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RESONANT NEUTRON SCATTERING FROM $YBa_2Cu_3O_7$

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Abstract—We have developed a new scattering geometry for magnetic neutron scattering experiments on $YBa_2Cu_3O_7$ in which the phonon background around $\mathbf{q} \sim (\frac{\pi}{a}, \frac{\pi}{a})$, $\hbar\omega \sim$ 40meV is significantly reduced. We use this new approach to study the previously detected sharp magnetic excitation at $\sim$ 40meV in the superconducting state in detail. The excitation does not shift substantially in energy up to at least 75K ($\sim 0.8T_c$). Polarized neutron scattering experiments (horizontal minus vertical field) confirm the magnetic origin of the 40meV excitation and put stringent limits on the magnetic scattering intensity in the normal state.

Over the past seven years, numerous magnetic neutron scattering experiments on the underdoped $YBa_2Cu_3O_{6+x}$ system have been performed and have revealed a wealth of important information on the magnetic ground state and excitations [1,2]. Until recently similar experiments on the fully oxygenated compound $YBa_2Cu_3O_7$ have been more controversial [2,3], because the magnetic cross section is smaller and occurs at higher energies. Since in all neutron scattering experiments on $YBa_2Cu_3O_7$ (unpolarized as well as polarized) the background is comparable or larger than the signal, the background subtraction has to be carried out with extreme care. For unpolarized beam experiments, the background from one-phonon and multiphonon scattering is dominant. While multiphonon scattering gives a background which is featureless in energy and momentum, dispersion and dynamical structure factor effects in scattering from single optical phonons generally lead to distinct features of the scattering cross section in energy and momentum which are difficult to distinguish from magnetic excitations.

We have therefore begun to develop a detailed understanding of the phonon spectrum with emphasis on the energy range ($\hbar\omega \sim$ 40meV) in which magnetic excitations had previously been reported [2,3]. Detailed lattice dynamical calculations, together with experimental studies of the temperature and momentum dependence of the scattered intensity, allowed us to separate a phonon involving predominantly c-axis motion of the in-plane oxygen from a magnetic excitation with a similar energy and dynamical structure factor [4]. Our measurements were performed at the High Flux Beam Reactor at Brookhaven at the H7, H8 and H4M triple axis spectrometers.

Figure 1 shows the scattering geometry we developed for this purpose. As first reported by Rossat-Mignod *et al.* [2], the magnetic excitation occurs at $\sim$40meV and $\mathbf{Q} = \left(\frac{1}{2}(2i+1), \frac{1}{2}(2j+1), 1.7(2k+1)\right)$ with the momen-

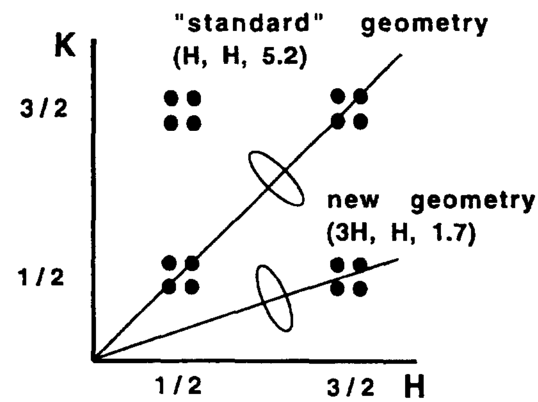

Fig. 1. Geometries used for magnetic neutron scattering experiments on $YBa_2Cu_3O_7$. The long axis of the resolution ellipsoid is perpendicular to the (horizontal) scattering plane. The four peaks shown would be expected if the scattering were peaked at $\mathbf{q} = (k_F, k_F)$ instead of $(\frac{\pi}{a}, \frac{\pi}{a})$.

tum transfer $\mathbf{Q} = (H, K, L)$ measured in units of the reciprocal lattice vectors $\frac{2\pi}{a}$, $\frac{2\pi}{b}$ and $\frac{2\pi}{c}$, and i, j and k integer. As the point $(\frac{1}{2}, \frac{1}{2}, 1.7)$ cannot be studied because of kinematical constraints, and the magnetic form factor suppresses the magnetic intensity for $(\frac{3}{2}, \frac{3}{2}, 1.7)$, all previous neutron scattering experiments had been carried out at the point $(\frac{1}{2}, \frac{1}{2}, 5.2)$. However, we found that the phonon dynamical structure factor is peaked at this point, which makes it difficult to separate the magnetic excitation from the phonon background. For $\mathbf{Q} = (\frac{3}{2}, \frac{1}{2}, 1.7)$, on the other hand, the phonon cross section is very small and the magnetic excitation can be isolated. The phonon can be isolated by increasing the momentum transfer to $L = 14$, where the magnetic form factor suppresses the magnetic intensity almost completely, but the phonon intensity is greatly enhanced. (The phonon cross section contains a term proportional to Q^2.) While the phonon experiences a momentum dependent softening below T_c [5], its *intensity* is unaffected by superconductivity. By contrast, the 40meV magnetic excitation exists in the superconducting state *only*, that is, there is no evidence in our measurements of any significant magnetic peak centered around an energy of 40meV in the normal state. We note that the same conclusion was recently reached independently by Bourges *et al.* [6] using very different (but equally valid) reasoning.

