Magnetic Behavior of the Cuprate Superconductors

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I review recent work [1–6] on magnetic dynamics of the high temperature superconductors using a model that combines two weakly interacting species of low-energy excitations: the antiferromagnetic spin waves which carry spin-1 and no charge, and Fermi-liquid-like quasiparticles which carry spin-$1/2$ and charge $e$. The model allows conversion of spin waves into electron-hole pairs; however, the low-energy spin waves are not collective modes of the quasiparticles near the Fermi surface, but rather are a separate branch of the low-energy spectrum. With certain experimentally justified assumptions, this theory is remarkably universal: the dependence on the detailed microscopic Hamiltonian and on doping can be absorbed into several experimentally measurable parameters. The $z = 1$ theory of the insulators and $z = 2$ theory of the overdoped materials, are both reproduced as limiting cases of the theory described here, which predicts that the underdoped materials remain in $z = 1$ universality class at sufficiently high temperature. This theory provides a framework for understanding both the experimental results and microscopic calculations, and in particular yields a possible explanation of the spin gap phenomenon. I also discuss some of the important unresolved issues.

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I. INTRODUCTION

The evolution of the normal state properties of the high temperature superconductors with doping is schematically described by the phase diagram in Fig. 1. The stoichiometric insulators La$_2$CuO$_4$ and YBa$_2$Cu$_3$O$_6$ undergo an antiferromagnetic transition at $T_N$, and exhibit short-range antiferromagnetic correlations well above $T_N$. Upon doping by more than several per cent strontium or oxygen, these systems become metallic and no longer have a long-range antiferromagnetic order, but short-range magnetic correlations remain. It is universally agreed that the normal state properties of this metallic state are far from the conventional metallic behavior, and the term “strange metal” has been coined to describe them. Some of the key properties of the “strange metal” are: (i) short-range antiferromagnetic correlations, seen by NMR and neutron scattering; (ii) both the resistivity and the uniform magnetic susceptibility increase as the temperature increases; (iii) some, but not all, of the materials exhibit a suppression of the low-frequency spectral weight for magnetic excitations for $T < T^* \sim 150K$ (spin gap). At higher doping, the normal state properties become increasingly similar to the Fermi liquid (FL) behavior with short-range antiferromagnetic correlations. While Landau Fermi liquid theory in the orthodox sense requires temperature-independent spin correlations, the temperature dependence is weak in YBa$_2$Cu$_3$O$_7$ and other fully doped materials, where close proximity of the FL state is evident.

High-temperature superconductivity occurs in the intermediate strange metal phase in Fig. 1. Currently, there is no consensus regarding the precise microscopic Hamiltonian of this phase. In what follows, I describe a theoretical approach to this problem which bypasses the missing information about the microscopic Hamiltonian by assuming continuous evolution of the low-energy magnetic and charge excitation spectrum between the antiferromagnetic insulator and the Fermi liquid phases, through the intermediate strange metal phase (see, e.g. [5,6], and...
references therein, and relevant earlier work \cite{10}.

II. NEARLY ANTIFERROMAGNETIC FERMI LIQUID

The approach of Refs. \cite{1,2} is based on combining the low-energy excitations encountered in the two extreme doping limits in Fig.1: the undoped antiferromagnetic insulators where the low-energy excitations are spin waves, and the overdoped limit where the low-energy excitations are the usual Fermi liquid quasiparticles. I emphasize that such an approach makes no explicit assumptions about the microscopic Hamiltonian, and also it makes no assumptions regarding the mechanism through which the two types of low energy excitations are formed. Instead, the theory is based on the premise that at low energies, the spectral weight of the system is shared between the spin waves and the quasiparticles, and that the primary interaction mechanism is spin wave to electron-hole pair conversion. A microscopic basis for this theory is provided by the mean-field spin density wave (SDW) calculations, described in \cite{3}.

The presence of the first type of low-energy excitations, the quasiparticles, is evident from photoemission experiments. Such quasiparticles at low energies must be similar to the quasiparticles of the Landau Fermi liquid theory, and carry both charge $e$ and spin $S = 1/2$, in order to account for the sharp quasiparticle peak near the Fermi energy, observed in photoemission. The quasiparticles are gapless and form a Fermi surface, the shape of which is very important for the interaction between the quasiparticles and spin waves.

