were the spin-wave velocity appreciably smaller, the high-frequency behavior of Eq. (20) would be quite different from that obtained using the MMP expression; with the latter, the spin-fluctuation peak is at ω_{SF}, while Eq. (20) in the absence of strong spin-wave damping predicts a spin-fluctuation peak at

$$\Delta=\left[\frac{c^2}{\xi^2}+c^2(\mathbf{q}-\mathbf{Q})^2\right]^{1/2}$$

even though one is in a $z=2$ regime. However, for our choice of ω_J that high-energy peak, $\Delta_Q(100\text{ K})\sim 60$ meV, is never well defined; for example, at $\mathbf{Q}$ and $T=100$ K, one finds, on making use of Eq. (23)

$$\gamma_Q(100\text{ K})=\frac{\Delta(100\text{ K})}{\omega_{\mathrm{SF}}(100\text{ K})}=\frac{J}{\xi\omega_{\mathrm{SF}}}=4.3 \ .$$

Thus the spin waves introduced by an energy scale of magnetic origin are always significantly overdamped, and as a result the high-frequency behavior of $\chi(q,\omega)$ is close to that obtained using the MMP expression.

Spin-pseudogap behavior in the underdoped systems

The underdoped cuprate superconductors ($YBa_2Cu_3O_{7-x}$ for $x\geq 0.15$; $La_{2-x}Sr_xCuO_4$) demonstrate low-frequency magnetic behavior which is quite different from that measured in $YBa_2Cu_3O_{7-x}$ for $x\lesssim 0.1$: the long-wavelength static magnetic susceptibility χ_0 becomes markedly temperature dependent, decreasing as T decreases, while the product $(^{63}T_1T)^{-1}$ turns over as T decreases; thus it initially rises, reaches a maximum, and then decreases, as T is decreased from, say, 300 K. Moreover, for $YBa_2Cu_3O_{6.63}$, the only underdoped system for which $^{63}T_{2G}$ has been measured,[14] the product $^{63}T_1T/^{63}T_{2G}^2$ is no longer independent of T; rather it increases as $(a+bT)^{-1}$ as T is decreased.

As has been discussed by many authors (see Ref. 15 for a review), this behavior suggests that a "spin pseudogap" forms in the quasiparticle system, which affects the magnetic behavior but does not give rise to superconductivity. At long wavelengths it can be characterized by an effective temperature-dependent density of states $N_0(T)$, so that

$$\chi_0(T)\sim N_0(T) \ , \tag{24a}$$

where $N_0(T)$ might, for example, resemble the Yosida function introduced by Yosida to explain the fall off of $\chi_0(T)$ in conventional superconductors.[16] As Loram[17] has shown, one can understand in this way the specific heat of the underdoped cuprate superconductors.

In considering the behavior of $\tilde{\chi}(\mathbf{q},\omega)$ for the underdoped cuprate superconductors at wave vectors in the vicinity of $\mathbf{Q}$, it would therefore seem reasonable to introduce the phenomenological expression, valid at low ω,

$$\tilde{\chi}''(\mathbf{Q},\omega)=\tilde{\chi}_QN_Q(T)\omega \ , \tag{24b}$$

where $\tilde{\chi}_Q=\alpha\tilde{\xi}^2$ is assumed to be weakly temperature dependent, as in $YBa_2Cu_3O_7$, and $N_Q(T)$ is an effective temperature-dependent quasiparticle density of states which reflects the spin-pseudogap suppression of the low-frequency magnetic behavior. On comparing Eqs. (24) and (9), we see that this implies that in the underdoped system $\tilde{\Gamma}$ becomes temperature dependent, being given by

