Pseudogap and incommensurate magnetic fluctuations in YBa$_2$Cu$_3$O$_{6.6}$

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Abstract

Unpolarized inelastic neutron scattering is used to study the temperature and wave vector dependence of the dynamical magnetic susceptibility, $\chi''(q, \omega)$, of a well characterized single crystal YBa$_2$Cu$_3$O$_{6.6}$ ($T_c = 62.7$ K). We find that a pseudogap opens in the spin fluctuation spectrum at temperatures well above $T_c$. We speculate that the appearance of the low frequency incommensurate fluctuations is associated with the opening of the pseudogap. To within the error of the measurements, a gap in the spin fluctuation spectrum is found in the superconducting state.

Keywords: High-$T_c$ superconductivity, magnetic excitations

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It is generally recognized that the determination of the spin dynamical properties of the cuprates is crucial to the understanding of the physical origin of high-temperature ($T_c$) superconductivity. Neutron scattering is a unique technique that can provide direct information on the wave vector and energy dependence of the imaginary part of the dynamical susceptibility, $\chi''(q, \omega)$. Over the past several years, intensive experimental work on the single layer La$_{2-x}$Sr$_x$CuO$_4$ (214) \cite{1,2} and the bilayer YBa$_2$Cu$_3$O$_{7-x}$ [(123)O$_{7-x}$] \cite{3-9} cuprates has yielded valuable information concerning the magnetic response in the normal and superconducting states. To summarize the advances of the field would be difficult in this short paper, so we limit ourselves to recent low frequency inelastic neutron scattering measurements on the underdoped bilayer cuprate (123)O$_{6.6}$ at the Oak Ridge National Laboratory (ORNL).

The unpolarized experiments were performed at the High-Flux Isotope Reactor at ORNL using the HB-3 triple-axis spectrometer with pyrolytic graphite (PG) as monochromator and analyzer. For the experiment, we index reciprocal $(Q)$ space by using the orthorhombic unit cell so that momentum transfers ($q_x$, $q_y$, $q_z$) in units of Å$^{-1}$ are at positions $(H, K, L) = (q_xa/2\pi, q_yb/2\pi, q_zc/2\pi)$ reciprocal lattice units (r.l.u.). The sample used in present experiment is a well characterized (123)O$_{6.6}$ showing the onset $T_c$ of 62.7 K with a transition width that is 3.3 K wide \cite{8}.

In previous work \cite{8,10}, we have demonstrated that the magnetic response in (123)O$_{6.6}$ is complex with incommensurate fluctuations for energies below the commensurate resonance at low temperatures. The low frequency spin fluctuations change from commensurate to incommensurate on cooling with the incommensuration first appearing at temperatures somewhat above $T_c$. The incommensurate fluctuations were first discovered with the filter integration technique \cite{10,11}. For a linear response function [$\chi''(q_x, q_y, \omega) \propto \omega F(q_x, q_y)$], the integration range is mostly between 10 and 30 meV with the weight centered around 23 meV for an incident neutron energy of $\sim 59$ meV. Thus, the observed incommensurate fluctuations with this technique should mostly stem from fluctuations with an energy transfer of $\sim 23$ meV. In the subsequent triple-axis \cite{10} and time-of-flight measurements \cite{12}, magnetic
fluctuations are confirmed to be incommensurate for energies around 25 meV in the low temperature superconducting state. The intensity of the incommensurate peaks increases on cooling below $T_c$, accompanied by a suppression of fluctuations at the commensurate positions. However, the energy transfers of these inelastic neutron scattering measurements are still large compared to that probed by the nuclear magnetic resonance (NMR) experiments [13]. In order to follow the incommensurate fluctuations to lower frequencies and to compare the results with the NMR experiments, we have performed additional triple-axis measurements in the ($H, H, L$) zone at energies lower than previously investigated [8,10].

Figure 1 shows the constant-energy scans along the ($H, H, 1.8$) direction. The measurements were done using a collimation of $48''$-$40''$-$120''$ in the usual notation. For an energy transfer of 6 meV [see Fig. 1(a)], there is no detectable difference in the normal and the superconducting states. The scattering is featureless with nonobservable magnetic intensity around $H = 0.5$ rlu. These data suggest the presence of a normal state spin gap (or pseudogap), consistent with previous observations [3,4]. The same scan at an energy transfer of 10 meV is shown in Fig. 1(b). In contrast to the 6 meV data, the scattering in the normal state appears to be enhanced around the expected incommensurate positions indicated by the arrows. However, the weakness of the signal and the statistics of the data do not allow a conclusive identification about the nature of the scattering.

