Commensurate and Incommensurate Spin Fluctuations in YBa\(_2\)Cu\(_3\)O\(_{6+y}\)

Khee-Kyun Voo and W. C. Wu

Department of Physics, National Taiwan Normal University, Taipei 11650, Taiwan

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We present an interpretation of the recent neutron data on the commensurate and incommensurate spin fluctuations found in YBa\(_2\)Cu\(_3\)O\(_{6+y}\) based on a special configuration of the electronic dispersion and intervention from the \(d_{x^2-y^2}\)-wave superconducting phase. The observed switch over between the commensurate and incommensurate fluctuation spectra at the change of frequency or temperature is naturally accounted within this scenario.

Recent inelastic neutron scattering (INS) experiments on YBa\(_2\)Cu\(_3\)O\(_{6+y}\) (YBCO) compounds show a lot of new boggling data in spin dynamics. Since magnetic fluctuations in the high-\(T_c\) cuprates are long thought to be intimately related to their mechanism of superconductivity, it has attracted very much attention.

We briefly review the INS experiments which measure spin susceptibility Im\(\chi_s\) on YBCO. The INS in low-temperature superconducting (SC) phase optimal-doped YBCO shows a peak at frequency \(\omega_0(T=0) = 41\) meV and momentum \(Q_\pi = (\pi, \pi)\). The frequency width of the peak is within 10 meV and momentum width is within 0.1 \(\pi\) – 0.5 \(\pi\). In underdoped YBCO, the resonance frequency is slightly softened, and some damping is developed both in the frequency and momentum space. When the temperature is raised, the resonance frequency \(\omega_0(T)\) is softened only very little and intensity slightly suppressed before it abruptly disappears at the transition to normal state. Recently it was found that the incommensurate fluctuation, which was found previously only in La\(_{2-x}\)Sr\(_x\)CuO\(_4\) (LSCO) compounds, also exist in YBCO. The spin fluctuation in low-temperature YBCO at frequencies either lower or higher than \(\omega_0(0)\) is incommensurate in nature, characterized by four peaks at \((\pi, \pi \pm \delta)\) and \((\pi \pm \delta, \pi)\) as in the case of LSCO. At frequencies just below \(\omega_0(0)\) the deviation of the incommensurate peak from \(Q_\pi\) is also found to be slightly less than those at lower frequencies, where in contrast the deviation grows with frequency at \(\omega > \omega_0(0)\). There is also evidence that at frequency substantially below \(\omega_0(0)\), raising the temperature from below to high above \(T_c\) brings the fluctuation from incommensurate to commensurate. Contradictory, in a similar underdoped YBCO, a weak incommensurate structure is found recently by Arai \textit{et al.} at a similar high temperature regime.

On the other hand, a similar commensurate peak was also found very recently in Bi\(_2\)Sr\(_2\)CaCu\(_2\)O\(_y\) (BSCCO)\(^6\). Though less definite, an incommensurate fluctuation also occurs in these compounds at lower frequencies\(^3\).

Since in earlier times commensurate fluctuation was specific in YBCO while incommensurate in LSCO, the fluctuations were believed to be mutually unrelated and hence theoretical approaches to them were independent. The recent found interrelation thus sets a new constraint on the candidate theory of these systems.

The incommensurate peaks are believed as, due to Fermi surface nesting in one form or another\(^\text{i,ii}\). Whereas for the commensurate peak, various possibilities were proposed. Some focused on its peak feature frequency space \(^{\text{iii,iv}}\) while others gave more comprehensive treatments including the overall behavior of Im\(\chi_s\) in momentum space \(^{\text{v,vi}}\). Because of the recent discovery of incommensurate fluctuation in YBCO, unified treatments of the fluctuations were also put forward \(^{\text{vii,viii}}\). A common feature of these theories is that most of them incorporate some interaction effect into the susceptibility via Random-Phase-Approximation (RPA) in some form to result in a collective mode at \(Q_\pi\) \(^{\text{ix,xi,}xii,}xiii\). In this Letter we address the mentioned observations to a property of the band structure in conjunction with the intervention from the \(d_{x^2-y^2}\)-wave SC phase. Thus in contrast to the collective mode via RPA scenarios, our view of the 41 meV peak is based on the bare susceptibility. Furthermore we also include the discussion of the switch-over between commensurate and incommensurate fluctuations as driven by temperature, which so far absent from the literature.