The other species of low energy excitations, the spin waves, are the only low-energy modes in the antiferromagnetic insulators La$_2$CuO$_4$ and YBa$_2$Cu$_3$O$_6$. Below $T_N$, the spin waves are gapless, and in small-$q$ limit have a linear spectrum $\omega_q \approx cq$ and a mean-free path that is longer than the wavelength. When elevated temperature or doping destroy the long-range order, and only short-range antiferromagnetic correlations remain (the correlation length $\xi$ is finite), the spin waves are no longer gapless and also are overdamped for $q < \xi^{-1}$. Nevertheless, for larger wavevectors $q > \xi^{-1}$, the spin waves remain nearly the same as in the presence of long-range order, because they sample only the local order for distances of order wavelength $\lambda = 2\pi/q \ll \xi$, and therefore are nearly insensitive to the absence of antiferromagnetic correlations at distances larger than $\xi$. The evidence for their existence in the strange metal phase is based primarily on NMR and neutron scattering measurements, and is discussed in what follows. The spin waves carry spin $S = 1$ and no charge.

Whereas on the microscopic level an antiferromagnetic spin wave can be regarded as a coherent electron-hole pair, the contribution from the quasiparticle states near the Fermi surface accounts for only a fraction of the total spectral weight of the spin wave, if there is no nesting. The spin waves are therefore a separate branch of excitations, rather than a collective mode of low-energy quasiparticles. In that sense, the theory described here is somewhat similar to the spin-charge separation theory, where low-energy spin excitations cannot be represented as collective modes of low-energy charge excitations, even though on the microscopic level both originate from electrons. The difference between our model \cite{1,2} and the spin-charge separation picture applied to the high temperature superconductors \cite{3}, is that in our model one species of excitations (spin waves) carries only spin, while the other (quasiparticles) carries both spin and charge, therefore there is charge separation, but not spin separation. Recently, Sachdev \cite{4} and Laughlin \cite{12} have pointed out that in a system with spin-charge separation, some of the spinon and holon excitations may form bound states which carry both spin and charge, and in many respects are similar to conventional quasiparticles.

FIG. 2. Magnetic excitation spectrum of type (B) model (classification due to Millis \cite{13}), where $Q = (\pi/a,\pi/a)$ can connect two points on the Fermi surface. The minimum of the spin wave dispersion $\omega_Q = \left(c^2|q - Q|^2 + \Delta^2\right)^{1/2}$ is located inside the electron-hole continuum.

One of the key factors that affect the magnetic and charge properties is the position of the minimum of the spin wave spectrum, $Q = (\pi/a,\pi/a)$ for the commensurate short range order discussed here, with respect to the electron-hole continuum. If the spin wave spectrum is located inside the electron-hole continuum, as it is illustrated in Fig.2, the spin waves can convert into electron-hole pairs. This conversion process becomes the dominant contribution to spin wave damping at low energies, and has a profound effect on the magnetic properties. In the classification introduced by Millis, this situation is called model B. For a discussion of the opposite case, when $Q$ cannot connect two points on the Fermi surface (model A), see Refs. \cite{14,15}.
The results of recent photoemission measurements indicate that model B is relevant to the Y- and Bi-based high-temperature superconductors. In what follows, I concentrate exclusively on model B.

III. SPIN GAP

The spin gap behavior is the suppression of the low frequency spectral weight for magnetic excitations, which can be observed by NMR and neutron scattering. In the model at hand, this suppression is expected already in a very crude approximation which treats spin wave and quasiparticle excitations as noninteracting, free modes. Below, I describe a qualitative picture of the spin gap behavior suggested by Sokol and Pines, and derived starting from model B by Sachdev, Chubukov, and Sokol.

In the non-interacting approximation, the density of states for magnetic excitations is a sum of spin wave and quasiparticle contributions. For frequencies below the gap for spin wave excitations, \( \omega < \Delta = c/\xi \), only the quasiparticles contribute to the magnetic density of states. For frequencies \( \omega > \Delta \), both the spin waves and the quasiparticles contribute. In a measurement of the total magnetic density of states, for example in a NMR relaxation or neutron scattering measurement at low temperatures, one expects to see a gap-like suppression of the density of states for magnetic excitations for \( \omega < \Delta \).

