Linear Dependence of Peak Width in $\chi(\mathbf{q}, \omega)$ vs T_c for $YBa_2Cu_3O_{6+x}$ Superconductors

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It is shown that the momentum space width of the peak in the spin susceptibility, $\mathrm{Im}\chi(\mathbf{q}, \omega)$, is *linearly* proportional to the superconducting T_c: $T_c = \hbar v^* \Delta q$ with $\hbar v^* \simeq 35$ meV Å. This relation is similar to the linear relation between incommensurate peak splitting and T_c in LaSrCuO superconductors, as first proposed by Yamada *et al.* [Phys. Rev. B **57**, 6165 (1998)]. The velocity $\hbar v^*$ is smaller than Fermi velocity or the spin-wave velocity of the parent compound and remains the same for a wide doping range. This result points towards strong similarities in magnetic state of $YBa_2Cu_3O_{6+x}$ and LaSrCuO. [S0031-9007(99)09478-8]

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Recent progress in neutron scattering in high-T_c superconductors system, $YBa_2Cu_3O_{6+x}$ (YBCO), allowed us to gather a wide variety of inelastic neutron scattering data which reveal a nontrivial structure of the antiferromagnetic (AF) susceptibility $\chi(\mathbf{q}, \omega)$ in both the energy and momentum spaces [1–24]. Using these data one can try to understand what is the relation between the superconducting and magnetic properties of high-T_c superconductors. A nontrivial feature that has attracted a lot of attention is the so-called resonance peak appearing in the superconducting state and seems to be directly related to the formation of the superconducting state [1–12].

Here, we will focus on the completely different feature of $\mathrm{Im}\chi(\omega, \mathbf{q})$, namely on the off-resonance spectrum. Substantial interest has been recently devoted to that contribution as incommensurate peaks have been observed away from the resonance peak in $YBCO_{6.6}$ [13,14]. However, it was observed so far in limited doping, energy, and temperature ranges. Generally, in the *normal state* $\chi(\omega, \mathbf{q})$ is peaked at the commensurate wave vector (π, π). This contribution is then simply characterized by a q width in momentum space, Δq (HWHM).

Considering the neutron scattering data in YBCO for oxygen concentrations between $x = 0.45$–0.97 with respective T_c up to 93 K, we find a surprisingly simple *linear* relation between superconducting transition temperature T_c and HWHM Δq for the whole doping range:

$$T_c = \hbar v^* \Delta q, \qquad \hbar v^* = 35 \text{ meV Å}. \tag{1}$$

This observation is based on analysis of the data and we used no theory assumptions in extracting the velocity v^* from the data. The left-hand side of the above equation has dimension of energy, Δq has an inverse distance dimension, hence the coefficient relating them should have dimension of *velocity*. *A priori*, it is not clear that this relation implies the existence of the excitation with such a velocity. We believe it does.

Below, we explain how Eq. (1) is obtained. The spin susceptibility in the metallic state of YBCO is experimentally found to have a maximum at any energy at the *commensurate* in-plane wave vector $q_{\mathrm{AF}} = (\frac{h}{2}, \frac{k}{2})$ (with h, k even integer), referred to as (π, π) [1–12,16–24]. This generic rule is found to be violated in two cases.

First, in the underdoped $YBCO_{6.6}$, Dai *et al.* [13] reported low-temperature q scans at $\hbar\omega = 24$ meV which display well-defined double peaks [15]. Recent measurements with improved q resolution confirm this observation [14]. However, this behavior is mostly observed at temperatures below T_C. In the normal state, a broad commensurate peak is restored in the same sample (unambiguously above 75 K) [9].

The other case where the spin susceptibility was not found maximum at (π, π) is above ~50 meV in the weakly doped $YBCO_{6.5}$ [18]. Dispersive quasimagnons behavior is observed in this high energy range. Most likely, this is reminiscent of spin waves observed in the undoped AF parent compound $YBCO_6$.

