Spin susceptibility of underdoped cuprates: the case of Ortho-II YBa$_2$Cu$_3$O$_{6.5}$

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Recent inelastic neutron scattering measurements found that the spin susceptibility of detwinned and highly ordered ortho-II YBa$_2$Cu$_3$O$_{6.5}$ exhibits, in both the normal and superconducting states, one-dimensional incommensurate modulations at low energies which were interpreted as a signature of dynamic stripes. We propose an alternative model based on quasiparticle transitions between the arcs of a truncated Fermi surface. Such transitions are resonantly enhanced by scattering to the triplet spin resonance. We show that the anisotropy in the experimental spin response is consistent with this model if the gap at the saddle points is anisotropic.

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Recent experiments$^{\text{1,2,3}}$ have addressed the magnetic spectrum in detwinned and highly ordered ortho-II YBa$_2$Cu$_3$O$_{6.5}$ which has an average doping per planar Cu $x \sim 0.09$ and $T_c \sim 60$ K. The ortho-II phase is characterized by a periodic alternation of filled and empty Cu-O b-axis chains, doubling the size of the unit cell in the a direction. The oxygen ordering reduces the disorder and quasi-elastic peaks would be expected. Dimensionality has been reported by Hinkov$^{\text{4}}$ et al.\textsuperscript{4} centered at $(\pi, \pi)$ and a ring-like high energy branch dispersing upwards.\textsuperscript{5} At lower energies, there is inelastic scattering from one-dimensional modulations at incommensurate wavevectors stretching down to zero energy but without elastic or quasielastic peaks. On entering the superconducting state, the scattering at energies less than 16 meV is suppressed, but not eliminated. In this strongly underdoped regime the incommensurability $\delta$ at low energies is very small.\textsuperscript{5} Contrary to what has been observed at optimal doping the incommensurability below the resonance persists in the normal pseudogap phase.\textsuperscript{1} The feature associated with the one-dimensional modulations, which were interpreted as a signature of dynamic stripes,\textsuperscript{1} is a flat top lineshape centered at $(\pi, \pi)$ along the direction perpendicular to the chains. An anisotropic response, but no sign of one-dimensionality has been reported by Hinkov et al\textsuperscript{2} on untwinned YBa$_2$Cu$_3$O$_{6+\delta}$.

Static stripes should show up as elastic magnetic peaks and quasi-elastic peaks would be expected\textsuperscript{2} from slow fluctuating stripes, but these are not observed. Also, the dramatic drop of the magnetic scattering at low energies, at the onset of superconductivity, is not expected if ordered antiferromagnetic regions between hole stripes are involved. The stripe-based model also has difficulties to explain the isotropy found above the resonance.\textsuperscript{1}

Many authors have used RPA\textsuperscript{17} (random phase approximation) schemes to describe the magnetic response near optimal doping. This model relates the resonance peak and incommensurate branches with a particle-hole collective mode bounded below the superconducting gap. An extension to the normal pseudogap phase at underdoping can be made by assuming an energy gap from another origin (e.g. d-density wave order) but even then careful tuning of the parameters is required since the resonance decreases while the gap increases in energy with decreasing doping. Alternatively one can interpret the resonance as a collective mode of a spin liquid which goes soft as the antiferromagnetic instability at strong underdoping is approached or as an undamped spin-wave excitation brought about by strong antiferromagnetic correlations.

In this letter we introduce a simple phenomenological model for the pseudogap phase and focus on the anisotropic incommensurate low energy response. We start from a Fermi surface of quasiparticles which is truncated near the saddle points leaving only four Fermi arcs centered on the diagonals, similar to the form observed in ARPES\textsuperscript{12} experiments. Although the dispersion we use is derived from a staggered flux phase,\textsuperscript{13,14} we propose it as a phenomenological form for the normal state of a doped spin liquid (SL). Arguments that a Fermi surface truncation can occur without symmetry breaking have been given by Ledermann et al\textsuperscript{15}, based on an analysis of multi-leg Hubbard ladders and by Honerkamp et al\textsuperscript{16} and also Läuchli et al\textsuperscript{17} from a functional renormalization group analysis of a 2-dimensional Hubbard model. In addition to the quasiparticle scattering we introduce a resonant spin triplet mode at $(\pi, \pi)$ dispersing upwards, in both normal and superconducting phases. We view the resonance as the collective mode of the spin liquid analogous to that found, for example, in coupled ladder systems\textsuperscript{18,19,20} and in the slave boson approach.\textsuperscript{10}