Beyond the non-interacting approximation, the lifetime of spin waves primarily is due to their conversion into electron-hole pairs. Upon increasing doping, the spin gap is washed out by a combination of two separate effects: first, the spin waves become overdamped because the rate of conversion increases; second, the gap for spin-wave excitations \( \Delta = c/\xi \) increases as \( \xi \) decreases. The remaining spin waves, which are pushed up to much larger energies, can in principle be seen by neutron scattering. At least two recent experiments seem to allow such an interpretation: the evidence for the magnetic character of the 41 meV peak in YBa\(_2\)Cu\(_3\)O\(_7\) by Keimer et al., and the observation of the zone-boundary magnon in La\(_2\)-xSr\(_x\)CuO\(_4\) by Aeppli et al.

The zone boundary high-energy spin wave (a magnon), which continuously evolved from the identical mode in the insulator, seems to be most likely explanation of Aeppli’s measurements; however, this data is very preliminary.

IV. UNIVERSAL THEORY OF MAGNETIC DYNAMICS

In this section, I describe recent work by Sachdev, Chubukov, and Sokol, where the universal behavior of the magnetic correlations near \( Q \), and of the bulk susceptibility, was calculated using the rate of the Landau damping of spin waves as an input parameter. Several important assumptions about the microscopic model are built into this theory. First, we limit our study to systems with short-range order at \( T = 0 \). The region at low doping where the long range Néel order exists at \( T = 0 \) requires separate consideration. Second, we require that there is no nesting, i.e. the areas of the Fermi surface that are adjacent to the points connected by \( Q \), are not parallel to each other. The photoemission measurements show that this is the case in Y- and Bi-based superconductors. Third, we assume that there is no substantial \( g - \omega \), and \( T \)-dependence of the Landau damping for \( |q - Q| \sim 1/\xi \) and \( \omega \sim \Delta \), respectively. This assumption is more difficult to verify experimentally; it holds in mean field theory on the disordered side if the correlation length is large enough.

Under these assumptions, the additional damping due to the spin wave to electron-hole pair conversion can be included into the theory by inserting its rate \( \Gamma \) into the noninteracting spin wave dynamical response function (a similar expression was introduced by Barzykin, Pines, Sokol, and Thelen on phenomenological grounds):

\[
\chi(q, \omega) \sim \text{const} \left( \frac{\omega_q^2 - \omega^2}{\omega_q^2 - \omega^2 - i\omega\Gamma} \right),
\]

where the spin wave spectrum for finite \( \xi \) (short-range correlations) has the following form:

\[
\omega_q = \sqrt{c^2|q - Q|^2 + \Delta^2}, \quad \Delta = c/\xi.
\]

The exact dynamical susceptibility of the model is obtained by calculating the effects of mutual scattering of spin waves, primarily the additional damping, on \( \chi(q, \omega) \) given by Eq. (1). When the Landau damping processes dominate dissipation, the result of such a calculation differs only slightly from Eq. (1).

With these assumptions, the dynamical magnetic susceptibility near the staggered wavevector, \( |q - Q| \ll a^{-1} \), is given by:

\[
\chi(q, \omega) = \frac{Z}{T - \eta} \left( \frac{c}{T} \right)^2 \Phi_s \left( c|q - Q| T \omega, \Delta T, \frac{\Gamma}{T} \right),
\]

and the temperature-dependent part of the uniform magnetic susceptibility, \( \chi_u \), by:

\[
\chi_u(T) - \chi_u(T = 0) = (1 + \alpha') \frac{T}{c^2} \Phi_u \left( \frac{\Delta}{T}, \frac{\Gamma}{T} \right).
\]

Here, \( \alpha' \) is a non-universal constant, both \( \Phi_s \) and \( \Phi_u \) are universal and computable functions of their arguments,
and $\eta$ is a universal critical exponent which is very small and for all practical purposes can be replaced by zero.