$$\tilde{\Gamma}=[N_Q(T)]^{-1} \ . \tag{25}$$

To the extent this description is appropriate, we can then understand, from a Fermi-liquid perspective, how the low-temperature magnetic scaling regime, the quantum disordered regime posited by SP, comes about. In this regime, found in $YBa_2Cu_3O_{6.63}$ for $T\lesssim 120$ K,[14] the antiferromagnetic correlations are frozen; both the correlation length ξ and T_2 are independent of temperature. This in turn implies that $\chi_Q=\alpha\xi^2$ becomes independent of temperature, as does F^a_Q. On the other hand,

$$\frac{1}{^{63}T_1T}\sim\frac{\chi_Q}{\xi^2\omega_{\mathrm{SF}}}=\frac{\chi_Q}{\tilde{\xi}^2\tilde{\Gamma}}=\alpha\left[\frac{\xi^2}{\tilde{\xi}^2}\right]N_Q(T) \tag{26}$$

simply tracks the spin-gap-induced suppression of the effective quasiparticle density of states $N_Q(T)$, as does the product $(^{63}T_1T/^{63}T_{2G}^2)$.

In a more speculative vein, we note that the freezing of the antiferromagnetic correlations signaled by the temperature independence of the effective quasiparticle interaction, $F^a_Q=f^a_Q\tilde{\chi}_Q$ in the NAFL description, is just what might be expected if the effects of negative feedback in this underdoped system are comparable to those found in the Hubbard-model-conserving calculations of the effective interaction in the superconducting state of the fully doped system carried out by Monthoux and Scalapino[18] and Pao and Bickers.[19] Thus as the spin pseudogap begins to be fully developed, it both reduces χ_0 and increases ω_{SF}; the resulting reduction in the feedback of the spin-fluctuation excitations on the quasiparticle motion then opposes what would otherwise be a reduction in χ_Q, thereby maintaining an effectively temperature-independent F_Q^a.

What happens as the temperature increases? According to SP and Barzykin *et al.*[9] for $T \gtrsim a$ crossover temperature T^* (~175 K for $YBa_2Cu_3O_{6.63}$), the system enters into a quantum-critical, $z=1$, magnetic scaling region, in which ω_{SF} varies inversely with ξ, so that

$$\omega_{SF} \sim (a+bT) \sim \xi^{-1} . \quad (27)$$

This behavior is confirmed by NMR experiments on $YBa_2Cu_3O_{6.63}$, which show that for $T > T^*(^{63}T_1T/^{63}T_{2G})$ is independent of temperature, with

$$\omega_{SF}\xi = \hat{c} \cong 60 \text{ meV} . \quad (28)$$

In our NAFL description, since $\omega_{SF} = \bar{\Gamma}\bar{\xi}^2/\xi^2$, this means that above T^* one obtains a result equivalent to QC $z=1$ scaling if the temperature variation of $N_Q(T)$ is proportional to that of $\xi^{-1}(T)$, that is, if

$$N_Q(T) \sim \frac{1}{\xi(T)} \sim a+bT . \quad (29)$$

This constraint appears reasonable, since $\chi_0(T)$ [and by inference $N_0(T)$] is found experimentally, for $T > T^*$, to display an approximately linear variation with T for the underdoped cuprates.[9,20] As was the case for the fully (and over-) doped systems, in this temperature regime we expect f_Q^a to follow Eq. (11a), and hence to be weakly temperature dependent. Because ξ is greater for the underdoped systems,[20,21] the actual temperature dependence of f_Q^a will not be appreciable; it will just suffice to yield the temperature dependence of $\xi(T)$.

We note that, in the underdoped systems, this NAFL scenario then implies that $\tilde{\chi}_Q\bar{\Gamma}_Q \sim (^{63}T_1T/^{63}T_{2G}^2)$ will not change its character appreciably over the entire temperature domain, since our assumption that $\tilde{\chi}_Q$ is weakly temperature dependent means that the temperature dependence of this quantity simply tracks that of $N_Q^{-1}(T)$, which is found to be $(a+bT)^{-1}$ in both the QC $z=1$ regime and the QD $z=1$ regimes. Our NAFL description thus provides a natural explanation of the nearly monotonic increase in $(^{63}T_1T/^{63}T_{2G}^2)$ measured by Takigawa[14] in $YBa_2Cu_3O_{6.63}$. We note that experiment shows that, while $N_Q(T)$ and $N_0(T)$ display comparable temperature variations between T_c and 300 K, $N_Q(T)$ does not scale with $N_0(T)$.