We propose that the low-energy spin response is due to particle-hole excitations across the Fermi arcs. In the absence of other effects the bare spin susceptibility, due to particle-hole excitations, is too small to explain the experimental data and has a much richer structure than the one observed. In our model such transitions are resonantly enhanced by scattering into the triplet spin resonance. The enhancement is strongest close to $(\pi, \pi)$. We analyze the possible sources of anisotropy between directions parallel and perpendicular to the chains and find that results similar to those found experimentally can be obtained if the gap at the saddle points is sufficiently
anisotropic.

We start from a two-dimensional dispersion with hopping to first and second nearest neighbors. Truncation is introduced through the opening of a gap in the particle-hole channel at the boundary of the Antiferromagnetic Brillouin zone (AFBZ). Note, as argued above, we assume that this gap can occur in a spin liquid without symmetry breaking. We neglect bilayer splitting of the bands and work with a single-planar band with dispersion:

\[ \epsilon_k = 4t' \cos kx \cos ky - \mu \]
\[ \pm \sqrt{4t^2 (\cos kx + \cos ky)^2 + \Delta_{SL}^2(k)} \]  

(1)

The sign follows the opposite of \(\cos kx + \cos ky\). The gap is assumed to have the form \(\Delta_{SL}(k) = \Delta_{ST}(\cos kx - \cos ky + \alpha [\cos^2 kx + \cos^2 ky])\). If \(\alpha\) is zero the gap has d-wave symmetry and the same magnitude at \((0, \pi)\) and \((\pi, 0)\). When \(\alpha\) is negative (positive) the magnitude of the gap is anisotropic and larger at \((\pi, 0)\), (respectively \((0, \pi)\)). The 2\(0\) periodicity due to the oxygen ordering breaks the tetragonal symmetry and splits this band into two: \(\alpha\) and \(\beta\), folding the Brillouin zone in the \((0, 0) - (\pi, 0)\) direction, and opening a gap \(V\) at \(k_x = \pi/2\), see Bascones et al. In the reduced Brillouin zone, \(k_x \in (-\pi/2, \pi/2)\) and \(k_y \in (-\pi, \pi)\),

\[ \epsilon_{k_x}^{\alpha, \beta} = \frac{\epsilon_k + \epsilon_{k+\pi_x}}{2} \pm \frac{1}{2} \sqrt{\frac{(\epsilon_{k+\pi_x} - \epsilon_k)^2 + V^2}{(\epsilon_{k+\pi_x} - \epsilon_k)^2 + V^2}} \]  

(2)

with \(\pi_x = (\pi, 0)\). In the superconducting state, the energy of the quasiparticles is \(E_{k_x}^{\alpha, \beta} = \left[ (\epsilon_{k_x}^{\alpha, \beta})^2 + \Delta_{k_x}^{\alpha, \beta} \right]^{1/2}\). Due to the ortho-II ordering and the breaking of the tetragonal symmetry the superconducting gap is modified from a pure d-wave form to \(\Delta_{k_x}^{\alpha, \beta} = \Delta_{k_x}^{\alpha, \beta} \sqrt{g(k) \cos kx \cos ky}\) with

\[ g(k) = (\epsilon_{k+\pi_x} - \epsilon_k) \left/ \left[ (\epsilon_{k+\pi_x} - \epsilon_k)^2 + V^2 \right]^{1/2} \right. \]  

(3)