Therefore, concentrating on the low energy spin excitations (below 50 meV), $\mathrm{Im}\chi(\mathbf{q}, \omega)$ is characterized in the *normal state* by a broad maximum at the commensurate wave vector. The neutron scattering function is then empirically found to be well accounted for by a Gaussian line shape [2,8,16] such as

$$S(Q, \omega) = I_{\max}(\omega) \exp\left[-\log 2 \, \frac{(q - q_{\mathrm{AF}})^2}{\Delta_q^2(\omega)}\right], \tag{2}$$

where $\Delta q(\omega)$ is the half width at half maximum. In principle, $\Delta q(\omega)$ is an increasing function of energy. However, a rather weak energy dependence is found for $\Delta q(\omega)$ with only a slight increase with the energy [2,16,19]. Furthermore, this energy dependence becomes less pronounced for the higher doping range.

The situation is even more subtle for $x \geq 0.6$ as $\mathrm{Im}\chi(\mathbf{q}, \omega)$ is characterized by two distinct (although interrelated) contributions: one occurs exclusively in the superconducting state, the resonance peak, the second one appears in both states and is characterized by a broad peak (around ~30 meV). They mainly differ by their energy dependences as the resonance peak is basically resolution limited in energy [1,5,8–11]. With increasing doping, the off-resonance spectrum is continuously reduced (becoming too weak to be measured in the overdoped regime $YBCO_7$ [5,7,12]) whereas the resonant peak becomes the major part of the spectrum [12]. The recent incommensurate peaks measured below the resonance peak in $YBCO_{6.6}$ [13,14] confirms the existence of two contributions [20] as the low energy incommensurate excitations cannot belong to the same excitation as the commensurate resonance peak.

At each doping, the peak intensity at the resonance energy is characterized by a striking temperature dependence either resembling to an order parameterlike dependence for the higher doping range ($x > 0.9$) [2,3,8] or just displaying a marked kink at T_C [4,9,10,21]. In contrast, a much smoother temperature dependence is observed for the off-resonance spectrum [10,12]. This "normal" contribution has not received much attention so far. However, the knowledge of the nonresonant peak in the normal state is important and is crucial for some proposed mechanisms for the high-T_C superconductivity based on antiferromagnetism, e.g., [25].

The resonance peak is related to smaller q values (and hence larger real space distance) as $\Delta q(\omega)$ exhibits a minimum at the energy of the resonance peak [6,8,10]. Furthermore, its q width remains almost constant whatever the doping, $\Delta q^{\mathrm{reso}} = 0.11 \pm 0.02$ Å^{-1} [6]. Recent data [9,10,21] agree with that conclusion. Applying the simple relation $\xi = 1/\Delta q$, it yields a characteristic length for the resonance peak, $\xi \simeq 9$ Å. In contrast, the "normal" contribution is characterized by a doping dependent q width which in terms of the nearly AF liquid approach [25] would yield surprisingly small correlation length $\xi/a \simeq 1 - 2$ (for $x \geq 0.6$).

Moreover, in all inelastic neutron scattering experiments (see, e.g., [2,7,16,22]), the q width is found temperature independent at any doping. For larger doping, the low temperature q width is already large and the AF intensity vanishes without any sign of q broadening when increasing temperature [2]. Therefore, these q widths might be related to new objects essentially dependent on the doping level.

To emphasize the precise value of the q width, we have summarized in Table I the neutron data obtained over the last decade by a few different groups. We consider only the low energy results for each oxygen content, where Δq is weakly energy dependent. The energy range of interest is indicated in Table I. The Δq value reported here has been mostly taken along the [110] reciprocal direction. Other data have been also taken along the [310] reciprocal direction [13,18,21] which basically agree with the hypothesis of an isotropic q width.

Δq versus the oxygen content displays a double plateau shape [6] which reminds the standard x dependence of T_C in YBCO. For the 90-K phase, $\Delta q^{\mathrm{HWHM}} = 0.22$ Å^{-1} yielding a very short AF correlation length within CuO_2 planes $\xi/a \simeq 1.1$.