We turn next to a consideration of the high-frequency magnetic behavior. In the QD (frozen-correlation-length) regime, as might be expected, $\Delta_Q = c/\xi$ is independent of temperature; for $YBa_2Cu_3O_{6.63}$, with $c \sim J$ and $\xi \sim 4.2$,[9] $\Delta \sim 30$ meV at temperatures below ~120 K. The corresponding value of $\gamma(T)$ is minimum at 60 K, where it is determined by T_1 measurements to be

$$\gamma_Q(60 \text{ K}) = \frac{\Delta(60 \text{ K})}{\omega_{SF}(60 \text{ K})} \cong 1.5$$

on taking $\alpha \sim 15$ states/eV. Thus, even in the QD regime at just above T_c, the spin waves are considerably overdamped; as T increases that damping becomes more substantial. Above T^*, in the QC $z=1$ regime, it becomes independent of temperature, being given by

$$\gamma_Q = \frac{J}{\hat{c}} \cong 2.2 .$$

These estimates suggest that quite generally, although the spin-wave energies are considerably lower in the underdoped cuprates (because ξ is larger), these excitations continue to be so strongly damped as not to be observable in a neutron-scattering experiment. Indeed, for $\gamma_Q \gtrsim 1.5$, spin-wave damping is so strong that the high-frequency peak of $\chi''(\mathbf{Q},\omega)$ will be close to that predicted by MMP theory. These conclusions are consistent with the results of the Brookhaven neutron-scattering experiments on $YBa_2Cu_3O_{6.6}$ (Ref. 22) and $YBa_2Cu_3O_{6.5}$ (Ref. 23) which find no evidence for well-defined spin-wave excitations at $\mathbf{Q}$.

The remaining set of experimental constraints on the underdoped systems are from measurements of the ^{17}O spin-lattice relaxation time, which show quite generally that

$$(^{17}T_1T)^{-1} \sim \chi_0(T) .$$

This result, which is found for $YBa_2Cu_3O_{6.63}$,[5,20] $YBa_2Cu_4O_8$,[24] and $La_{1.85}Sr_{0.15}CuO_4$,[25] may be understood along the lines proposed by Monien, Pines, and Takigawa.[20] In the present notation it corresponds to taking for $\tilde{\chi}(q,\omega)$ a long-wavelength analogue of Eq. (24b),

$$\tilde{\chi}_0''(\mathbf{q},\omega) \cong N_0(T)\omega/\Gamma_0 . \quad (30)$$

Here $\Gamma_0 \sim E_F$, while $N_0(T)$ is the temperature-dependent density of states introduced in Eq. (24a).

A somewhat more general, one-component, account of both the long-wavelength behavior and the nearly antiferromagnetic behavior of the underdoped cuprates is obtained using Eq. (2), with

$$\tilde{\chi}(q,\omega) = \alpha\xi_q^2[1+i\omega N_q(T)] . \quad (31)$$

For wavelengths which are long (but not so long that one is in the *very* long-wavelength limit in which $\tilde{\chi}'' \sim 1/qV_F$), on identifying $\alpha\xi_0^2$ with Γ_0^{-1} this expression goes over to Eq. (30), while it also clearly reproduces our results for wave vectors near $\mathbf{Q}$. With a specific model for $f_a(\mathbf{q},0)$ and $N_q(T)$ it should then be possible to obtain a quantitative fit to both the ^{17}O and ^{63}Cu NMR experiments on the underdoped cuprates, analogous to that found by Thelen, Pines, and Lu[26] for the normal and superconducting states of $YBa_2Cu_3O_7$.