The resonantly enhanced spin susceptibility at low energies is given by:

\[ \text{Im} \chi_0(q, \omega) = J \text{Re} \chi^{res}(q, \omega) \text{Im} \chi_0(q, \omega) \]  

(4)

\(J\) is a constant of order the exchange energy, \(\text{Im} \chi_0(q, \omega)\) is the imaginary part of the bare spin susceptibility of the truncated Fermi surface and \(\text{Re} \chi^{res}(q, \omega)\) is the real part arising from the resonant mode. For simplicity, we assume that the high energy part of the spin fluctuation spectrum is a single mode with dispersion taken from experiment:

\[ \omega_{res}(q) = (\Delta_{spin}^2 + (Aq^2))^{1/2} \]  

(5)

Here \(\Delta_{spin} = 33\ \text{meV}\) and \(A = 365\ \text{meV}\ \text{Å}\). From Kramers-Krönig the real part

\[ \text{Re} \chi^{res}(q, \omega) = 1/ [\omega - \omega_{res}(q)] \]  

(6)

At zero temperature, applying a Kubo formula,

\[ \text{Im} \chi_0(q, \omega) = \frac{1}{2} \sum_k \{ F_{k_q}^\pm \sum_{m, m' = \alpha, \beta} \Lambda_{k_q}^{m, m'} \}

(7)

\[ \delta \left( \omega - \left[ E_{k+\alpha}^{m} + E_{k}^{m'} \right] \right) \delta \left( \omega + \left[ E_{k+\alpha}^{m} + E_{k}^{m'} \right] \right) \]

Plus (minus) sign applies when \(m\) and \(m'\) are equal (different), and

\[ F_{k_q}^\pm = \frac{(\epsilon_{k+\pi_x} - \epsilon_{k+q}) (\epsilon_{k+\pi_x} - \epsilon_k) + V^2}{(\epsilon_{k+\pi_x} - \epsilon_{k+q})^2 + V^2 (\epsilon_{k+\pi_x} - \epsilon_k)^2 + V^2} \]

\[ \Lambda_{k_q}^{m, m'} = \frac{1}{4} \left( 1 - \frac{\epsilon_{k+\pi_x} - \epsilon_{k+q}}{E_{k+\alpha}^{m} + E_{k+\alpha}^{m'}} \right) \]  

(8)

Neutron scattering experiments are affected by the resolution factor of the measurement apparatus. In the experiments by Stock et al., the resolution factor in \(q\) space is anisotropic and comparable to the observed incommensurability. In order to compare with their results we convolute \(\text{Im} \chi(q, \omega)\) with an anisotropic gaussian\(\delta\) with standard deviation along directions perpendicular and parallel to the chains \(\sigma_x = 0.078\) and \(\sigma_y = 0.058\). We set \(t' = 0.15\), \(\Delta_{SP} = 0.31\), \(V = 0.6\), and \(\mu = -0.70\), in units of \(t\), corresponding to hole doping \(x = 0.09\). In the following, we assume \(t = 180\ \text{meV}\), then \(\Delta_{spin} = 0.183\) and \(A = 0.52\).

We first consider the case \(\Delta_0 = 0\) \(\alpha = 0\) and analyze the possibility that the observed anisotropy is a consequence of the modification of the Fermi surface due to ortho-II ordering. The truncated Fermi surface obtained with these parameters is shown, in the extended Brillouin zone, in Fig. 1a). The breaking of the tetragonal symmetry is clear. The magnetic response (not shown) has two
peaks close to \((\pi, \pi)\), along the directions \((\pi + \delta, \pi)\) and \((\pi, \pi + \delta)\). The position of these peaks depends on the band parameters and their distance from \((\pi, \pi)\) increases with doping. The spin susceptibility, convoluted with the resolution factor, along \((\pi + \delta, \pi)\) and \((\pi, \pi + \delta)\) is shown in Fig. 1b). As the value of \(J\) is uncertain, the susceptibility is given in arbitrary units, but these units are the same throughout. In spite of the clear anisotropy of the Fermi surface, once the resolution factor is included, the spin response in the directions perpendicular and parallel to the chains is very similar. We have repeated the calculations for different Fermi surface parameters. The anisotropy we obtained is very weak or it gives larger incommensurability in \((\pi, \pi + \delta)\), contrary to the experiment. We have checked the effect which, combined with the ortho-II ordering, could have the addition of a third nearest neighbor hopping term, the reduction of the spectral weight along the Fermi surface as the saddle points are approached or the inclusion of finite lifetime of the quasiparticles. None of these effects gives an incommensurability comparable to the observed value. We conclude that the modification of the Fermi surface due to the ortho-II symmetry breaking alone cannot explain the experimental results.