Our approach was initiated by recent angle resolved photoemission spectroscopy (ARPES) measurement on YBCO and BSCCO. The measurement shows the existence of an extended van Hove singularity (VHS) at the \(M\) points \((0, \pm \pi)\) and \((\pm \pi, 0)\) of the Brillouin zone situated within 20 meV below the Fermi level \(^{\text{xiv}}\). The authors relates this to the occurrence of higher \(T_c\) of these compounds as enhanced by the VHS \(^{\text{xv}}\), compared to NdCeCuO compounds where the VHS is found hundreds of meV below the Fermi level \(^{\text{xvi}}\). On the other hand, both YBCO and BSCCO were found to exhibit commensurate fluctuation, and incommensurate fluctuation at lower frequencies. We believe that these common features are not accidental. Therefore in this paper we start out from an electronic dispersion with Fermi level near the VHS at \(M\) to describe the INS experiment on YBCO. Previously there were also interpretations of the commensurate peak based on the VHS effect. But the authors considered the RPA-type susceptibility in bilayer systems \(^{\text{xvii}}\) and a \(s^\pm\)-wave gap \(^{\text{xviii}}\). A mono-layer
VHS scheme closer to ours also exist but the discussion on the bare susceptibility was limited to zero temperature and specific to commensurate peaks [14].

Our description of the spin fluctuations in YBCO is in good agreement with experiments. The absence of commensurate magnetic response in LSCO is probably due to the remoteness of Fermi level from the VHS at $\overline{M}$ as it has a lower $T_c$.

We start with the single-band bare spin susceptibility

$$\chi_s^0(\mathbf{q}, \omega) = -\frac{1}{4} \sum_k \left[ 1 - \frac{\varepsilon_k + \Delta_k \Delta_{k+\mathbf{q}}}{E_k E_{k+\mathbf{q}}} \right] \times \left[ \frac{1 - f(E_k) - f(E_{k+\mathbf{q}})}{\omega - E_k - E_{k+\mathbf{q}} + i\delta} - \frac{1 - f(E_k) - f(E_{k+\mathbf{q}})}{\omega + E_k + E_{k+\mathbf{q}} + i\delta} \right] - \left[ \frac{f(E_k) - f(E_{k+\mathbf{q}})}{\omega - E_k - E_{k+\mathbf{q}} + i\delta} - \frac{f(E_k) - f(E_{k+\mathbf{q}})}{\omega + E_k - E_{k+\mathbf{q}} + i\delta} \right],$$

where $f(E_k)$ is the Fermi function and $E_k = (\varepsilon_k^2 + \Delta_k^2)^{1/2}$ is the quasiparticle excitation spectrum with $\varepsilon_k$ and $\Delta_k$ the electronic dispersion and superconducting gap respectively. We use a two-dimensional tight-binding electronic dispersion

$$\varepsilon_k = -2t(\cos k_x + \cos k_y) - 4t' \cos k_x \cos k_y - \mu,$$

where $t$ and $t'$ are the nearest-neighbor (NN) and next-nearest-neighbor (NNN) hopping respectively. We have fixed $t' = -0.178t$ throughout this paper and $\mu$ is the chemical potential that depends on doping. With YBCO in mind, the gap is taken as $\Delta_k = \Delta(T)(\cos k_x - \cos k_y)/2$. The maximum gap at zero temperature is taken as $\Delta(0) = 0.3t$ and this point will be further elaborated. The numerical integration width is taken as $\delta = 0.004t$ and the slicing is $2000 \times 2000$.

