Magnetic Coherence in Cuprate Superconductors

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Recent inelastic neutron scattering (INS) experiments on La$_{2-x}$Sr$_x$CuO$_4$ [1–5] observed a magnetic coherence effect, i.e., strong frequency and momentum dependent changes of the spin susceptibility, $\chi''$, in the superconducting phase. We show that this effect is a direct consequence of changes in the damping of incommensurate antiferromagnetic spin fluctuations due to the appearance of a d-wave gap in the fermionic spectrum. Our theoretical results provide a quantitative explanation for the weak momentum dependence of the observed spin-gap. Moreover, we predict (a) a Fermi surface in La$_{2-x}$Sr$_x$CuO$_4$ which is closed around $(\pi, \pi)$ up to optimal doping, and (b) similar changes in $\chi''$ for all cuprates with an incommensurate magnetic response.

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The spin excitation spectrum in La$_{2-x}$Sr$_x$CuO$_4$ [1–5] in the normal and superconducting state has been intensively studied during the last few years in inelastic neutron scattering (INS) experiments. The normal state spectrum for compounds with $x > 0.04$ is characterized by peaks in $\chi''(\mathbf{q}, \omega)$ at incommensurate wave-vectors $\mathbf{Q}_1 = (1 \pm \delta, 1)\pi$ and $\mathbf{Q}_3 = (1, 1 \pm \delta)\pi$, where $\delta$ increases with increasing doping. Recent INS experiments in the superconducting state of La$_{2-x}$Sr$_x$CuO$_4$ (LSCO) by Mason et al. (x=0.14) [6] and Lake et al. (x=0.16) [7] show striking momentum and frequency dependent changes in $\chi''$ upon entering the superconducting state, which the authors called the magnetic coherence effect. For both compounds, $\chi''(\mathbf{Q}_i)$ in the superconducting state is considerably decreased from its normal state value below $\omega \approx 7$ meV, while it increases above this frequency. For frequencies in the vicinity of 7 meV, the incommensurate peaks sharpen in the superconducting state, while at higher frequencies the peak widths in the normal and superconducting state are approximately equal. Moreover, by employing a Kramers-Kronig transformation, the authors found that the static susceptibility, $\chi'$, at $\mathbf{Q}_i$ decreases in the superconducting state [8].

In this communication, we show that the magnetic coherence effect is a direct consequence of changes in the damping of incommensurate antiferromagnetic spin fluctuations due to the appearance of a d-wave gap in the fermionic spectrum. We obtain results for the frequency and momentum dependence of $\chi''$ that are in good qualitative, and to a large extent quantitative agreement with the experimental data, and also explain the weak momentum dependence of the spin-gap. We show that INS data in the superconducting state provide information on the symmetry of the order parameter and the topology of the Fermi surface (FS) and that for La$_{2-x}$Sr$_x$CuO$_4$, INS experiments suggest a FS closed around $(\pi, \pi)$. We predict that the magnetic coherence effect is to be expected for any cuprate superconductor with an incommensurate spin spectrum, and thus in particular for YBa$_2$Cu$_3$O$_{6+x}$ (YBCO), in which an incommensurate spin structure at low frequencies has been observed [9–11].

The starting point for our calculations is a spin-fermion model [11] in which the damping of incommensurate spin-excitations arises from their interaction with fermionic quasi-particles. In this model, the spin propagator, $\chi$, is given by

$$\chi^{-1} = \chi_0^{-1} - \Pi,$$

where $\chi_0$ is the bare propagator, and $\Pi$ is the bosonic self-energy given by the irreducible particle-hole bubble. $\chi_0$ is in general obtained by integrating out the high-energy fermionic degrees of freedom. However, since the form of fermionic excitations at high frequencies is so far not well understood, a microscopic calculation of $\chi_0$ is not yet feasible. We therefore make the experimentally motivated ansatz