The anisotropy in the hopping matrix element has been suggested, alone or with other effects, as the origin of the one-dimensionality of the spin spectrum reported by Mook et al. in YBa\(_2\)Cu\(_3\)O\(_6\). The case in which the hopping along \((t_y)\) and perpendicular \((t_x)\) to the chains are inequivalent is shown in the inset of Fig. 1b). We have taken \(t_y = 1.3t_x = 1.3t\), keeping the rest of the parameters as above. With this modification of the Fermi surface the tail of the peak at \((\pi, \pi)\) decays more slowly along \((\pi + \delta, \pi)\), than along \((\pi, \pi + \delta)\). But this broadening is different to the one found in ortho-II YBa\(_2\)Cu\(_3\)O\(_6\). We have also checked the effect of a modulated doping, which could follow the ortho-II oxygen ordering, with no
success.

Next we examine the effect of finite $\alpha$. The gap at the AFBZ loses its $d$-wave symmetry and for $\alpha = -0.33$, at $(\pi, 0)$ it is twice than at $(0, \pi)$. In spite of this large asymmetry, the effect on the shape of the Fermi arc is not unreasonable, see Fig. 2 a). The crossing between the arcs and the AFBZ moves towards $(0, \pi)$ in the first and second quadrants and towards $(0, -\pi)$ in the third and fourth quadrants. The color map in Fig. 2 c) shows the spin susceptibility at $\omega = 0.05$, without the resolution factor. The inequivalence of the peaks is clear. This anisotropy remains when the resolution factor is included. The shape of the peaks along $(\pi + \delta, \pi)$ and $(\pi, \pi + \delta)$ are plotted in Fig. 2 b), and compare well with those reported. As shown in Fig. 3 (top figure) the anisotropy is maintained with increasing energy. As the resonance is approached the incommensurability vanishes due to the enhancement factor. The anisotropy is robust and survives also in the superconducting state, see Fig. 2 b). In this plot it is clear that at low energies, the magnetic intensity has been reduced in the superconducting state. The suppression in the superconducting state is due to the opening of a gap along the arcs. It is also evident in Fig. 3 (bottom figure) which plots the susceptibility at $(\pi, \pi)$ as a function of energy. The signal increases with energy, as reported experimentally.

In conclusion, we have presented a simple phenomenological model which is able to account for the main features of the spin scattering in ortho-II $YBa_2Cu_3O_6.5$, at low energies, without involving one-dimensional. The model should be applicable to other underdoped cuprates. The spin response is larger close to $(\pi, \pi)$, but sensitive to the parameters which determine the Fermi surface. It is characterized by two peaks along the Cu-O axis. Below $T_c$ the opening of the superconducting gap on the arcs produces a reorganization of the spectral weight at low energies. The superconducting state can influence the spin susceptibility also through a better definition of the quasiparticles. The model is intended for low energies in the underdoped regime. The high energy part observed experimentally, including the resonance, is modelled with a collective triplet mode. Recently, Tranquada et al. has suggested that the high energy mode is due to disordered bond- stripes, which behave as weakly coupled two-leg ladders. However in our view the ring form of the dispersion at high energies suggests a 2-dimensional character for the spin liquid. Our model can be seen as a phenomenological extension for the pseudogap phase of the RVB (resonant valence bond) theory, whose success was recently reviewed.

