Frequency Evolution of Neutron Peaks Below \( T_c \): Commensurate and Incommensurate Structure in LaSrCuO and YBaCuO

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We study the evolution of the neutron cross-section with variable frequency \( \omega \) and fixed \( T \) below \( T_c \) in two different cuprate families. Our calculations, which predominantly probe the role of \( d \)-wave pairing, lead to generic features, independent of Fermi surface shapes. Among our findings, reasonably consistent with experiment, are (i) for \( \omega \) near the gap energy \( \Delta \), both optimal LaSrCuO and slightly underdoped YBCO exhibit (comparably) incommensurate peaks (ii) peak sharpening below \( T_c \) is seen in LaSrCuO, (iii) quite generically, a frequency evolution from incommensurate to commensurate and then back to incommensurate structure is found with increasing \( \omega \). Due to their narrow \( \omega \) regime of stability, commensurate peaks in LaSrCuO should be extremely difficult to observe.

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The field of neutron scattering in high temperature superconductors has seen a variety of recent experimental discoveries associated with incommensurate and commensurate structure at \( T < T_c \) [4,5, 21]. These neutron data remain of central importance in the field of high \( T \) superconductivity: the combined momentum and frequency range covered by this technique is wider than that in virtually all other spectroscopies. It is mainly through this extended range that these neutron results have direct bearings on such important issues as dynamical stripes [8] and where the condensation energy comes from [4].

The goal of the present paper is to systematically address these observations over the entire momentum and frequency range that the experiments have covered, in the two different cuprate families (LaSrCuO and YBaCuO). In the process, we show that all of the above commensurate and incommensurate features are compatible with \( d \)-wave pairing superposed onto the normal state Fermi surfaces. In contrast to \( T > T_c \), the details of the Fermi surface shape are of relatively less importance, and serve primarily to select out the \( \omega \) regime where various commensurate or incommensurate features can be observed. The importance of the present work derives from the panoply of different experimental observations which are semi-quantitatively addressed here. These calculations have no adjustable parameters (besides those which were used originally [9, 11] to fit some aspects of normal state data), so that their success or failure, upon comparison with experiment, should help select out viable theories of the cuprates. Here, following previous work above [4] and below [4, 14, 17], we apply an RPA, three band scheme which we have developed to treat the effects of very strong Coulomb correlations [12]. It should be stressed that our RPA approach is not a weak coupling RPA. The Lindhard function \( \chi_o \) used here is appropriate whenever the spin excitations are associated with spin 1/2 and with an underlying Fermi surface—be it in a Fermi liquid [13-17], or in a spin-charge separated metal [18-20]. Our starting point is the dynamical susceptibility \( \chi(q, \omega) = \chi_o(q, \omega)/[1 + J(q)\chi^o(q, \omega)] \) where, at low \( T \), the dominant contribution to the imaginary part of \( \chi^o \) is given by

\[
Im \chi^o(q, \omega) = \sum_k u(k, q)\delta(\omega - E_2(k, q))
\] (1)

Here \( u(k, q) = (1 - (\xi_k\xi_{k+q} + \Delta_k\Delta_{k+q})/E_kE_{k+q}) \), and \( \xi_k \) represents the “bare” particle energy relative to the chemical potential while \( E_k \) is that of the superconducting quasiparticles. The important function \( E_2(k, q) = E_k + E_{k+q} \) will play a key role in our analysis.

The RPA neutron cross section reflects a competition between effects associated with the Fermi surface shapes and pairing symmetry [via \( \chi_o \)] and those from the residual exchange interaction \( J(q) = J_o[\cos q_x + \cos q_y] \), which derives from Cu-Cu interactions via the mediating oxygen band. While the YBaCuO system is a two layer material, our past experience [9, 11] has shown that most of the peak structures associated with the neutron cross section are captured by an effective one layer band calculation, which we will investigate here. For definitiveness, we have fixed the temperature at 4 K and assume the electronic excitation gap to be described by an ideal \( d \)-wave, \( \Delta(q) = \Delta(\cos q_x + \cos q_y) \), where at \( T = 4 \) K, \( \Delta \) is taken to be 17 meV in YBaCuO [6] and 8 meV in optimally doped LaSrCuO. The breakdown of the Fermi liquid state is addressed only insofar as there may be precursor pairing or pseudogap effects, which lead to an excitation gap in the Lindhard function \( \chi_o \) above \( T_c \). Our calculations were based on a numerical procedure in which the Brillouin zone is subdivided into tetrahedral microzones [21]. Our peak heights are represented in arbitrary units, which are best quantified by
noting that in the normal state, the peak values are around 2 for 
LaSrCuO and for underdoped YBaCuO, whereas for the latter 
compound at optimal doping, the value is around 1. Presum-
ably all peak structure with intensity less than this is not cur-
cently observable (since the normal state peak of YBaCuO$_7$
 is essentially absent experimentally (22)).

