Linear dependence of peak width in $\chi(q, \omega)$ vs $T_c$ for YBCO superconductors

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It is shown that the momentum space width of the peak in the spin susceptibility, Im$\chi(q, \omega)$, is linearly proportional to the superconducting $T_c$: $T_c = h\nu^* \Delta q$ with $h\nu^* \approx 35$ meVÅ. 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. B57, 6165, (1998)). The velocity $h\nu^*$ 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 YBCO and LaSrCuO.

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Recent progress in neutron scattering in high-$T_c$ superconductors system, YBa$_2$Cu$_3$O$_{6+x}$ (YBCO), allowed to gather a wide variety of inelastic neutron scattering data which reveal a nontrivial structure of the antiferromagnetic susceptibility $\chi(q, \omega)$ 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 have 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 Im$\chi(\omega, q)$, 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 $\chi(\omega, q)$ is peaked at the commensurate wavevector $(\pi, \pi)$. This contribution is then simply characterized by a $q$-width in momentum space, $\Delta q$ (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 $\Delta q$ for the whole doping range:

$$T_c = h\nu^* \Delta q, \quad h\nu^* = 35\text{meVÅ}$$  \hspace{1cm} (1)

This observation is based on analysis of the data and we used no theory assumptions in extracting the velocity $\nu^*$ from the data. The left-hand side of the above equation has dimension of energy, $\Delta q$ 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 mode with such a velocity. We believe it does: the magnetic properties of the YBCO are described by two velocities $v_{SW}$ and $\nu^*$. Below, we explain how the 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 wavevector $q_{AF} = (\frac{k}{2}, \frac{k}{2})$ (with $h, k$ even integer), referred to as $(\pi, \pi)$ [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 reported low temperature q-scans at $\omega_w = 24$ meV which display well-defined double peaks. Recent measurements with improved q-resolution confirm this observation [4]. 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).

The other case where the spin susceptibility was not found maximum at $(\pi, \pi)$ is above ~ 50 meV in the weakly doped YBCO$_{6.5}$ [8]. Dispersive quasi-magnons 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), Im$\chi(q, \omega)$ is characterized in the normal state by a broad maximum at the commensurate wavevector. This justifies an analysis in terms of a single peak centered around $q_{AF}$. However, the shape in q-space is systematically found to be sharper than a Lorentzian shape usually assumed to describe such a disordered magnetic system. The neutron scattering function is then empirically found to be well accounted for by a Gaussian line-shape $\propto e^{-(q-q_{AF})^2}$ such as

$$S(Q, \omega) = I_{max}(\omega) \exp \left(-\frac{(Q-q_{AF})^2}{\Delta q^2(\omega)}\right)$$  \hspace{1cm} (2)

where $\Delta q(\omega)$ is the half width at half maximum (HWHM). 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 [4]. Furthermore, this energy dependence becomes less pronounced for the higher doping range.

The situation is even more subtle for $x \geq 0.6$ as Im$\chi(q, \omega)$ is characterized by two distinct (although inter-related) 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 \(\sim 30\) meV). They mainly differ by their energy dependences as the resonance peak is basically resolution limited in energy \([3,11]\). With increasing doping, the off-resonance spectrum is continuously reduced (becoming too weak to be measured in the overdoped regime YBCO\(\_\_\_\_\) whereas the resonant peak becomes the major part of the spectrum \([12]\). The recent incommensurate peaks measured below the resonance peak in YBCO\(\_\_\_\_\) \([13,14]\) 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 parameter-like dependence for the higher doping range \((x>0.9)\) \([3,3]\) or just displaying a marked kink at \(T_c\) \([3,4,21]\). Therefore, this mode is a novel signature of the superconducting state in the cuprates, and most likely is due to electron-hole pair production across the superconducting energy gap \([3,12]\). In contrast, a much smoother temperature dependence is observed for the off-resonance spectrum \([14,3]\). This ”normal” contribution has not received much attention so far. However, the knowledge of the non resonant 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 \([3,3,14]\). Furthermore, its q-width remains almost constant whatever the doping, \(\Delta_q^{\text{reso}} = 0.11 \pm 0.02\) \(\text{Å}^{-1}\) \([7]\). Recent data \([3,7,12]\) agree with this conclusion. Applying the simple relation \(\xi = 1/\Delta_q\), it yields a characteristic length for the resonance peak, \(\xi \approx 9\) Å which might be related to the superconducting coherence length as the resonance peak is intimately linked to the high-\(T_c\) superconductivity. In contrast, the ”normal” contribution is characterized by a doping dependent q-width which in terms of the Nearly AF Liquid approach \([23]\) would yield surprisingly small correlation length \(\xi \approx 1 - 2\) (for \(x \geq 0.6\)).