The anisotropy of the spin response found in Ortho-II $YBa_2Cu_3O_6.5$ is ascribed to an asymmetric deformation of the Fermi arcs close to the boundary of the AFBZ. We found that such a deformation could originate from an anisotropic $\Delta_{SL}$ -the energy gap that truncates the Fermi surface in the normal pseudogap phase. A substantial anisotropy of $\Delta_{SL}$ was required to explain the experiment. The origin of this anisotropy remains to be an open question, but could be related to the chain ordering.

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1. C. Stock et al., Phys. Rev. B 66, 024505 (2002).
2. C. Stock et al., Phys. Rev. B 69, 014502 (2004).
3. C. Stock et al., Phys. Rev. B 71, 024522 (2005).
4. R. Liang et al., Physica C 336, 57 (2000).
5. N.H. Andersen et al., Physica C 317-318, 259 (1999).
6. V. Hinkov et al., Nature 430, 650 (2005).
7. S.A. Kivelson et al., Rev. Mod. Phys. 75, 1201 (2003).
8. M.R. Norman, Phys. Rev. B 63, 092509 (2001). A. Abanov et al., Phys. Rev. Lett. 89, 177002 (2002). I. Eremin et al., Phys. Rev. Lett. 94, 147001 (2005).
9. S. Tewari et al., Phys. Rev. B 64, 224516 (2001). In the absence of a superconducting gap, at the RPA level, the low-energy incommensurate branch would be absent, E. Bascones (unpublished).
10. J. Brincmann and P.A. Lee, Phys. Rev. Lett. 82, 2915 (1999).
11. D.K. Morr and D. Pines, Phys. Rev. Lett. 81, 1086 (1998).
12. A. Damascelli et al., Rev. Mod. Phys. 75, 473 (2003).
13. P.A. Lee et al [cond-mat/0410445].
14. S. Chakravarty et al., Phys. Rev. B 63, 094503 (2001)
15. U. Ledermann et al., Phys. Rev. B 62, 16383 (2000).
16. C. Honerkamp et al., Phys. Rev. B 63, 035109 (2001).
17. A. Läuchli et al., Phys. Rev. Lett. 92, 037006 (2004).
18. E. Dagotto and T.M. Rice, Science 271, 618 (1996). L. Balents and M.P.A. Fisher, Phys. Rev. B 53, 12133 (1996).
19. E. Dagotto et al., Phys. Rev. B 45, 5744 (1992). H. Tsunetsugu et al., Phys. Rev. B 49, 16078 (1994). M. Troyer et al., Phys. Rev. B 53, 251 (1996).
20. B. Normand and T.M. Rice 54, 7180 (1996). M. Troyer et al Phys. Rev. B 55, R6117 (1997).
21. E. Bascones et al., Phys. Rev. B 71, 012505 (2005).
22. This enhancement is intermediate between the one resulting from Fermi-Golden rule and the one obtained from an RPA-coupling between the bare particle-hole susceptibility and the high-energy mode.
23. We have neglected finite resolution in energy. Due to the robustness of the anisotropy with energy we do not expect any effect of the finite resolution in energy on the anisotropy found.
24. All the calculations have been done with a finite lifetime $\Gamma = 0.008$, which results in finite susceptibility at zero energy. In those done to check the impact of lifetime effects on the anisotropy, $\Gamma$ was larger and could be $q$ dependent.
25. I. Eremin and D. Manske, Phys. Rev. Lett. 94, 067006 (2005). A. P. Schnyder et al., cond-mat/0510790. T. Zhou
and J-X. Lin, Phys. Rev. B 69, 224514 (2004).
26 H.A. Mook et al, Nature 404, 729 (2000).
27 J.M. Tranquada et al., Nature 429, 534 (2004).
28 P.W. Anderson et al, J. of Phys. Cond. Mat. 16, R755 (2004). A. Paramekanti et al, Phys. Rev. B 70, 054504 (2004).