$$\chi_0^{-1} = \xi_0^{-2} + (\mathbf{q} - \mathbf{Q}_0)^2 \alpha,$$

where $\xi_0$ is defined as the “bare” magnetic correlation length (unrenormalized by the coupling to low-frequency particle-hole excitations) and $\alpha$ is a temperature independent constant. In general one would expect a frequency term in Eq. (2) which is omitted here because experimentally there is no observed dispersion in the spin excitation spectrum below $\omega \approx 25$ meV [12], well above the frequency range we consider here. The above form of $\chi_0$ thus only determines the position of the incommensurate peaks in momentum space; it does not affect the frequency dependence of $\chi''$, which arises solely from $\Pi$. In the following we define the renormalized magnetic correlation length as $\xi^{-2} = \xi_0^{-2} - \alpha \text{Re} \Pi$. We first consider $\chi''$ at $\mathbf{Q}_i$, in the normal state. Calculating $\Pi_N$ to lowest order in the spin-fermion coupling $g$ yields $\text{Im} \Pi_N \sim \omega$, while $\text{Re} \Pi_N \approx \text{const.}$ [13], yielding $\xi^{-2}_N(\omega) = \text{const.}$, and a frequency dependent dynamic susceptibility, $\chi''(\mathbf{Q}_i, \omega)$, of the MMP form [12] which
quantitatively describes the results of INS experiments in the normal state of LSCO \[12\] and YBCO \[13\].

In the superconducting state, \( \Pi_{SC} \) is given by (to lowest order in \( g \))

\[
\Pi_{SC}(\mathbf{q}, i\omega_n) = -g^2 T \sum_{\mathbf{k},m} \left\{ G(\mathbf{k}, i\Omega_m) G(\mathbf{k} + \mathbf{q}, i\Omega_m + i\omega_n) + F(\mathbf{k}, i\Omega_m) F(\mathbf{k} + \mathbf{q}, i\Omega_m + i\omega_n) \right\},
\]

(3)

where \( G \) and \( F \) are the normal and anomalous Green’s functions

\[
G = \frac{i\omega_n + \epsilon_k}{(i\omega_n)^2 - \epsilon_k^2 - \Delta_k^2}, \quad F = \frac{-\Delta_k}{(i\omega_n)^2 - \epsilon_k^2 - \Delta_k^2},
\]

(4)

\( E_k = \sqrt{\epsilon_k^2 + |\Delta_k|^2} \) is the fermionic dispersion in the superconducting state, \( \Delta_k = \Delta_0 \left( \cos(k_x) - \cos(k_y) \right)/2 \) is the d-wave gap and

\[
\epsilon_k = -2t \left( \cos(k_x) + \cos(k_y) \right) - 4t' \cos(k_x) \cos(k_y) - \mu,
\]

(5)

is the electronic tight-binding dispersion where \( t, t' \) are the hopping elements between nearest and next-nearest neighbors, respectively, and \( \mu \) is the chemical potential.

Since our theoretical results for both doping levels of LSCO \( x = 0.14(0.16) \) are quantitatively similar, we consider for definiteness \( x = 0.16 \) and choose \( t'/t = -0.22 \) and \( \mu/t = -0.84 \), a choice which will be seen to yield agreement with the experimental data. The superconducting gap, \( \Delta_0 \approx 10 \text{ meV} \), is taken to be that extracted from Raman scattering experiments by Chen et al. [14] and the incommensurate wave-vector \( \mathbf{Q} \), is at \( \delta \approx 0.25 \).

Our theoretical results for the spin-damping, \( \text{Im} \Pi \) in Eq.(3) at \( \mathbf{Q} \), are presented in Fig. 1. Since \( \mathbf{Q} \) is incommensurate, we obtain four decay channels for spin excitations; the two channels in the first Brillouin zone are shown in the inset of Fig. 1. In the normal state all four channels for particle-hole excitations are excited in the low frequency limit, which yields \( \text{Im} \Pi_N \sim \omega \), as noted above. In the superconducting state, the four channels split into two pairs with degenerate non-zero threshold energies, \( \omega^{(1,2)} \), that are determined by the momentum dependence of the order parameter and the shape of the Fermi surface. In particular, we find

\[
\omega^{(1,2)} = |\Delta_k| + |\Delta_{k+\mathbf{Q}}|,
\]

where \( \mathbf{k} + \mathbf{Q} \) are on the Fermi surface, as shown in the inset of Fig. 1. For the band parameters chosen, the threshold energies are \( \omega^{(1,2)} = 0.70 \Delta_{SC} \) for quasiparticle excitations close to the nodes of the superconducting gap (excitation 1), and \( \omega^{(1,2)} = 1.86 \Delta_{SC} \) for excitations which connect momenta around \((0,\pi)\) and \((\pi,0)\) (excitation 2). Note that due to the superconducting coherence factors in Eq.(3), \( \text{Im} \Pi_{SC} \) exhibits sharp jumps at the threshold frequencies. Since for \( T = 0 \) and \( \omega < \omega^{(1)} \), \( \text{Im} \Pi_{SC} \equiv 0 \), and thus \( \chi''_{SC} \equiv 0 \), \( \omega^{(1)} \) is often referred to as the spin-gap in the superconducting state.

