Quantum Spin Excitations through the Metal-to-Insulator Crossover in $YBa_2Cu_3O_{6.45}$ (T_c = 48 K)

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Abstract

We use inelastic neutron scattering to study the temperature dependence of the spin excitations of a detwinned superconducting $YBa_2Cu_3O_{6.45}$ (T_c = 48 K). In contrast to earlier work on $YBa_2Cu_3O_{6.5}$ (T_c = 58 K), where the prominent features in the magnetic spectra consist of a sharp collective magnetic excitation termed "resonance" and a large ($\hbar\omega$= 15 meV) superconducting spin gap, we find that the spin excitations in $YBa_2Cu_3O_{6.45}$ are gapless and have a much broader resonance. Our detailed mapping of magnetic scattering along the *a*/b**-axis directions at different energies reveals that spin excitations are anisotropic and consistent with the "hourglass"-like dispersion along the a*-axis direction near the resonance, but they are isotropic at lower energies. Since a fundamental change in the low-temperature normal state of $YBa_2Cu_3O_{6+y}$ when superconductivity is suppressed takes place at y ~ 0.5 with a metal-to-insulator crossover (MIC), where the ground state transforms from a metallic to an insulating-like phase, our results suggest a clear connection between the large change in spin excitations and the MIC. The resonance therefore is a fundamental feature of metallic ground state superconductors and a consequence of high-T_c superconductivity. Here we describe our findings that are published in [1].

Materials

A solute-rich liquid pulling method was used to grow a large pure YBCO crystal without any impurity phase for our neutron scattering study. The crystal was cut into four pieces with a total mass of 6 grams and the oxygen content was set to y = 0.45 at one atmosphere with 0.5% oxygen partial pressure at 550°C for 5 days. The samples were mechanically de-twinned at 220°C and then annealed in sealed tube at 90°C for more than three weeks. The samples have well-established Ortho-II CuO chain ordering with 90% de-twinning ratio and sharp T_c.

Methods

The neutron scattering measurements were taken on the C5 thermal triple axis spectrometer with E_f = 14.7 meV and with PG(002) as both a vertically focusing monochromator and flat analyzer. Two PG filters with a total thickness 10 cm in the scattered beam removed high-order neutron wavelengths. Fast neutrons were removed from the incident beam by liquid nitrogen cooled sapphire filter before monochromator. The horizontal collimations were controlled with Soller slits and set at 30'-48'-51'-144' for [*H,H,L*] zone or 30'-28.6'-33.4'-144' for [*H,K,4K/3*] and [*H,K,4H/3*] zones.

Results

To search for a neutron spin resonance in $YBa_2Cu_3O_{6.45}$, we note that the intensity of the neutron spin resonance increases below T_c like an order parameter and its energy tracks T_c as the oxygen composition is varied via $E_R = 5.8\ k_BT_c$. Since $YBa_2Cu_3O_{6.45}$ has T_c = 48 K, we expect the mode to occur at energies around 20 meV. Figure 1a shows energy scans at wave vector $\boldsymbol{Q}$ = (1/2, 1/2, 5) below and above T_c. Consistent with earlier results on higher-doping YBCO, the raw data are dominated by phonon scattering at 20 meV and ~ 30 meV at both temperatures. However, when one takes the temperature difference spectra below and above T_c, a broad peak with a full-width-half-maximum (FWHM) of ~ 15 meV emerges at $\hbar\omega \approx 19$ meV (Figure 1c). Since intensity of phonons should decrease with decreasing temperature and the Bose population factor does not much affect the magnetic scattering above 10 meV from 5 to 55 K, the net intensity gain in Figure 1a must be the result of enhanced dynamic susceptibility below T_c. Although such intensity gain below T_c is a hallmark of the resonance, the observed broad energy peak is quite different from the instrumental resolution-limited resonance for YBCO at higher doping levels.

