Spin dynamics in high-$T_C$ superconductors

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Abstract. Key features of antiferromagnetic dynamical correlations in high-$T_C$ superconductors cuprates are discussed. In underdoped regime, the sharp resonance peak, occurring exclusively in the SC state, is accompanied by a broader contribution located around $\sim 30$ meV which remains above $T_C$. Their interplay may induce incommensurate structure in the superconducting state.

INTRODUCTION

Over the last decade, a great deal of effort has been devoted to show the importance of antiferromagnetic (AF) dynamical correlations for the physical properties of high-$T_C$ cuprates and consequently for the microscopic mechanism responsible for superconductivity [1,2]. To elucidate how these electronic correlations are relevant, it is then necessary to put the spectral weight of AF fluctuations on a more quantitative scale. Inelastic neutron scattering (INS) provides essential information
on this matter as it directly measures the full energy and momentum dependences of the spin-spin correlation function. Recently, efforts have been made to determine them in absolute units by comparison with phonon scattering. The following definition, corresponding to \( \frac{1}{3} \) of the total spin susceptibility, is used [3],

\[
\chi^{\alpha\beta}(Q, \omega) = -(g \mu_B)^2 \hbar \int_0^\infty dt \exp^{-i\omega t} [S^\alpha_Q(t), S^{\beta}_{-Q}] >
\]  

(1)

Our results are then directly comparable with both Nuclear Magnetic Resonance (NMR) results and theoretical calculations. Here, some aspects of the spin dynamics obtained in bilayer system will be presented in relation with recent results reported by other groups [4,5]. However, it is before useful to recall the main features of magnetic correlations in the YBa\(_2\)Cu\(_3\)O\(_{6+x}\) (YBCO) system over doping and temperature [6–11].

**ENERGY-DEPENDENCES**

We first emphasize the energy dependence of the spin susceptibility at the AF wave vector, \( Q_{AF} = (\pi, \pi) \), for \( x \geq 0.6 \) (or \( T_C \geq 60 \) K). \( Im\chi \) in the normal state is basically well described in the underdoped regime by a broad peak centered around \( \simeq 30 \) meV (see Fig. 1) [11]. Upon heating, the AF spin susceptibility spectral weight is reduced without noticeable renormalization in energy. Going into the superconducting state, a more complex line shape is observed essentially because a strong enhancement of the peak susceptibility occurs at some energy. This new feature is referred to as the resonance peak, as it is basically resolution-limited in energy (see e.g. [6,9,14]). With increasing doping, the resonant peak becomes the major part of the spectrum [11]. At each doping, the peak intensity at the resonance energy is characterized by a striking temperature dependence displaying a pronounced kink at \( T_C \) [12–15]. Therefore, this mode is a novel signature of the unconventional superconducting state of cuprates which has spawned a considerable theoretical activity. Most likely, the magnetic resonance peak is due to electron-hole pair excitation across the superconducting energy gap [9,11].

The resonance peak may or may not be located at the same energy as the normal state peak. Fig. 1 displays a case where both occurs at different energies. However, at lower doping, these two features are located around similar energies, \( \hbar \omega \sim 30-35 \) meV for \( x \sim 0.6-0.8 \) [11,13,15]. Indeed, the resonance energy more or less scales with the superconducting temperature transition [11–13] whereas the normal state maximum does not shift much over the phase diagram for \( x \geq 0.6 \) [11].

Apart from the sharp resonance peak, the broad contribution (around \( \sim 30 \) meV) is still discernible below \( T_C \) as a shoulder, shown around \( \hbar \omega \simeq 35 \) meV in Fig. 1 [11]. In the superconducting state, the situation looks more complex as the low energy spin excitations are removed below a threshold, so-called spin gap [6,7,11], likely related to the superconducting gap itself. The non-resonant contribution has not received much attention so far. However, its spectral weight in the normal state
FIGURE 1. Low temperature (closed circles) and T=100 K (open squares) spin susceptibility at \(Q = (\pi, \pi)\) in absolute units in YBCO\(_{6.92}\) (2T-Saclay) (from [8]).

is important and may be crucial for a mechanism for the high-\(T_C\) superconductivity based on antiferromagnetism [2].

With increasing doping, the latter peak is continuously reduced: it becomes too weak to be measured in INS experiments in the overdoped regime YBCO\(_7\) [7,9–11]. Using the same experimental setup and the same sample [7,11], no antiferromagnetic fluctuations are discernible in the normal state above the nuclear background. Consistently, in the SC state, an isolated excitation around 40 meV is observed corresponding to the resonance peak. Above \(T_C\), an upper limit for the spectral weight can be given [10] which is about 4 times smaller than in YBCO\(_{6.92}\) [11]. Assuming the same momentum dependence as YBCO\(_{6.92}\), it would give a maximum of the spin susceptibility less than 80 \(\mu_B^2/\text{eV}\) at \((\pi, \pi)\) in our units. Therefore, even though YBCO\(_7\) may be near a Fermi liquid picture [11] with weak magnetic correlations, the spin susceptibility at \(Q = (\pi, \pi)\) can still be \(\sim 20\) times larger than the uniform susceptibility measured by macroscopic susceptibility or deduced from NMR knight shift [2].