We now turn to the calculation of \( \text{Re} \Pi_{SC} \). The gap in \( \text{Im} \Pi_{SC} \) gives rise to a \( \omega^2 \)-term in \( \text{Re} \Pi_{SC} \) for \( \omega \ll \omega^{(1)} \), while \( \text{Re} \Pi_{SC} \approx \text{const.} \) for \( \omega \gg \omega^{(2)} \). The steps in \( \text{Im} \Pi_{SC} \) at \( \omega^{(1,2)} \) give rise to logarithmic divergences in \( \text{Re} \Pi_{SC} \); as has recently been demonstrated [15] these are an artifact of our restriction to the second order bosonic self-energy correction. When fermionic lifetimes are calculated within a self-consistent strong-coupling approach, the authors of Ref. [15] found that the steps in \( \text{Im} \Pi_{SC} \) are smoothed out, while the gap below a frequency \( \approx \omega^{(1)} \) still persists. The weak logarithmic divergences in \( \text{Re} \Pi_{SC} \) become a smooth function of frequency. Since the spin-gap survives the inclusion of realistic fermionic lifetimes, we expect the conclusions we draw in the following to be valid beyond the current level of approximation.

In Fig. 2 we present a fit of our theoretical results for \( \chi'' \) to the experimental data of Ref. [3] in the normal and superconducting state. The fit to the experimental data in the superconducting state for \( \omega^{(1)} < \omega < 16 \text{ meV} \) was obtained by making the ansatz that at these frequencies, \( \xi_{SC}(\omega) \) is frequency independent and given by

\[
\xi_{SC}^2(\omega) \approx \frac{3}{2} \xi_N^2 = \text{const.}
\]

(6)

To account for the experimental energy resolution we convolute our theoretical results with a Gaussian distribution of width \( \sigma \approx 2 \text{ meV} \).

The “high frequency” result, Eq.(8), is a consequence of the redistribution in the spectral weight of \( \chi''(\mathbf{Q}, \omega) \) in the superconducting state. By using the Kramers-Kronig relation, we find \( \xi_{SC}(\omega = 0) < \xi_N(\omega = 0) \) while,
as seen in Fig. 2 quite generally, for $\omega_c^{(1)} < \omega < \omega_c^{(2)}$, $\chi''_N(\omega)$ exceeds $\chi''_N(\omega)$, so that $\xi_{SC}(\omega) > \xi_N(\omega)$ in this frequency range. As may be seen in Fig. 2, the simple ansatz, Eq. (3), yields good agreement with experiment. Because the form of both $\chi''_{SC}(\omega)$ and $\chi''_N(\omega)$ above $\omega_c^{(2)}$ is not well known, one cannot at present arrive at a self-consistent description of the frequency dependence of $\xi_{SC}$ using the Kramers-Kronig relation. We note, however, that upon restricting the frequency integration in the Kramers-Kronig relation to $\omega < \omega_c^{(2)}$, we find $\chi''_{SC}(\omega = 0) \approx 0.65\chi''_N(\omega = 0)$, in agreement with the results of Ref. [5].

To understand the momentum dependent changes in $\chi''$ between the normal and superconducting state, we consider the momentum dependence of the spin-gap, $\omega_e^{(1)}(q)$. In Fig. 3 we plot the experimental intensity in the $\langle \omega, q \rangle$-plane for the momentum space path shown in the inset of Fig. 3b, together with our theoretical results for $\omega_e^{(1)}(q)$ (red line). We also included $\omega_e^{(1)}(q)$ as a dashed red line into the normal state data so as to demonstrate the transfer of spectral weight between the normal and the superconducting state from frequencies below $\omega_e^{(1)}(q)$ to frequencies above the spin-gap. A comparison of Fig. 3a and b clearly shows that the experimental intensity that exists in the normal state for $\omega < \omega_e^{(1)}(q)$ vanishes as expected in the superconducting state. Note that the momentum dependence of the spin-gap is rather weak; it only changes from $\Delta_{sg}^{\text{min}} \approx 5.5$ meV at its minimum (close to $Q_i$) to $\Delta_{sg}^{\text{max}} \approx 8$ meV at its local maximum midway between the incommensurate positions. We thus conclude that our theoretical result for the momentum dependence of the spin gap provides a good quantitative description of the area in the $\langle \omega, q \rangle$-plane where the spectral weight vanishes in the superconducting state.