Moreover, in all inelastic neutron scattering experiments (see e.g. \([4,6,2])\), the q-width is found temperature independent at any doping. This finding is especially clear for \(x \approx 0.5\) where the q-width at low temperature is small enough to increase upon heating. But, in contrast, no evolution is seen within error bars (about 10 %) up to room temperature \([2]\). 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 \([3]\). 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 \(\_\_\_\_\_\) the neutron data obtained over the last decade by few different groups. We consider only the low energy results for each oxygen content, \(\Delta_q\) is weakly energy dependent. The energy range of interest is indicated in Table \(\_\_\_\_\_\). The \(\Delta_q\) value reported here has been mostly taken along the \([110]\) reciprocal direction. Other data have been also taken along the \([310]\) reciprocal direction \([13,14,22]\) which basically agree with the hypothesis of an isotropic q-width.

\(\Delta_q\) versus the oxygen content displays a double plateau shape \([1]\) which reminds the standard x dependence of \(T_c\) in YBCO. For the 90-K phase, \(\Delta_q^{\text{HWHM}} = 0.22\) \(\text{Å}^{-1}\) yielding a very short AF correlation length within CuO\(\_\_\_\_\) planes \(\xi \approx 1.1\).

![FIG. 1. Q-width (closed circles) and \(T_c\) (open squares) versus oxygen content.](image1)

![FIG. 2. Superconducting transition versus q-width \([20]\). The full square corresponds to locus of the maximum of incommensurate magnetic excitations \(\delta\) recently reported below \(T_c\) \([14]\).](image2)

Summarizing the data in this Table, we plot both \(T_c(x)\) and \(\Delta_q(x)\) in Fig. \(\_\_\_\_\) and find the linear relation between \(T_c\) and \(\Delta_q\) (Fig. \(\_\_\_\)) in the whole oxygen doping range, Eq. \(\_\_\_\_\_\)., where \(T_c\) is the respective superconducting transition temperature at a given oxygen concentration \(x\) and \(\Delta_q\) is the corresponding half-width of the peak at \((\pi,\pi)\) in \(\chi'(\textbf{q},\omega)\). The velocity \(hv^* = 35\) meV.Å is about a factor
of two larger than the equivalent velocity in LaSrCuO, $hv_{214} = 20 \text{ meV.A}$, inferred from $T_c$ vs $\delta$ plot (Fig. 3), see below. The Eq. (1) does imply that the magnetic correlations, as measured by $\chi(q, \omega)$, and superconducting transition are closely related.

The recent incommensurate splitting $\delta$ of the peak at $(1/2 + \delta, 1/2) = (1/2, 1/2 + \delta)$, observed by Dai et al. [14] and subsequently by Mook et al. [15] in YBCO$_{6.6}$ have been included in Fig. 2 (full square). Interestingly, the incommensuration $\delta$ by Mook et al fall on the same linear plot.

First, we can make 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 two orders of magnitude smaller than typical Fermi velocity $\hbar v_F \sim 1 \text{ eV.A}$ in these compounds 25. This perhaps is not surprising as we are considering the magnetic response where localized Cu spins provide the main contribution.

c) More importantly, $v^* << v_{SW}$ is about an order of magnitude smaller than the spin wave velocity, $\hbar v_{SW} \simeq 0.65 \text{ eV.A}$ [27], of the parent compound but also much smaller than the spin velocity in the metallic state $\hbar v_{spin} \simeq 0.42 \text{ eV.A}$ [15]. This is a nontrivial fact. It may suggest that some magnetic soft mode is present. 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 $\chi''(q, \omega)$.