Therefore, \(\text{Im}\chi\) is then naturally characterized in the superconducting state by two contributions having opposite doping dependences, the resonance peak becoming the major part of the spectrum with increasing doping. The discussion of \(\text{Im}\chi\) in terms of two contributions has not been emphasized by all groups [14]. However, we would like to point out that this offers a comprehensive description consistent with all neutron data in YBCO published so far. In particular, it provides an helpful description of the puzzling modification of the spin susceptibility induced by zinc substitution [16,17] by noticing that, on the one hand, zinc reduces the resonant part of the spectrum and, on the other hand, it restores AF non-resonant correlations in the normal state [11]. Interestingly, the incommensurate peaks re-
FIGURE 2. Spin-flip Q-scans at 24 meV along the (11̅) direction in YBCO$_{6.7}$ ($T_C = 67$ K): $T = 14.5$ K (right) and 70 K (left) (IN20-Grenoble). Polarized beam field was applied either parallel to $Q$ (closed circles) or perpendicular to $Q$ (dashed squares). The bar represents the q-resolution.

Recently observed below the resonance peak in YBCO$_{6.6}$ [4,5,18] support the existence of two distinct contributions as the low energy incommensurate excitations cannot belong to the same excitation as the commensurate sharp resonance peak. Finally, these two contributions do not have to be considered as independent and superimposed excitations: the occurrence of the sharp resonance peak clearly affects the full energy shape of the spin susceptibility [6,11–14]. We shall see below that the spin susceptibility q-shape is also modified below $T_C$.

MOMENTUM-DEPENDENCES

In momentum-space, although both contributions are most generally peaked around the commensurate in-plane wavevector ($\pi, \pi$), they exhibit different q-widths. The resonance peak is systematically related to a doping independent q-width, $\Delta q_{reso} = 0.11 \pm 0.02$ Å$^{-1}$ [8] (HWHM), and hence to a larger real space distance, $\xi = 1/\Delta q_{reso} \approx 9$ Å in real space. Recent data [14,13,15,18] agree with that conclusion. In contrast, the non-resonant contribution exhibits a larger and doping dependent q-width, so that, the momentum width displays a minimum versus energy at the resonance peak energy [8,13,18].

Recently, in the underdoped regime $x = 0.6$, Dai et al [4] reported low temperature q-scans at $\hbar \omega = 24$ meV which were peaked at an incommensurate wavevector. Later, Mook et al [5] have detailed the precise position of these features, displaying a complex structure of the incommensurability with a squared-like shape with more intense four corners at $Q = (\pi, \pi(1 \pm \delta))$ and $Q = (\pi(1 \pm \delta), \pi)$ with $\delta = 0.21$. Interestingly, the energy where this structure is reported is systematically located in a small energy range below the resonance energy, $E_r = 34$ meV [14,18]. Further, this structure is only clearly observed at temperatures below $T_C$. In the normal state, its existence remains questionable owing to background subtraction.
difficulties in such unpolarized neutron experiments [5,18]. A broad commensurate peak is unambiguously recovered above 75 K in polarized beam measurements [14].

To clarify that situation, we have performed a polarized neutron triple-axis experiment on an underdoped sample YBCO$_{6.7}$ with $T_C = 67$ K [12,15]. The experiment on IN20 at the Institut Laue Langevin (Grenoble) with a final wavevector $k_F = 2.662$ Å$^{-1}$ (Experimental details will be reported elsewhere [15]). Fig. 2 displays $q$-scans at $\hbar\omega = 24$ meV in the spin-flip channel at two temperatures: $T=14.5$ K and $T= T_C + 3$ K. The polarization analysis, and especially the comparison of the two guide field configurations ($H // Q$ and $H \perp Q$), allows unambiguously to remove the phonon contributions [10]. Surprisingly, the magnetic intensity is basically found commensurate at both temperatures. Tilted goniometer scans have been performed to pass through the locus of the reported incommensurate peaks [5]: less magnetic intensity is measured there meaning that there is no clear sign of incommensurability in that sample. However, Fig. 2 shows different momentum shapes at both temperatures: a flatter top shape is found at low temperature indicating that the momentum dependence of the spin susceptibility evolves with temperature. Fig. 3 underlines this point as it displays the temperature dependence of the intensity at both the commensurate wavevector and at the incommensurate positions (along the (310) direction as reported in Ref. [4]). Two complementary behaviors are found: at the commensurate position, the peak intensity is reduced at $T_C$ [14] whereas at the incommensurate position the intensity increases at a temperature which likely corresponds to $T_C$. As quoted by Dai et al [4], on cooling below $T_C$, the spectrum rearranges itself with a suppression at the commensurate point accompanied by an increase in intensity at incommensurate positions.

Therefore, even though our YBCO$_{6.7}$ sample does not exhibit well-defined incommensurate peaks, quite similar temperature dependences are observed in both samples. Superconductivity likely triggers a redistribution of the magnetic response.
in momentum space, that may marginally result in an incommensurate structure in a narrow energy range. Interestingly, the sharp resonance peak simultaneously occurs. So that, superconductivity affects the spin susceptibility shape in both the momentum and the energy spaces. Then, the interplay between the resonant and the non-resonant contributions may induce the incommensurate structure. In this respect, the magnetic incommensurability found in the La$_{2-x}$Sr$_x$CuO$_4$ system would have a different origin as the wavevector dependence of Im$\chi$ in LSCO remains essentially the same across the superconducting transition [19].

CONCLUDING REMARKS

Energy and momentum dependences of the antiferromagnetic fluctuations in high $T_C$ cuprates YBCO have been discussed. The sharp resonance peak occurs exclusively below $T_C$. It is likely an intrinsic feature of the copper oxides as it has been, recently, discovered in Bi$_2$Sr$_2$CaCu$_2$O$_{8+\delta}$ [20]. This resonance peak is accompanied in underdoped samples by a broader contribution remaining above $T_C$.

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