In Figure 1 we show the evolution of the neutron peaks 
in underdoped YBaCuO as a function of $\omega$. These incom-
mensurate peaks are first seen at $\omega \approx \Delta$: as frequency in-
creases, the incommensurability is found to continuously de-
crease. This decrease is most apparent in the immediate vicin-
ity of the onset of the resonance, [or ($\pi, \pi$) peak] which can 
be read off from the lower part of Figure 1, to be at around 
27 meV, somewhat less than 2$\Delta$. Just above resonance, the 
($\pi, \pi$) peak becomes flat-topped possibly weakly incommen-
surate. It then broadens and remains structureless between 30-
40 meV. Finally, above 45 meV, clear incommensurate struc-
ture re-appears. We find that our low $\omega$ incommensurate peak 
heights are in the ratio of about 1:2. Experimentally 
(4), the ratio of spectral weights is found to be 1: 3.8 .

The lower panel shows the detailed frequency evolution of 
the dominant peak position quantified as $(\pi, (1 \pm \delta)\pi) = 
(0.5, 0.5 \pm \delta/2) = (0.5, Q)$ in reciprocal-lattice units (r.l.u.). 
The peaks evolve much as is seen experimentally (5,6). The 
primary difference between our observations and these partic-
ular experiments (4) is that over a range of frequencies, the 
incommensurate features coexist (although, not explicitly in-
dicated in the lower panel) with the more dominant resonant 
peak. By contrast, experimentally, an energy scale $E_c$ is asso-
ciated with the frequency at which the various peaks merge. 
It should be stressed, however, that here we have not incorpo-
rated resolution limiting effects which may affect this detailed 
comparison between theory and experiment. A very early pre-
diction for this lowest energy scale incommensurability was 
presented by our group in Ref. (7), where it was shown to be a 
consequence of $d$-wave pairing and relatively independent of 
the fermiology. Subsequent insights, using a related but 
differently motivated formalism, were provided in Ref \[15\], 
which explicitly showed the influence of $d$-wave pairing on 
$Im \chi$. 

To understand the origin of the various commensurate and 
incommensurate structures, in the main body of Figure 2 we 
plot the prototypical behavior of $Re \chi_0$ and $Im \chi_0$ for $Q$ at the 
commensurate point $Q_o = (\pi, \pi)$; in the inset is shown the 
analogous plot for the incommensurate peaks. These plots, 
which were chosen to correspond to YBaCuO, contain, in ef-
effect, a summary of the key energy scales (23) which appear in 
$Im \chi_0$. Here we emphasize how they are reflected in $Re \chi_0$. 
These $Re \chi_0$ effects are essential because, through the RPA 
denominator they serve to greatly enhance a given character-
istic feature in $Im \chi_0$. The four important energy scales which 
determine the behavior of $Im \chi$ (via simultaneous effects on 
$Im \chi_0$ and $Re \chi_0$) are given as (i) $\omega_o(q) = \min E_2(k, q)$, (ii) 
$\omega_{coh}$, the saddle point of $E_2(k, Q_o)$ (see point B in the inset), 
(iii) $\omega_{coh}$ the frequency where the rate of change of $u(k, q)$ 
drops abruptly. and, (iv) the onset for commensurate peaks 
$\Omega_o = \omega_o(Q_o)$ (see point A in the inset).