In concluding this section on the underdoped curprates, it is important to note that the temperature dependence of both $\Delta_Q(T)$ and the crossover temperature T^* are such that both quantities increase as the doping increases. This contrasts with the behavior of the spin pseudogap $\Delta_{\rm eff}$, which one might introduce to describe phenomenologically the evolution with doping of $N_0(T)$ and $N_Q(T)$; as Slichter[15] and Loram *et al.*[17] have shown, $\Delta_{\rm eff}$ *decreases* as the hole doping increases, presumably going to zero at the crossover from underdoped to fully doped behavior.

In concluding this section we note that, in contrast to Randeira *et al.* and Trivedi *et al.*,[27] we do not regard the spin-pseudogap behavior considered here as a precursor to superconductivity, in the sense that spin pseudogap and superconductivity originate in the same physical phenomena. In our view, the spin pseudogap describes a quite subtle modification in quasiparticle behavior brought on by the presence of holes and strong antiferromagnetic correlations. As the hole concentration increases, that modification becomes less and less important, disappearing altogether in the fully doped and overdoped systems. Superconductivity, on the other hand, originates in spin-fluctuation exchange between quasiparticles; T_c increases as the doping increases, almost certainly because the "strength" of the spin-fluctuation spectrum increases with increased doping. Thus the formation of a spin pseudogap in the normal-state quasiparticle spectrum acts to reduce T_c, not increase it. The difference between the influence of the spin pseudogap and the influence of superconductivity on the uniform spin susceptibility is also clearly visible in Knight shift experiments on the underdoped superconductors, which show clearly an inflection point at T_c.

IV. CONCLUDING REMARKS

If a NAFL description is to be applicable to the underdoped systems, it seems evident that nonlinear feedback effects must play a significant role in the temperature evolution of $\chi_0(T)$, $\tilde{\Gamma}(T)$, $\omega_{\rm SF}(T)$, and $\xi(T)$. Let us suppose, for example, that it is the long range of the antiferromagnetic correlations which is responsible for spin-pseudogap behavior, and, further, that there may be a threshold ξ^* for the onset of the suppression of the quasiparticle density of states which characterizes the spin pseudogap. On this scenario, once ξ exceeds ξ^*, as a result of $f_Q^a(T)$ antiferromagnetic correlations act to initiate a reduction in $N_0(T)$ and $\tilde{\chi}(\mathbf{q},\omega)$; since however, in a one-component description it is the quasiparticles themselves which are responsible for $\chi(\mathbf{q},\omega)$, this reduction in $\tilde{\chi}(\mathbf{q},\omega)$ will cause both the correlation length ξ and $\chi(\mathbf{q},\omega)$ to grow less rapidly at low frequencies. Since we are dealing with a strong-coupling problem, this change in $\chi(\mathbf{q},\omega)$ will, as a result of the coupling of the quasiparticles to the spin fluctuations, act to further reduce $N_0(T)$ and $\tilde{\chi}(\mathbf{q},\omega)$, etc. One therefore has *positive* feedback in the vicinity of the onset of spin-pseudogap behavior at some temperature T^*. It will lead to a comparatively rapid evolution with decreasing temperature of the effective pseudogap $\Delta_{\rm eff}$, which might be invoked to describe that suppression. On the other hand, as we have discussed earlier, negative feedback likely acts to suppress the continued growth of ξ as T decreases, leading to a constant value ξ_0 at low temperatures in the underdoped systems.

The approach we have described represents a Fermi-liquid alternative to an approach based on the quantum nonlinear σ model of localized spins modified by holes. It appears capable of explaining the "universal" behavior of $\chi_0(T)$ found in the 2-1-4 system by Johnston,[28] Nakano *et al.*,[29] and Hwang *et al.*,[30] a topic to which, together with its applicability to neutron-scattering experiments and calculations of the superconducting transition temperature, we shall return in a future publication.

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