40meV thus appears to be an energy characteristic of the superconducting state. Of course, because of the significant background our data do not rule out magnetic scattering at 40meV in the normal state if it is very weak (conservatively, at least a factor of 3 weaker than in the superconducting state) or broadly distributed in energy and momentum. Polarized beam experiments (see below) put even more stringent limits on the magnetic scattering intensity in the normal state, as compared to the superconducting state. The fact that the magnetic excitation can be clearly observed at two symmetry-related positions of reciprocal space also rules out any spurious processes as the origin of the signal. Experimental artefacts such as accidental Bragg scattering generally do not have the symmetry of the reciprocal lattice. We have therefore ruled out any other explanation for the 40meV feature in the superconducting state, and even from unpolarized beam measurements alone we can conclusively identify it as a magnetic excitation.

Figure 2(a) shows a scan through the $(\frac{3}{2}, \frac{1}{2}, 1.7)$ position. As indicated in the figure, the intrinsic width of the profile is consistent with a sharp peak at $\mathbf{q}_{2D} = (k_F, k_F)$ and its Umklapp counterparts. If the scattering were indeed peaked at $\mathbf{q}_{2D} = (k_F, k_F)$, the peaks could not be resolved because of the poor vertical resolution of our triple axis spectrometer [long axis of the resolution ellipsoid shown in Fig. 1(a)]. The intrinsic momentum width of the excitation may thus indicate a Fermi surface effect, but alternative explanations have also been given [8]. All theories must explain the sinusoidal modulation of the scattering intensity as a function of the momentum transfer perpendicular to the CuO_2 layers [4].

As a crosscheck of our unpolarized beam experiments, we have performed polarized beam experiments both in the "standard" scattering zone around $(\frac{1}{2}, \frac{1}{2}, 5.2)$ and in the newly developed zone around $(\frac{3}{2}, \frac{1}{2}, 1.7)$. As in the case of unpolarized neutron scattering experiments the weakness of the signal makes an extremely careful background subtraction indispensable. In particular, it is difficult to discriminate between genuine magnetic scattering processes (Bragg scattering from monochromator and analyser; inelastic scattering from the sample) and accidental nuclear Bragg scattering (Bragg scattering from monochromator and sample; incoherent, diffuse or inelastic scattering from the analyser). Although the latter process does not involve a spin flip at the sample, limitations of the polarized beam setup nevertheless allow some such neutrons to reach the detector. We have conducted extensive checks for these spurious effects