Summarizing the data in Table II, we plot both $T_c(x)$ and $\Delta q(x)$ in Fig. 1, and find the linear relation between T_c and Δq (Fig. 2) in the whole oxygen doping range, Eq. (1), where T_c is the respective superconducting transition temperature at a given oxygen concentration x and Δq is the corresponding *half-width* of the peak at (π, π) in $\chi''(\mathbf{q}, \omega)$. The velocity $\hbar v^* = 35$ meV Å is about a factor of 2 larger than the equivalent velocity in LaSrCuO, $\hbar v^*_{214} = 20$ meV Å, inferred from T_c vs δ plot (Fig. 3); see below. Equation (1) does imply that the magnetic correlations, as measured by $\chi(\mathbf{q}, \omega)$, and superconducting transition are closely related, but through their *momentum* dependence. In contrast, the peak intensity of $\mathrm{Im}\chi(\mathbf{q}, \omega)$ in the normal state and its characteristic frequency do not exhibit obvious relations with T_C as the former decreases with increasing doping [7,12] and the latter is weakly doping dependent [2,6,7,12]. (Here, we do not speak about the doping dependence of the resonance peak energy in the SC state which actually roughly follows T_c [6,10–12]).

The recent incommensurate splitting δ of the peak at $(1/2 + \delta, 1/2) = (1/2, 1/2 + \delta)$, observed by Dai *et al.* [13] and subsequently by Mook *et al.* [14] in $YBCO_{6.6}$ have been included in Fig. 2 (full square).

TABLE I. q widths (HWHM) of the AF intensity as a function of the oxygen content at energies corresponding to the nonresonant contribution. q widths have been mostly determined along the [110] direction (see text). $\Delta_q^{\mathrm{resol}}$ denotes the HWHM of the Gaussian resolution of the spectrometer. The intrinsic q widths have been then obtained after deconvolution from the spectrometer linewidth assuming a Gaussian shape wave vector dependence for $\mathrm{Im}\chi(\mathbf{q}, \omega)$ [Eq. (2)]. Energy range from where the q width has been taken is given (* only reported value). Fully oxidized $YBCO_7$ is not quoted in this table as the normal AF contribution is not detectable in this overdoped regime [7,5,12].

x	T_C (k)	Energy range (meV)	Δ_q^{mes} (Å^{-1})	$\Delta_q^{\mathrm{resol}}$ (Å^{-1})	Δ_q (Å^{-1})	Refs.
0.4	25	3–15	0.075	0.023	0.07	[23]
0.45	45	3–15	0.08	0.023	0.075	[23]
0.5	47	4–15	0.12	0.023	0.115	[2,7]
0.5	50	2–15	0.115	0.05	0.11	[8,21]
0.5	52	4–15	0.115	0.05	0.1	[22]
0.6	53	6–15	0.14	0.035	0.14	[16,17]
0.6	63	24*	0.18	0.07	0.17	[9]
0.69	59	15–20	0.17	0.06	0.16	[24]
0.7	67	15–25	0.17	0.07	0.16	[21]
0.8	82	20–25	0.21	0.09	0.18	[10]
0.83	85	15–25	0.23	0.11	0.2	[4]
0.92	91	28–38	0.25	0.11	0.23	[1,7]
0.97	92.4	33–37	0.25	0.11	0.23	[8]

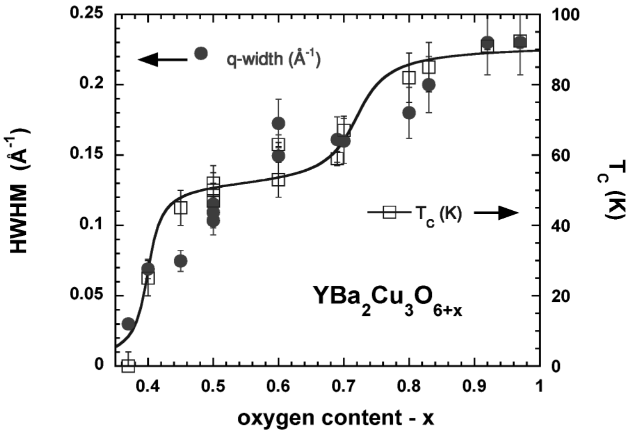

FIG. 1. q width (closed circles) and T_C (open squares) versus oxygen content.