To see if the intensity gain below T_c is consistent with the bilayer Cu^{2+} acoustic magnetic excitations from YBCO, we carried out energy scans at the equivalent acoustic wavevector $\boldsymbol{Q}$ = (0.5, 0.5, 1.8) and Figure 1b summarizes the temperature dependence of the susceptibility $\chi''(Q,\omega)$. Consistent with the cold neutron data measured at SPINS, NIST, $\chi''(Q,\omega)$ is proportional to $\hbar\omega$ above T_c, and increases with decreasing temperature. The difference spectrum $\Delta\chi''(Q,\omega)$ in Figure 1d shows a clear peak in susceptibility. Figures 1e-g show wavevector dependence of $\chi''(Q,\omega)$ at $\hbar\omega$ = 8, 12, and 24 meV below and above T_c. The superconductivity-induced susceptibility gain increases from 12 to 24 meV (see Figure 1), and there is substantial magnetic scattering even at 250 K.

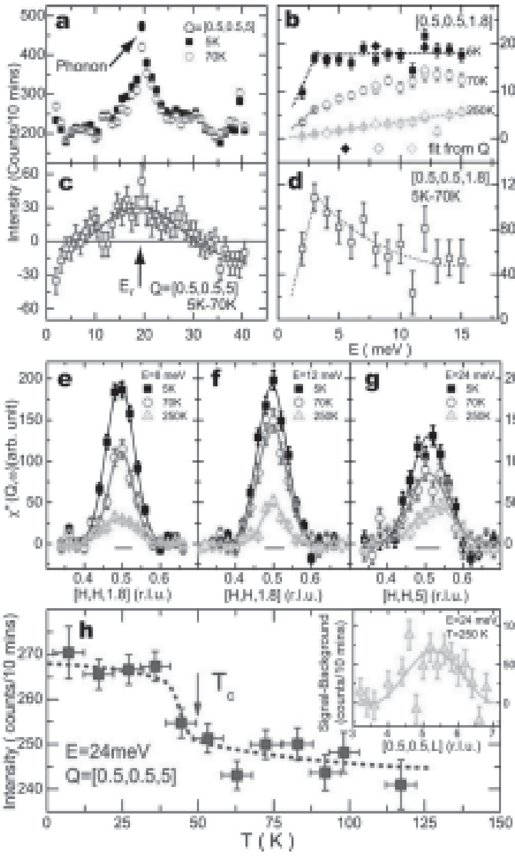

Fig. 1 *(a), Energy-scans at* $\boldsymbol{Q} = (1/2, 1/2, 5)$ *taken below and above* T_c*. The difference in (c) shows a clear peak centered around 20 meV with a FWHM of 15 meV. (b), Temperature dependence of the dynamic susceptibility at the equivalent position* $\boldsymbol{Q} = (1/2, 1/2, 1.8)$ *showing clear magnetic intensity gain on cooling. (d) The temperature difference in dynamic susceptibility. (e)-(g) Wavevector dependence of dynamic susceptibility along the [H,H] direction at different energies and temperatures. (h), The temperature dependence of the scattering at 24 meV and (1/2, 1/2, 5) shows an order-parameter-like increase below* T_c*.*

To confirm that the observed scattering at 250 K is from acoustic magnetic excitations in YBCO, we carried out *Q*-scans along the *c*-axis direction and found that the L-modulation of the $\hbar\omega = 24$ meV excitation at 250 K follows the expected acoustic bilayer structure factor (see inset of Figure 1h). Finally, the temperature dependence of the scattering at $\boldsymbol{Q} = (0.5, 0.5, 5)$ and $\hbar\omega = 24$ meV shows an order parameter-like increase below T_c similar to the temperature dependence of the resonance in the higher-doping YBCO. These results thus demonstrate that the broad peak centered at $\hbar\omega = 19$ meV is indeed the magnetic resonance similar to other superconducting cuprates.