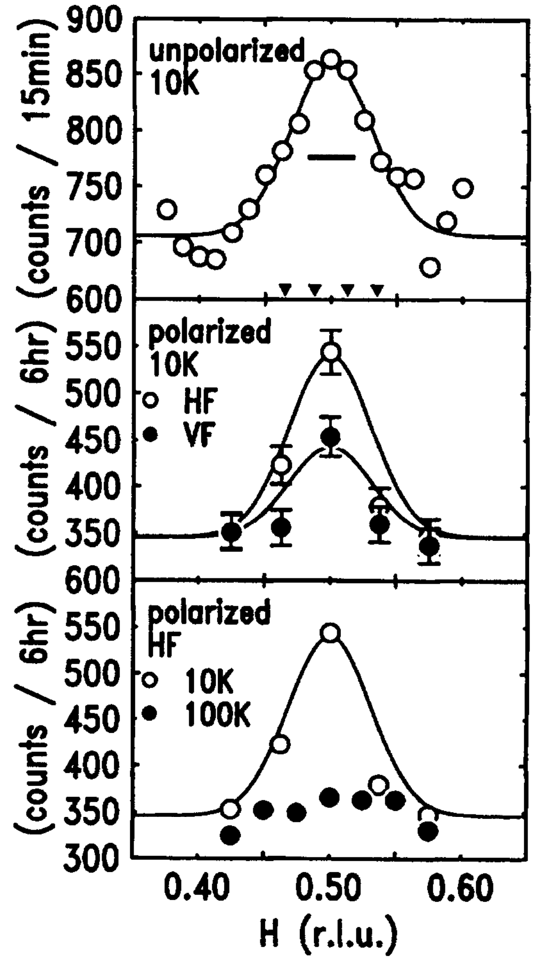

Fig. 2. (a) Scattering profiles along $(3H, H, 1.7)$ at $\hbar\omega = 41$meV. The approximate locations of the four peaks of Fig. 1 are indicated by arrows. k_F was taken from the photoemission data of Ding *et al.* [7] on $Bi_2Sr_2CaCu_2O_{8+\delta}$, which has a structure and T_c very similar to $YBa_2Cu_3O_7$. The bar indicates the momentum resolution. (b) $(3H, H, 1.7)$ scan taken with a polarized beam, with horizontal (HF) and vertical (VF) neutron guide fields at the sample. The lines are the same as in panel a), rescaled without adjustable parameters. (c) Horizontal field scans in the same geometry at 10K and 100K.

and found that in the standard geometry they dominate the signal, so that polarized beam experiments are very difficult. Spurious effects are in fact the origin of the small 41 meV "resonance" in the normal state observed in the polarized-beam experiments of Mook *et al.* [3] Fortuitously, the new scattering geometry is far less affected by this contamination, and data taken in this mode allowed us to confirm the magnetic origin of the 40meV excitation in the superconducting state unambiguously [Fig. 2(b)]. The solid line through the points is the line of panel a), rescaled to adjust for the reduced efficiency of the polarized beam equipment. This confirms that all the intensity which is peaked around $\mathbf{q}_{2D} = (\frac{\pi}{a}, \frac{\pi}{a})$ in the superconducting state arises from magnetic scattering.

For fixed neutron guide field at the sample, one measures the magnetic cross section plus an extrinsic background. The standard way of removing the background is to measure the intensity for vertical guide field (yielding only half magnetic cross section because of polarization effects) and subtracting it from the intensity for horizontal guide field (yielding the full magnetic cross section). Figure 2(b) shows that the the 40meV excitation survives this test as well. Figure 2(c) confirms that the the magnetic cross section at 40meV in the normal state is much smaller than in the superconducting state. While on general grounds one expects some magnetic scattering at any temperature, the magnetic scattering intensity at 40meV in the normal state is indistinguishable from zero within our present errors.

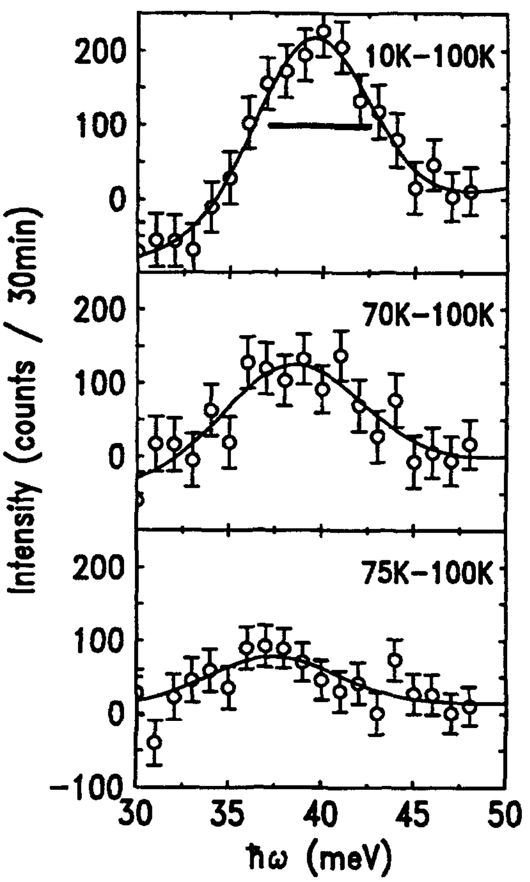

Fig. 3. Energy scans of the magnetic excitation at $Q = (\frac{3}{2}, \frac{1}{2}, 1.7)$. The data were taken under different experimental conditions, and the relative intensities were normalized approximately. The bar indicates the energy resolution.

In Fig. 3 energy scans at $\mathbf{Q} = (\frac{3}{2}, \frac{1}{2}, 1.7)$ are shown. The intensity of the magnetic excitation (and concomitantly the data quality) diminishes rapidly as T_c is approached. A slight shift (~ 2 meV) of the excitation energy is suggested by the data taken at 75K ($\sim 0.8T_c$), but is within the experimental uncertainty. As there is no evidence of scattering centered around 40meV in the normal state, we may associate this energy with the spectroscopic energy gap (2Δ) in the superconducting state. If this interpretation is correct, the gap must be essentially temperature independent below $\sim 0.8T_c$. Further, the coherence factor for quasiparticle creation by magnetic neutron scattering necessitates a sign reversal of the energy gap on the Fermi surface [4]. Other interpretations in which the excitation energy is determined by weakly temperature dependent microscopic parameters have also been proposed [8].

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