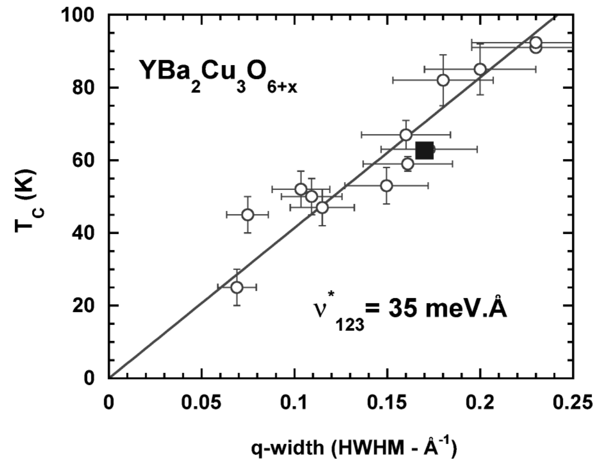

FIG. 2. Superconducting transition versus q width [26]. The full square corresponds to locus of the maximum of incommensurate magnetic excitations δ recently reported below T_C [14]. Note that for this sample the resolved incommensuration δ turns out to be close to Δq. The double peaks reported in Refs. [13,14] could probably be broadened in previously measured samples. Whether the incommensurate peak structure in $\text{Im}\chi(\mathbf{q},\omega)$ exists in the whole doping range in YBCO remains to be proved. It also could be a specific feature seen in some finite doping range near $YBCO_{6.6}$.

Interestingly, the incommensuration δ by Mook *et al.* falls on the same linear plot.

First, we can make a few comments on what one can extract from such a simple relationship as Eq. (1) regardless of the particular mechanism responsible for v^*:

(a) Proportionality between the width of the peak and the critical temperature implies that there is a characteristic velocity $\hbar v^*$ which is the same (within experimental resolution) for a wide range of oxygen doping in YBCO.

(b) Velocity $\hbar v^*$ is 2 orders of magnitude smaller than typical Fermi velocity $\hbar v_F \sim 1$ eV Å in these compounds [28]. This perhaps is not surprising as we are considering the magnetic response where localized Cu spins likely provide the main contribution.

(c) More importantly, $v^* \ll v_{\text{SW}}$ is about an order of magnitude smaller than the spin wave velocity, $\hbar v_{\text{SW}} \simeq 0.65$ eV Å [27], of the parent compound but also much smaller than the spin velocity in the metallic state $\hbar v_{\text{spin}} \simeq 0.42$ eV Å [18]. This is a nontrivial fact. We do not have a model to explain the data presently. On the other hand, on general grounds for any approach, based on the simple spin-wave theory, one would expect the typical spin-wave velocity to characterize the width in $\chi''(\mathbf{q},\omega)$.

(d) If, as we are proposing, the characteristic velocity $\hbar v^*$ does correspond to some propagating or diffusive excitation then there should be a way to directly observe it in other experiments [30].

Now we would like to discuss the possible origin of $\hbar v^*$. It is likely caused by some phase fluctuation mode associated with the slow motion of density excitations. These could be caused by "stripe" fluctuations. Recent tunneling and photoemission studies indicate that the gap in the SC state increases as T_c decreases on underdoping [31]. The T_c would then been determined by phase fluctuations, as emphasized by Emery and Kivelson [32]. Recently, based on the phase fluctuations model, the similarly small velocity (60 meV Å for LaSrCuO) was obtained by Castro Neto [33]. It is therefore natural that phase mode velocity will determine the superconducting temperature.