Having shown the presence of the resonance in our $YBa_2Cu_3O_{6.45}$, it is important to determine its dispersion to allow a direct comparison between the magnetic spectra of underdoped YBCO and LSCO. Previous neutron scattering work on YBCO with y = 0.5, and 0.6 have shown [2] that the dispersion of the resonance has the hour-glass shape, with incommensurate scattering below the resonance being anisotropic, having a magnetic anisotropy with a larger incommensurability along the *a**-axis direction than the *b**-axis direction. Since the low-energy spin fluctuations in our $YBa_2Cu_3O_{6.45}$ are commensurate, it will be interesting to determine the dispersion of spin excitations along *H* and *K* directions near the resonance. To accomplish this, we co-aligned the samples in either the [*H,K*,4/3*K*] or [*H,K*,4/3*H*] zone by simply rotating them 90 degrees along the *c**-axis in the [*H,K*,0] zone before tilting around the *a**(*b**)-axis. The unique advantage of such experimental geometries is that one can carry out scans along the [*H*,1.5,2] or [-1.5,*K*,2] directions with identical instrumental resolution, thus allowing a direct comparison of the possible magnetic anisotropy in this material (Figures 2a,b).

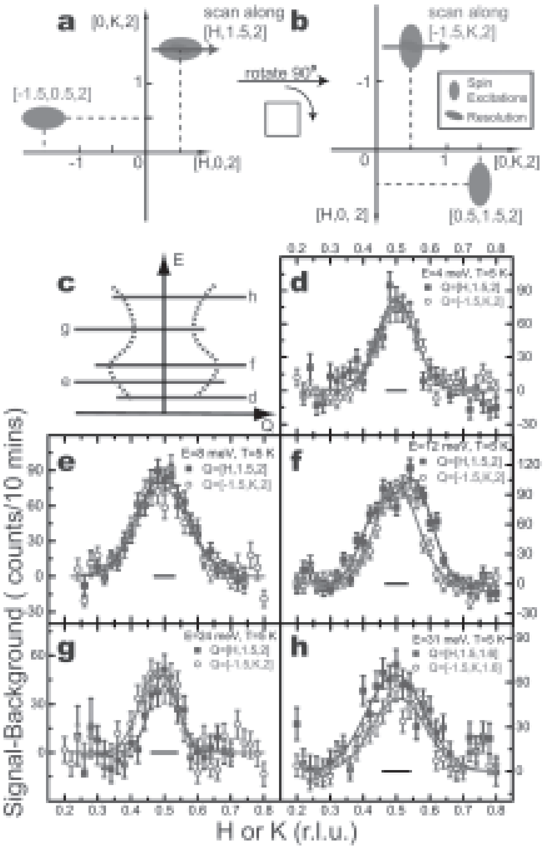

Fig. 2 *(a)-(b) The measurements were carried out in the [H,K,4K/3] and [H,K,4H/3] zones by rotating the sample 90 degrees along c*. The advantage of such a setup is that the instrumental resolutions are identical in a* and b* scan directions. (c) Schematic Q-scans at different energies. (d)-(h) Q-scans along the [H,1.5,2] and [-1.5,K,2] directions at different energies in the low-temperature superconducting state. At 12 meV, the data show clear flattish top and we fit the data with two Gaussian peaks with the incommensurability of* $\delta = 0.057 \pm 0.003$ *rlu. The Q-profiles become narrow and isotropic again near the resonance energy. The instrumental resolutions are shown as the horizontal bars.*

Figures 2d-h summarize the constant-energy scans along *H* and *K* directions for energy transfers of $\hbar\omega = 4, 8, 12, 24$, and 31 meV in the low temperature superconducting state. At $\hbar\omega = 4$ meV, *Q*-scans along the *H* and *K* directions show identical behavior and suggest that spin fluctuations are isotropic at this energy (Figure 2d). On increasing the energy to $\hbar\omega = 8$ meV, the excitations become broader in $\boldsymbol{Q}$ but are still the same along H and K directions (Figure 2e). Upon increasing the energy further to $\hbar\omega = 12$ meV, the Q-scan along the H direction shows a clear flattish top indicative of incommensurate spin excitations while the identical scan along the K direction is commensurate and has a smaller width than the Q-scan along the a^* direction. At energies near and above the resonance (at $\hbar\omega = 24$, and 31 meV, respectively), the scattering profiles become narrow again and the in-plane magnetic anisotropy essentially disappears (Figures 2g,h). Figure 2c summarizes the dispersions of the spin excitations along a^*-direction. The disappearing spin gap energy in the sample did not reveal more incommensurate scattering as expected from a naïve stripe picture but instead showed that the low-energy spin excitations are commensurate much different from the dispersion of the lower-doping LSCO [3].

References

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