Eqs. (3) apply when all dimensionful parameters and variables are smaller than the respective lattice cutoffs, which roughly translates into the following:

$$\omega, T, \Delta, \Gamma \ll \min(J, E_F), \quad \xi^{-1}, |q - Q| \ll a^{-1},$$  \hspace{1cm} (5)

where $J$ is the exchange constant, $E_F$ the Fermi energy, and $a$ the lattice spacing. If the conditions (5) apply, the magnetic dynamics near $Q$ depends on four dimensionful parameters, two of which describe the spin wave spectrum ($c$ and $\Delta$), one is set by the size of spin ($Z$), and one is determined by the rate of the Landau damping ($\Gamma$).

The temperature-dependent part of the bulk susceptibility, which adds to the Pauli term, is also universal up to a fixed doping as the temperature increases; it is however not observed experimentally because scaling fails altogether when at high temperatures the correlation length becomes very short, $\xi/a \lesssim 2$ (Barzykin and Pines [1]). The $z = 2$ phase shows a further crossover to the Landau Fermi liquid when $\Delta^2/\Gamma$ becomes larger than $\omega$ or $T$. Fig. 3 describes the sequence of crossovers observed as $\Gamma/\Delta$ increases.

### A. $z=1$ limit ($\Gamma/\Delta \lesssim 1$)

The limit $\Gamma/\Delta = 0$ and $\Delta > 0$ corresponds to an insulator with short-range antiferromagnetic correlations at $T = 0$ (Fig. 3a). Such an insulator has a true energy gap $\Delta$ because creating any combination of excitations (spin waves which have a gap) above the ground state requires a finite energy, hence $\chi''(\omega < \Delta) = 0$. While this limit has no direct relevance to the cuprate oxide insulators (which develop Néel long-range order at $T = 0$ and have gapless spin waves), it helps to understand the behavior of the underdoped materials where $\Gamma/\Delta \lesssim 1$.

The effect of small doping is shown in Fig. 3b: $\chi''(\omega)$ becomes finite for all $\omega$, but it remains much smaller for $\omega < \Delta$ compared to $\omega > \Delta$. The gap which existed for $\Gamma/\Delta = 0$ transforms into a knee-like feature at $\omega \sim \Delta$ for $\Gamma/\Delta \lesssim 1$. This behavior reproduces the essential features of the spin gap observed in some of the underdoped high-temperature superconductors.

At high temperatures $T \gg \Delta$, the behavior of $\Gamma/\Delta \lesssim 1$ underdoped system is similar to that of the $\Gamma/\Delta = 0$ insulator, because for energies $\omega \gtrsim \Delta$ the spectral weight of the two systems is nearly the same, and in both cases is dominated by the spin wave contribution (compare Figs. 3a,b). As a result, the magnetic dynamics in this temperature range is in the $z = 1$ universality class, and exhibits quantum critical behavior $\tilde{\omega} \sim \Delta \sim T$.

The NMR measurements in the underdoped materials $\text{YBa}_2\text{Cu}_3\text{O}_6.63$ (Takigawa [7]) and $\text{YBa}_2\text{Cu}_3\text{O}_8$ (Imai et al. [8], Stern et al. [19], and Corey et al. [20]) are consistent with $z = 1$ predictions by Sokol and Pines [2]: both materials have a spin gap at low temperatures, and $T_{\text{c}}/T_{\text{c}2} \approx \text{const}$ at high temperatures. In
La$_{1.85}$Sr$_{0.15}$CuO$_4$, $1/T_{2G}$ has not yet been measured at sufficiently high temperatures ($T = 500 – 1000K$), but $1/T_1$ has been, and it is nearly the same as in the insulator (Imai et al. [21]). Therefore, it has to be dominated by the spin wave contribution, which obeys the $z = 1$ theory. At low temperatures, the application of this theory to La$_{1.85}$Sr$_{0.15}$CuO$_4$ requires modifications due to the incommensurability of short range order. According to the theory described here, La$_{1.85}$Sr$_{0.15}$CuO$_4$ should have a smaller spin gap than the underdoped YBCO materials, which appears to be almost obscured by the superconducting phase (see Ref. [8] for a discussion).