Figure 2 summarizes the ($H, H, 1.8$) scans for an energy transfer of 16 meV at various temperatures. Although the statistics of the data could still be improved, the temperature evolution of the magnetic scattering is clear. At 11 K in the superconducting state [see Fig. 2(a)], there is no detectable magnetic signal around $H = 0.5$, similar to the data of Fig. 1. However, the same scan at 75 K [see Fig. 2(b)] displays a pair of incommensurate peaks at $(0.5 \pm \delta, 0.5 \pm \delta)$ ($\delta = 0.054 \pm 0.004$) rlu. The observed incommensurate wave vectors are consistent with the value obtained using the filter integration technique [10]. Warming the sample to 125 K, the incommensuration disappears and the profile is replaced by a single Gaussian peak as shown in the solid line of Fig. 2(c). On further warming, the multi-phonon background increases significantly. Figure 2(d) shows the data at 220 K, the scattering is
dominated by phonons and the magnetic signal around $H = 0.5$ has reduced drastically.

For underdoped (123)O$_{7-x}$, NMR experiments [13] suggested the presence of a pseudo-gap. The pseudogap temperature $T^*$ obtained from NMR measurements [13] is about 120 K for materials with a transition temperature of $\sim 60$ K. In previous neutron scattering experiments [3,4], the characteristic temperature $T^*$ has been associated with the opening of a gap (or pseudogap) in the spin fluctuations spectrum. The open circles in Figure 3 show the sum of the scattered intensity above the multi-phonon background at different temperatures obtained from constant-energy scans as those shown in Fig. 2. The closed circles are the corresponding susceptibility in arbitrary units after taking into account the Bose population factor. The dynamical susceptibility peaks at $\sim 120$ K, consistent with the opening of a pseudogap. The wave vector dependence of the fluctuations [see Figs. 2(c) and (d)] changes from commensurate above the $T^*$ to incommensurate below it. Therefore, it is tempting to associate the appearance of the incommensurate fluctuations to the opening of a spin pseudogap. However, we stress that the measurements presented here are still preliminary and more experiments are desirable. In particular, we would like to determine more precisely the temperature at which the incommensurate peaks first appear.

In summary, we have performed preliminary measurements on the wave vector dependence of the low frequency spin fluctuations for (123)O$_{6.6}$. Our data extend the earlier measurements [8,10] to lower frequencies. Two tentative conclusions are drawn from the present measurements: (1) There appears to be a gap in the spin fluctuations spectrum in the low temperature superconducting state. The magnitude of the gap is between 16 and 24 meV. (2) The appearance of the magnetic incommensurate fluctuations in (123)O$_{6.6}$ may be associated with opening of a pseudogap in the spin fluctuations spectrum.

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FIGURES

FIG. 1. (a) Triple-axis scans along \((H, H, 1.8)\) at 6 meV in the normal \((T = 75 \text{ K}, \bullet)\) and superconducting \((T = 11 \text{ K}, \circ)\) states. The data were collected with a final neutron energy of 14.78 meV, and a PG filter was placed before the analyzer. (b) Identical scans at 10 meV in two different temperatures. In this case, data were taken with a final neutron energy of 30.5 meV. Arrows indicate the expected positions for incommensurate magnetic fluctuations.

FIG. 2. Triple-axis scans along \((H, H, 1.8)\) at 16 meV with a final neutron energy of 35 meV for (a) 11 K, (b) 75 K, (c) 125 K, and (d) 220 K. The positions of incommensurate peaks are indicated by the arrows. The solid line in (b) is two Gaussians on a linear background. Solid lines in (c) and (d) are Gaussian peaks on a linear background.

FIG. 3. Temperature dependence of the magnetic scattering for an energy transfer of 16 meV. Since there is no observable peak at 11 K, the dynamical susceptibility is assumed to be zero at that temperature. For other temperatures, open circles represent the integrated magnetic intensity above the multi-phonon background. The closed circles are the corresponding \(\chi''(\omega)\) in arbitrary units. The vertical dashed line is the expected pseudogap temperature \(T^*\) and the superconducting transition temperature is marked by the vertical arrow.
Figure 1
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Figure 3
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(H, H, 1.8), $\Delta E = 16$ meV

Temperature (K)

Integrated intensity (arb. units)

$\chi''$ (arb. units)

Incommensurate
Commensurate
Pseudogap

$T_c$