The existence of the second magnetic velocity v^* we interpret as a closeness to the quantum critical point (QCP), controlled by some density instability with strong coupling to the spin channel. Based on the neutron scattering data for the LaSrCuO system this point was emphasized by Aeppli *et al.* [34].

Within the simple model, say *t-J*, the energy scales are set by t, which determines v_F and by J, determining v_{SW}. Hence one generally would not expect any excitations in this model with v^*. One possibility to generate a new energy scale in the problem is to allow some (microscopic) inhomogeneities. Phase separation into hole-rich and antiferromagnetic regions with fluctuations of the boundaries between regions will occur with some soft velocity that might be related to v^*.

Finally, we would like to relate the above discussion to the other well-studied system: LaSrCuO. Inelastic neutron scattering data by Yamada *et al.* [27] on LaSrCuO (La214) compounds show the existence of the incommensurate peaks at $(\pi \pm \delta, \pi)$ and $(\pi, \pi \pm \delta)$ [27]. Plotted vs δ, $T_c(\delta)$ was found to be a linear function of δ in the wide range of Sr doping, see Fig. 3, as appear in [27]. Using the same reasoning as for Eq. (1) from the data [27] we find the characteristic *velocity*,

$$T_c = \hbar v^*_{214}\delta, \qquad \hbar v^*_{214} = 20 \text{ meV Å}. \qquad (3)$$

Thus inferred velocity is much smaller that the Fermi velocity on La214 $\hbar v_F \sim 1$–0.5 eV Å and smaller than the measured spin wave velocity $\hbar v_{\text{SW}} \sim 0.85$ eV Å [35].

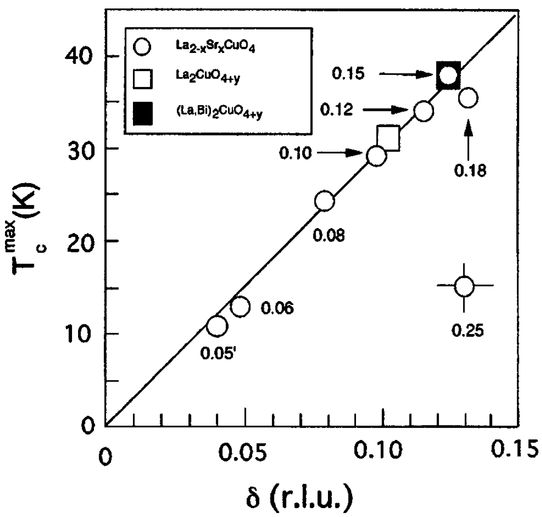

FIG. 3. Linear relation between the incommensurate peak splitting δ and T_c for the LaSrCuO superconductors. The linear slope of the curve means that $T_c = \hbar v^*_{214}\delta$. We find $v^*_{214} = 20$ meV Å. Note that the linear dependence is violated in the overdoped regime. The figure is taken from Yamada *et al.* (Fig. 10) [27].

We should again emphasize that the linearity T_c vs δ is an experimental fact. The coefficient relating energy scale T_c to the inverse length scale δ has a dimension of velocity. This result is similar to the small velocity we find for the Δq vs T_c plots in YBCO, except in YBCO the velocity v^* is about a factor of 2 larger than in LaSrCuO.

In conclusion, we find that the body of neutron scattering data on YBCO for a wide range of oxygen doping allows the simple linear relation between the width of the "normal" contribution, i.e., out of resonance peak, δq and corresponding T_c of the sample. Thus inferred velocity $\hbar v^* \simeq 35$ meV Å is anomalously small compared to known spin wave and Fermi velocities for these compounds. We suggest that this velocity indicates the existence of excitation that is closely related to the formation of the superconducting state. The $T_c \propto \delta q$ proportionality obtained over the whole phase diagram of YBCO suggests that antiferromagnetism is likely responsible for the high-T_C superconducting mechanism.

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