B. $z=2$ limit ($T/\Delta \gtrsim 1$)

Figs. 2c,d describe different regions of the same frequency dependence of $\chi^\prime_0(\omega)$ at $T = 0$ in the overdoped case, where $T/\Delta \gtrsim 1$: (c) corresponds to $\omega \sim \Delta^2/\Gamma$, and (d) to $\omega \ll \Delta^2/\Gamma$. Regime (c) is $z = 2$ quantum critical; regime (d) is $z = 2$ quantum disordered, which is equivalent to the Landau Fermi liquid. The theory of magnetic behavior in the $z = 2$ regime has been developed by Millis, Monien, and Pines [9] and Millis [10].

At low temperatures, the application of this theory to La$_{1.85}$Sr$_{0.15}$CuO$_4$, $1/T_{2G}$ corrections; detailed calculations must be performed to determine whether or not this speculation is correct. Millis, Ioffe, and Monien [24] recently presented a scenario of spin gap formation based on spin-charge separation, accompanied by singlet pairing of spin-carrying excitations (spinons). Since holons do not have spin and therefore do not contribute to the magnetic density of states, the bulk susceptibility must vanish upon singlet pairing of spinons at low temperatures. They argued that the observed decrease of the bulk susceptibility at low temperatures in underdoped YBCO can only be explained with this scenario.

However, their conclusion relies on the assumption that both $\chi^\prime_0(\omega \rightarrow 0, T)$ and $\chi_0(T)$ would extrapolate to zero at low temperatures even without the superconducting transition, a statement that cannot be verified experimentally. In our view, no conclusion can be drawn from the experimental data on $\chi_0(T)$ above $T_c$ as to whether at $T \rightarrow 0$ the magnetic density of states without superconductivity would decrease all the way down to zero, as it is required by their model, or would become much smaller than at high temperatures, but remain finite, as it is expected in our model.
VI. UNRESOLVED ISSUES AND CHALLENGES

The universal scaling theory yields a qualitative scenario for the evolution of magnetic behavior with doping which is consistent with the experiment. It also has been very successful in quantitatively explaining as well as predicting the results of some of the experimental measurements, notably the NMR relaxation rates in the insulators and doped materials. However, it fails to explain the detailed temperature dependence of $\chi_u(T)$ at high temperatures. This failure is likely to be caused by the lattice corrections in the broad sense: the influence of the Brillouin zone boundary on $q$-integrations, the non-linearity of the spin-wave spectrum at large wavevectors, bilayer coupling in YBCO, or energy dependence of the Landau damping rate $\Gamma$.

Different quantities are differently affected by the lattice corrections, and some are more robust than others. For instance, over a range of temperatures, $\chi_u$ in the Heisenberg model is affected by the lattice corrections, while the characteristic frequency $\tilde{\omega}$ is not. Furthermore, some of the lattice corrections that do appear, can be absorbed into the dimensionful parameters of the model, while the universal scaling functions remain nearly unaffected \[\text{[2]}\text{[20]. A detailed study of these lattice effects may allow their inclusion into a phenomenological extension of the scaling theory to expand its range of applicability.}

Another important challenge is to determine the precise role of bilayer coupling, which is central to the scenario of spin gap formation by Millis and Monien \[\text{[27]. In the theory described here, the bilayer coupling affects the dimensionful parameters of the model, but does not affect any observables expressed as a function of these parameters, unless the size of bilayer coupling is comparable to other low-energy scales. Note that in our model, the spin gap may form with or without bilayer coupling, but it is enhanced if bilayer coupling is present.}

Finally, it is very important to understand on the microscopic level how the spin waves and the quasiparticles share the spectral weight for intermediate doping, and in particular the mechanism of the experimentally observed reduction of the Pauli contribution to the uniform spin susceptibility in the underdoped case. The experimental data indicates that the spin wave to electron-hole pair conversion rate is also suppressed in the underdoped materials, which in the theory described here results in spin gap formation. The cause of such a reduction is not fully understood, and may be a consequence of a reduced density of states for the quasiparticles at low doping, which is also seen in $\chi_u(T = 0)$.

Studies of microscopic models for the high-Tc cuprates should help to clarify whether the experimentally observed evolution of the key parameters of the model discussed here is similar to that obtained in microscopic calculations, thereby allowing one to check the validity of the proposed theory.

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