We now turn to momentum dependence of $\chi''$ in the normal and superconducting state. Our theoretical results, which we present in Fig. 3, correspond to horizontal cuts in the $\langle \omega, q \rangle$-plane of Fig. 3 at $\omega = 7$ and 10 meV. For $\omega = 7$ meV (Fig. 3a), the peak intensity in the superconducting state is anisotropically reduced, with a stronger suppression of $\chi''_{SC}$ towards the center of the scan. The anisotropic suppression of $\chi''_{SC}$, is a direct consequence of the momentum dependence of the spin-gap which increases when moving from $Q_i$ towards the center of the scan, but decreases in the opposite direction. As a result, $\chi''_N$ is rapidly cut off by the spin-gap when moving towards the center of the scan, but is scarcely reduced in the opposite direction. This peak anisotropy should be observable for all frequencies between $\Delta_{sg}^{\text{min}}$ and $\Delta_{sg}^{\text{max}}$. For $\omega = 10$ meV $> \Delta_{sg}^{\text{max}}$ (Fig. 3b), the anisotropy vanishes, and the peak intensity increases in the superconducting state, as expected from Fig. 3. Since the anisotropy of $\chi''_{SC}$ around $Q_i$ is reduced with increasing frequency, the peak maximum seems to slightly shift towards the center of the scan. All these results, i.e., narrow peaks around 7-8 meV, a simultaneous increase in peak width and height and a shift of the peak maximum towards the center of the momentum scan with increasing frequency agree qualitatively with the experimental findings of Ref. [5] as may be seen by comparing Fig. 3a (Fig. 3a) with the bottom (top) part of Fig. 2 in Ref. [4] or with Fig. 2b (Fig. 2c) in Ref. [4]. Mason et al. considered the sharpening of the incommensurate peaks in the superconducting state as an effect of magnetic coherence which is shown here to arise solely from the momentum
dependence of the spin-gap.

Due to the symmetry of the Fermi surface, $\chi''_{SC}$ exhibits four different threshold frequencies for momenta away from $Q_i$. While the two upper thresholds remain close, the energy separation between the two lower threshold increases rapidly with distance from $Q_i$. We thus predict that $\chi''_{SC}$ will acquire additional frequency structure for $q \neq Q_i$.

The INS data also provide insight into the form of the FS in LSCO and thus complement the results of angle-resolved photoemission (ARPES) experiments. Since excitation (1) is located in the vicinity of the nodes where the superconducting gap changes rapidly with momentum, $\omega_{c1}$ sensitively depends on the form of the FS and the symmetry of the order parameter. The frequency location of $\omega_{c1}$ can therefore be used to extract information on the form of the Fermi surface, and, within the framework of Eq. (5), on the value of $t'/t$. In particular, we find that the INS data provide a lower bound for $t'/t$. Within our scenario, excitation (1) across the FS (see inset of Fig. 3) becomes impossible in the superconducting state for $|t'| < 0.2t$. Since this implies $\chi''(Q_i) = 0$ for frequencies below $\omega_{c2}$, in contradiction to the experimental results, we conclude $|t'| \geq 0.2t$. Assuming a weak doping dependence of $t'/t$, this constraint for $t'$ yields a FS of LSCO which is closed around $(\pi, \pi)$ up to optimal doping. The FS thus possesses the same topology as that in YBCO; this explains the occurrence of incommensurate peaks in the spin spectrum along the same direction in momentum space in the latter materials [5, 8].

Though the details of the magnetic coherence effect are sensitive to material specific parameters, e.g., Fermi surface topology, the extent of the incommensuration $\delta$, their experimental observation only depends on two criteria: the existence of an incommensurate spin structure and the d-wave symmetry of the superconducting gap. We thus predict a similar effect for all cuprate superconductors in which these criteria are met, and are currently studying its form in YBCO [11].

Finally, the theoretical scenario for the magnetic coherence effect presented here is conceptually different from that recently proposed for the resonance peak [16]. Not only do the effects take place in different wave-vector and energy regions of $\chi''$ [8], but the origin of the resonance peak is ascribed to a dispersing spin mode, while our scenario for the coherence effect is solely based on the existence of a relaxational spin mode.

In summary, we find that the frequency and momentum dependent changes of $\chi''$ in the superconducting state are a direct consequence of changes in the quasiparticle spectrum due to the appearance of a d-wave gap. We show that the available INS data constrain the Fermi surface topology, and suggest a Fermi surface in La$_{2-x}$Sr$_x$CuO$_4$ which is closed around $(\pi, \pi)$ up to optimal doping. We make several predictions for the frequency dependence of $\chi''(\omega)$ at and around $Q_i$ which await further experimental testing. Finally, we predict the presence of comparable changes in $\chi''$ in all cuprate superconductors with an incommensurate spin-structure.

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