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

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 30. The $T_c$ would then be determined by phase fluctuations, as emphasized by Emery and Kivelson [31]. Recently, based on phase fluctuations model, the similarly small velocity (60meV.A for LaSrCuO) was obtained by Casto Neto [32]. 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. The antiferromagnetic insulating compound with characteristic $v_{SW}$ determines the critical point at zero doping, where the transition into 3D antiferromagnetic state occurs at finite temperature. The second critical point with characteristic $v^*$ along the doping axis is close to the optimally doped compound and might be determined by some density wave or "stripe" instability. Based on the neutron scattering data for LaSrCuO system this point was emphasized by Aeppli et.al. [33].

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 [34] on LaSrCuO (La214) compounds show the existence of the incommensurate peaks at $(\pi \pm \delta, \pi)$ and $(\pi, \pi \pm \delta)$ [34]. Plotted vs $\delta$, $T_c(\delta)$ was found to be a linear function of $\delta$ in the wide range of Sr doping, see Fig. 3, as appear in [34]. Using the same reasoning as for Eq. (1) from the data [34] we find the characteristic velocity,

$$T_c = \hbar v_{214}^2 \delta, \hbar v_{214}^* = 20 \text{meV.A}$$

Thus inferred velocity is much smaller that the Fermi velocity on La214 $\hbar v_F \sim 1 - 0.5 \text{ eV.A}$ and smaller than the measured spin wave velocity $\hbar v_{SW} \sim 0.85 \text{ eV.A}$ [20]. We should again emphasize that the linearity $T_c$ vs $\delta$ is an experimental fact. The coefficient relating energy scale $T_c$ to the inverse length scale $\delta$ has a dimension of velocity. This result is similar to the small velocity we find for the $\Delta q$ vs $T_c$ plots in YBCO, except in YBCO the velocity $v^*$ is about a factor of two 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", i.e. out of resonance peak, δq and corresponding Tc of the sample. Thus inferred velocity hv* ≅ 35 meVÅ is anomalously small compared to known spin wave and Fermi velocities for these compounds. We suggest that this velocity indicates the existence of some new mode in these materials and this mode is closely related to the formation of superconducting state.

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| x   | 0.4 | 0.45 | 0.5 | 0.5 | 0.5 | 0.6 | 0.6 |
|-----|-----|-----|-----|-----|-----|-----|-----|
| $T_C$ (K) | 25  | 45  | 47  | 50  | 52  | 53  | 63  |
| Energy range (meV) | 3-15 | 3-15 | 4-15 | 2-15 | 4-15 | 6-15 | 24* |
| $\Delta_q^{\text{mes}}$ (Å$^{-1}$) | 0.075 | 0.08 | 0.12 | 0.115 | 0.115 | 0.14 | 0.18 |
| $\Delta_q^{\text{resol}}$ (Å$^{-1}$) | 0.023 | 0.023 | 0.023 | 0.05 | 0.05 | 0.035 | 0.07 |
| $\Delta_q$ (Å$^{-1}$) | 0.07 | 0.075 | 0.115 | 0.11 | 0.1 | 0.14 | 0.17 |
| Refs. | [23] | [23] | [2,7] | [18,21] | [22] | [16,17] | [9] |

| x   | 0.69 | 0.7 | 0.8 | 0.83 | 0.92 | 0.97 |
|-----|-----|-----|-----|-----|-----|-----|
| $T_C$ (K) | 59  | 67  | 82  | 85  | 91  | 92.4 |
| Energy range (meV) | 15-20 | 15-25 | 20-25 | 15-25 | 28-38 | 33-37 |
| $\Delta_q^{\text{mes}}$ (Å$^{-1}$) | 0.17 | 0.17 | 0.21 | 0.23 | 0.25 | 0.25 |
| $\Delta_q^{\text{resol}}$ (Å$^{-1}$) | 0.06 | 0.07 | 0.09 | 0.11 | 0.11 | 0.11 |
| $\Delta_q$ (Å$^{-1}$) | 0.16 | 0.16 | 0.18 | 0.2 | 0.23 | 0.23 |
| Refs. | [24] | [21] | [10] | [4] | [1,7] | [8] |

**TABLE I.** Q-widths (HWHM) of the AF intensity as a function of the oxygen content at energies corresponding to the non-resonant contribution. Q-widths have been mostly determined along the [110] direction (see text). $\Delta_q^{\text{resol}}$ 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 wavevector dependence for $\text{Im}\chi(q,\omega)$ (Eq. 8). 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.