The related implications for $Re \chi_0$ are illustrated in Figure 
2. The onset frequency $\Omega_o$ is accompanied by a substantial 
growth in $Re \chi_0$. However, once the frequency reaches the 
two-particle Van Hove energy $\omega_{coh}$, determined by the saddle 
point shown as B in the inset, $Re \chi_0$ shuts down, as does the 
resonance. Figure 2, thus, shows that because of these $Re \chi_0$ 
amplifications along with the $q$-structure of $J(q)$, the 
commensurate peak will tend to dominate incommensurate struc-
ture in the range $\Omega_o < \omega < \omega_{coh}$, because of the small size 
of the RPA susceptibility which, in turn, yields a pole-like 
behavior in $Im \chi$. Incommensurate peaks only appear at the 
lower frequencies because their threshold $\omega_o$ is less than that 
of the commensurate structure. The appearance of incommen-
surability is associated with the $d$-wave state and is best seen 
pictorially in the upper right inset of Figure 3, shown for the
LaSrCuO family which contrasts nesting processes in the normal state (left) and d-wave superconducting state (right). Here the spectral weight of a given process is indicated by the intensity of the various lines. The magnitude of the incommensurability of the peak is determined by (i) energy conservation through the delta function in Eq. (1) along with (ii) coherence factor $|u(k, q)|$ effects, which select out the most favorable regions from otherwise equivalent nesting vectors.

To summarize, we can consolidate our observations, along with a collection of some of the mechanisms which have been proposed for the resonance in YBaCuO into a single inequality: low $\omega$ incommensurate peaks appear for $\omega_0 < \omega < \omega_c$, and commensurate peaks appear for $\Omega_0 < \omega < \omega_{vh}$. At still higher frequencies the peaks are again incommensurate. $\Omega_0$ is always somewhat less than $2\Delta$ because of the nodal structure of the d-wave gap.

Indeed, the results of Figure 2 are rather generic and can be used to address the LaSrCuO family as well, where unusual incommensurate structures in the cross section have been experimentally reported below $T_c$ for a range of low $\omega$, above $\Delta$. These, and related “spin gap” features have not yet been addressed theoretically. Here, we demonstrate that, in contrast to Ref. [25], these features—which are closely connected to the (low energy scale) incommensurate peaks discussed above for YBaCuO—are unrelated to fermiology effects and to presumed “incommensurate spin structure”. They depend exclusively on the d-wave pairing symmetry. Figure 3 shows a comparison of the cross section in the normal (left) and superconducting (right) phases of optimally doped LaSrCuO at low $\omega$. The peak sharpening below $T_c$ was first observed experimentally [4]. Its origin can be traced to the differences (above and below $T_c$) in the initial and final scattering processes along constant energy contours, which contribute to $\text{Im}\chi_\omega$ at a given point. These processes are shown in the upper panels of Figure 3 for a particular point $q$ indicated on the normal state cross section. It can be seen that in the superconducting phase, as a consequence of the opening of the gap, there is relatively little weight at the $q$ point in question, thereby leading to a greatly reduced scattering in the region between the incommensurate peaks below $T_c$.

In order to gain more experimental insight into the behavior of the neutron peaks of LaSrCuO in the superconducting phase, the authors of Ref. [4] measured $\text{Re}\chi$ at low frequencies and at the incommensurate points. They also addressed the details in the frequency onset of the cross section, measured via $\text{Im}\chi$, for a range of different wave-vectors. To determine $\text{Re}\chi$, the cross section was fitted to a simple Lorentzian-like form [4] peaked at $\Delta_s$. Here, we use the directly calculated $\text{Re}\chi$ to extract $\Delta_s$. The resulting experimental curves look qualitatively similar to the theoretical plots shown in the right hand inset of Figure 4. A reduction in $\text{Re}\chi(\omega = 0)$ between the normal and superconducting phase can be associated (via general Kramers Kronig relations) with a low $\omega$ suppression in the spectral weight of $\text{Im}\chi$. In the present theoretical scheme, this suppression derives from the opening of a d-wave superconducting gap. It is important, however, to stress that the d-wave symmetry in the Lindhard inset compares $\text{Re}\chi$ at $\omega = 0$ in the normal and superconducting states.