The chosen electronic dispersion is meant to phenomenologically describe the empirical relation between the Fermi level and the VHS. The chosen NNN hopping $t' = -0.178t$ has a Fermi surface crossing $\overline{M}$ at doping level $x = 0.15$ [Fig.1(b)], which is here nominally taken as the optimal doped case. This is to simulate a most intense effect of the VHS at an optimal doped compound as to result at a highest $T_c$. We choose $x = 0.10$ throughout this paper unless otherwise stated, as to show that the commensurate peak exist even when the Fermi surface is not exactly situated at the VHS but sufficiently close to it. And we believe that the only crucial point is the small difference in energy between the VHS and Fermi level but not their distance in momentum space as seen in the ARPES experiment. Whatever the origin of the VHS is also out of our concern. Furthermore we adopt a rigid band approximation. As far as the chosen dispersion has a Fermi surface out-bowed from the origin of the Brillouin zone as seen in the ARPES experiment, the main conclusion of our discussion is believed to valid.

In Fig.1(a), the frequency dependence of zero-temperature $\text{Im}\chi_s^0(\mathbf{Q}_x, \omega)$ at several doping levels ranging from underdoped to overdoped are shown to exhibit a peak near $2\Delta(0)$. $\text{Im}\chi_s^0(\mathbf{Q}_x, \omega)$ is gapped out at low frequencies since $\mathbf{Q}_x$ spans regions of maximal gap. It shows a high intensity at a small window around $2\Delta(0)$ due to the enhancement by the coherence factor on transitions between opposite gap phase regions, and is most intense when the frequency is just enough to open up the transition [which is near $2\Delta(0)$]. Furthermore, these regions are situated near $\overline{M}$. Thus the peak arises due to a co-enhancement from the VHS and coherence factor. Note that since the gap is written in term of the NN-hopping, which is generally different from system to system, the absolute resonance frequencies and linewidths of different doped cases could not be directly compared.

But if we phenomenologically input the experimental fact that $\omega_0(0)$ is only moderately decreased at underdoping, the peak could be argued as always be broadened at underdoping. We give the argument as follows. Denoting $\Gamma$ as the half-height width of the peak. At doping $x = 0.05$, with choices of $\Delta(0)/t$ within 0.2~0.5, the ratio $\Gamma/\omega_0(0)$ runs within 0.14~0.07. While at $x = 0.15$, the same choice of $\Delta(0)/t$ give $\Gamma/\omega_0(0)$ within 0.05~0.04 (in both cases a smaller $\Delta(0)/t$ gives a larger $\Gamma/\omega_0(0)$). It is seen that if the decrement of $\omega_0$ is within 30 percent, the broadening in an absolute energy scale always exist regardless of the choice of $\Delta(0)/t$ in individual systems within a broad range.

The broadening of the peak in frequency space is due to a mismatch of both enhancement effects. As the compound is underdoped, the $\mathbf{Q}_x$ transition on the Fermi surface shifts away from the full-gap regions [see Fig.1(b)] and leads to a down shift of the leading edge of the peak. On the other hand the VHS remains to affect only when the frequency is sufficient to open up the transition to the $\overline{M}$ points. In the overdoped case, $\text{Im}\chi_s^0(\mathbf{Q}_x, \omega)$ is suppressed because the Fermi surface has shrunk to a

![Fig. 1](image-url)
nesting incommensurate peaks at frequencies just below \(\omega_0(0)\) [Fig.2(e)]. This is due to a dynamical nesting effect. Since the Fermi surface is out-bowed, the opened up energy contour \(E_k = \omega/2\) which determines the possible transitions [10] has a smaller (larger) curvature above (below) the Fermi surface. Thus local nesting is better between contour above the Fermi surface and this determines the location of the tip of the peak. As \(\omega\) increases, the contour surges away from the Fermi surface and that pushes the nesting peaks towards \(Q_x\).

At frequencies over \(\omega_0(0)\), due to the filling up of the valley at \(Q_x\) a hardly discernible incommensurate feature is seen [Figs.2(d) and 2(f)]. It is characterized by incommensurate peaks displaced from \(Q_x\) along both the zone diagonals and edges. The incommensurability grows with frequency in this regime [Fig.2(f)] and that agrees qualitatively with experiment [3]. Further comment will be made on this point at the end of this Letter.

In our following discussion of the temperature evolution, we take a convenient empirical relation between the gap and temperature \(\Delta(T)/\Delta(0) = [1 - (T/T_c)^2]^{1/2}\) [see inset in Fig.3(a)] and a typical ratio \(2\Delta(0)/T_c = 8\).

In Fig.3(a), \(\text{Im} \chi_0^0(Q_x, \omega(0))\) is seen to be suppressed by temperature as in experiments [2]. At temperature below \(T_c\), the main cause of the suppression is the shift away of the mode frequency \(\omega_0(T)\) from \(\omega(0)\), the diminishing of the peak intensity is actually less rapid [Fig.3(b)]. For temperatures \(T < 0.8T_c\), the mode frequency of the commensurate peak is softened a little from \(\omega(0)\) before abruptly softened to zero and disappears at \(T_c\). The softening is merely a manifestation of the diminishing gap and owing to \(T_c\) which is a small energy scale compared to the bandwidth, the peak feature is maintained well at \(T < T_c\).

While the temperature evolution of the commensurate peak at \(\omega = \omega(0)\) has been frequently discussed [12,13,16], the temperature evolution of the incommensurate peaks at \(\omega < \omega(0)\) has been overlooked. Nevertheless recent experiments show that this is not at all trivial [3]. At low frequency and temperature, \(\text{Im} \chi_0^0\) at \(Q_x\) is gapped out and leads to a clear appearance of the in-
commensurate peaks. As the temperature is raised, the particular frequency could equal to the temperature dependent resonance frequency and the fluctuation is then converted to commensurate at a $\omega < \omega_0(0)$ and $T < T_c$ [compare Fig.2(b) and Fig.4(a)]. Plotting $\Im \chi^0_s$ at the $\omega$ and $Q_s$ against the temperature shows the emergence of the peak at a temperature just below $T_c$ [Fig.3(a)]. As the temperature is raised further into the normal state, the fluctuation reverts to a very weak incommensurate feature [23]. Experimentally it may well escape from detection and seen as a broad commensurate structure. At further underdoping, say $x = 0.05$, even a well distinguished commensurate feature may appear in the normal state [Fig.4(b)] and it is suppressed as the temperature increases. Note that the intensity of this high temperature commensurate structure is of the same order of magnitude as its low temperature incommensurate counterpart as seen in the experiment [24]. In our case, the valley at $Q_s$ appears and leads to a pronounced incommensurate structure in the normal state only in the overdoped case [23]. This may resolve the apparent contradiction between the observation of a broad commensurate structure [23] and the observation of a weak incommensurate structure [24] at similar temperature ($> T_c$) and frequency ($< \omega_0$) regimes in an underdoped YBCO. In our calculation these weak incommensurate structures are deviated from $Q_s$ along the zone edges.

We make a last comment on our result. If a Hubbard repulsion of 1.0t is incorporated via a RPA spin susceptibility, structure at the vicinity of $Q_s$ will be more prominent than structures away from $Q_s$. Furthermore, at zero temperature a very sharp and intense resonance at $Q_s$ occurs at $\omega_0 = 1.8\Delta(0)$. The incommensurate structure at $\omega > \omega_0$ is prominently away from $Q_s$ along the Brillouin zone edges. If a smaller repulsion 0.5t is taken, every structure resembles those of the bare susceptibility. Since we have no reason to believe that the repulsion should be finely 1.0t, we believe that such a tuning is a less probable description of reality.

In conclusion, we have provided an unified explanation of the INS experiments on YBCO based on the close-

ness of the Fermi level to the VHS at $\overline{M}$ points and coherence effect from the $d_{x^2-y^2}$-wave SC phase. The results describe naturally the frequency and temperature dependence of the commensurate peak, the switch over between the incommensurate and commensurate spectra at the change of frequency or temperature, and the decrease [increase] of the incommensurateness at frequency $\omega \lesssim 2\Delta(0)$ [$\omega > 2\Delta(0)$]. Furthermore, the broadening in frequency space of the commensurate peak at underdoping is also accounted semi-phenomenologically.

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