Why then is there no d-wave signature in the spin gap frequency? This follows because the q structure associated with the d-wave gap appears inside the integral over $k$ in the Lind-
hard function $\chi_o$. Moreover, the $q$ points chosen in the main body of the figure and in the left hand inset, while consistent with those measured in Ref. [3], do not reflect most directly the superconducting gap. In our calculations the spin gap $\Delta_s$ is found to be associated with the coherence (coh) factor energy scale, $\omega_{coh}$, which is relatively wave-vector independent in the region studied. However, it is the slightly lower, threshold frequency at which $Im \chi$ first becomes non-zero ($\omega_c(q)$), which most closely reflects $\Delta_q$. Indeed, $\omega_c$ varies by a factor of 2 for the $q$ values indicated. By contrast with $\omega_{coh}$, at $\omega_c$, the cross section has relatively little detectable weight.

What, then, are the similarities between the LaSrCuO and YBaCuO families? There are claims in the literature [1,4] that the cross section has relatively little detectable weight. We find that this differs from incommensurate peaks in the neutron cross section (as shown by the lower panel in Figure 1) is a generic feature of the present approach, and because it appears to be observed experimentally in at least two cuprate families [15], it will be important to establish whether an alternative scheme, such as the “stripe” picture can lead to similar behavior.

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References

[1] H. A. Mook et al., Nature 395, 395 (1998).
[2] M. Arai et al., Phys. Rev. Lett. 83, 608 (1999).
[3] H. F. Hong et al., cond-mat/9910041 (unpublished).
[4] B. Lake et al., Nature 400, 43 (1999).
[5] H. A. Mook et al., cond-mat/9811100 (unpublished) and private communication.
[6] V. J. Emery and S. A. Kivelson, cond-mat/9809083 (to be published in J. of Supercond.).
[7] E. Demler and S.-C. Zhang, Phys. Rev. Lett. 75, 4126 (1995).
[8] E. Demler and S.-C. Zhang, Nature 396, 733 (1998).
[9] Q. M. Si, Y. Y. Zha, K. Levin, and J. P. Lu, Phys. Rev. B 47, 9055 (1993). In LaSrCuO, $E_p - E_d = 4$ eV, $V_{pd} = 0.6$ eV, and $t_{pp} = -0.15$ eV; in YBCO, $E_p - E_d = 5$ eV, $V_{pd} = 1.29$ eV, $t_{pp} = 1.2$ eV, and $t_{pp} = -1.0$ eV.
[10] Y. Zha, K. Levin, and Q. M. Si, Phys. Rev. B 47, 9124 (1993).
[11] D. Z. Liu, Y. Zha, and K. Levin, Phys. Rev. Lett. 75, 4130 (1995).
[12] Q. Si et al., Physica C 162-164, 1467 (1989).
[13] P. B. Littlewood et al., Phys. Rev. B 48, 487 (1993).
[14] P. Benard, L. Chen, and M.-M. S. Tremblay, Phys. Rev. B 47, 15217 (1992).
[15] N. Bulut and D. J. Scalapino, Phys. Rev. B 53, 5149 (1996).
[16] I. I. Mazin and V. M. Yakovenko, Phys. Rev. Lett. 75, 4134 (1995).
[17] N. Bulut and D. J. Scalapino, Phys. Rev. B 50, 16078 (1994).
[18] T. Tanamoto, H. Kohno, and H. Fukuyama, J. Phys. Soc. Japan 61, 1886 (1992).
[19] J. Brinckmann and P. A. Lee, Phys. Rev. Lett. 82, 2915 (1999); Related calculations were independently reported by Qimiao Si and K. Levin (unpublished, 1998).
[20] L. Yin, S. Chakravarty, and P. W. Anderson, Phys. Rev. Lett. 78, 3559 (1997).
[21] J. Rath et al., Phys. Rev. B 11, 2109 (1975).
[22] H. Fong et al., cond-mat/9902226 (unpublished).
[23] M. Lavagna and G. Stemmann, Phys. Rev. B 49, 4235 (1994).
[24] H. F. Fong et al., Phys. Rev. Lett. 75, 316 (1995).
[25] D. Morr and D. Pines, cond-mat/9807214 (unpublished).
[26] P. Dai, H. A. Mook, and F. Doğan, Phys. Rev. Lett. 80, 1738 (1998).
[27] K. Yamada et al., Phys. Rev. Lett. 75, 1625 (1995).