RAPID COMMUNICATIONS

PHYSICAL REVIEW B VOLUME 47, NUMBER 1 1 JANUARY 1993-I

# Neutron-scattering measurements as a test of theories of high-temperature superconductivity

Pierre Bénard, Liang Chen, and A.-M. S. Tremblay
*Département de Physique and Centre de Recherche en Physique du Solide, Université de Sherbrooke, Sherbrooke, Québec, Canada J1K 2R1*
(Received 3 August 1992)

It is shown that the Hubbard model in the intermediate-coupling regime can qualitatively explain neutron-scattering experiments in $La_{2-x}Sr_xCuO_4$ only if there are strong magnetic fluctuations in the system. By contrast, the marginal-Fermi-liquid approach explains the data without appealing at all to strong magnetic fluctuations. It is shown that the strength of the magnetic fluctuations can be estimated by detecting incommensurate peaks located near the zone center using neutron-scattering experiments.

The magnetic structure factor appears as an ideal quantity to make quantitative comparisons between theory and experiment in high-temperature superconductors. Indeed, this quantity can both be computed reliably and measured in detail as a function of wave vector and frequency. On the experimental side, there have been several detailed neutron-scattering measurements of this quantity in the new superconductors.[1-4] On the theoretical side, Monte Carlo calculations[5] have shown that up to the relevant[6-9] intermediate coupling regime ($U_0 \approx 4t$), standard generalized-random-phase-approximation (GRPA) calculations give extremely accurate results for the magnetic structure factor as long as one accounts for a renormalization of the bare interaction $U_0$ which comes from maximally crossed diagrams.[5] The renormalized $U$ can be estimated in two dimensions[5] by the formula $U \approx U_0/(1+0.2U_0)$.

Recent magnetic neutron-scattering experiments[2,3] in the *normal* phase of $La_{2-x}Sr_xCuO_4$ have shown clear incommensurate peaks whose intensity, relative to the background, decreases appreciably on a scale of 15 meV. The peaks are located at $\{(\pm\pi \mp \delta\pi, \pm\pi), (\pm\pi, \pm\pi \mp \delta\pi)\}$, in units where the lattice spacing is unity. Questions which arise are the following: (a) Why do the peaks appear further away from $(\pi,\pi)$ than one would expect from the simplest one-band Hubbard model with nearest-neighbor hopping? (b) Where does the small energy scale of 15 meV come from?

In Ref. 10, the position of the peaks was explained by a three-band model fit to the true band structure, while the energy dependence was ascribed purely to self-energy effects which arise in the marginal-Fermi-liquid (MFL) approach.[11] Magnetic fluctuations are small in this approach. Even if there is no enhancement by vertex corrections or by nesting of the Fermi surface, sharp incommensurate peaks appear at small frequency purely as a general property of *two-dimensional* Lindhard functions. By contrast, within the more standard one-band Hubbard model one must be very close to an incommensurate spin-density-wave (ISDW) instability to explain even only qualitatively the 15-meV energy scale. It is shown below that one can test for the importance of magnetic fluctuations by doing experiments which will compare the intensity of the already observed incommensurate peaks with the intensity of incommensurate peaks located around (0,0).

Let us first address the question of the experimental peak positions with the Hubbard Hamiltonian (in the electron representation)

$$H = \left[ -t \sum_{\langle i,j \rangle} c^{\dagger}_{\sigma i} c_{\sigma j} - t' \sum_{\langle\langle i,j \rangle\rangle} c^{\dagger}_{\sigma i} c_{\sigma j} + \text{H.c.} \right] + U_0 \sum_i n_{i\uparrow} n_{i\downarrow} \,. \quad (1)$$

$t'$ stands for the second-neighbor hopping matrix element ($-0.5t < t' < 0$). Other symbols are standard. Experimentally, the maxima in the neutron scattering cross section are displaced by $\delta(\pm\pi,0)$ and $\delta(0,\pm\pi)$ from $(\pi,\pi)$. Cheong *et al.* found in $La_{2-x}Sr_xCuO_4$ a value of $\delta$ equal to $0.25 \pm .01$ for $x = 0.14$ and of $0.14 \pm 0.02$ for $x = 0.075$. In the case of nearest-neighbor hopping only ($t' = 0$), the low-temperature small-frequency position of the peaks, $[q_x = \pm 2\cos^{-1}(-\mu/2t)\,,\ q_y = \pi]$ and $[q_x = \pi,\ q_y = \pm 2\cos^{-1}(-\mu/2t)]$, is determined by the bare chemical potential.[12] Assuming that the concentration $x$ is equal to the doping of the copper-oxygen planes, the prediction for $\delta$ is 0.087 when $x = 0.14$ and 0.038 when $x = 0.075$. These values are much smaller than allowed by the experimental data. Assuming that the real doping is smaller than $x$ gives corrections in the wrong direction and it does not appear chemically reasonable to assume that the doping is larger than $x$. Another discrepancy in comparing with experiment is that the observed peaks appear much smoother than predicted. Convolution with the experimental resolution[10] helps to solve both of these problems. However, the calculated shift $\delta$ is still smaller than observed by a factor of about 2.

Next-nearest-neighbor hopping can shift appreciably the incommensurate peaks from their positions in the nearest-neighbor model, especially close to half-filling. Let us first restrict ourselves to wave vectors along the zone boundary. The results for $\delta$, which can be obtained analytically in the small frequency limit, are summarized in Fig. 1. For $t' \neq 0$, the curves branch at $\mu_c^- = -t^2/(2t') - [t^4/(2t')^2 + 8t^2]^{1/2}$ because two peaks may occur. For dopings such that $\mu < \mu_c^-$, the dependence of $\delta$ on $\mu$ is the same as in the $t' = 0$ case, but $\mu$ also depends on $t'$ at fixed doping. For $4t' > \mu > \mu_c^-$, the two branches indicate the existence of two structures: a cusp whose position has again the same $[2\cos^{-1}(-\mu/2t),\ \pi]$

 

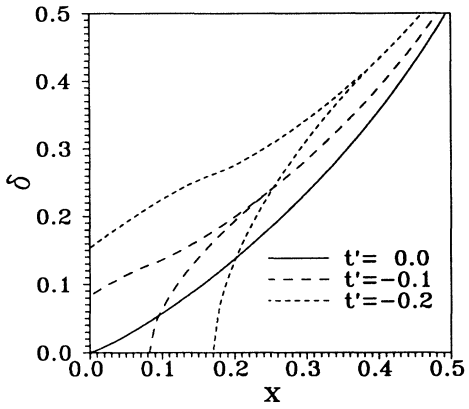


FIG. 1. Peak displacement $\delta$ vs dopant concentration $x$ (decreasing $\mu$) for three values of $t'(0, -0.1$, and $-0.2)$ at low temperatures and low frequencies ($T,\omega \ll 2|\mu|$), as predicted by GRPA with renormalized $U$.

dependence and an unambiguous maximum at

$$(2\cos^{-1}\{-4t'(\mu-4t')/[16t'^2-(t+t'\mu/t)^2]\}^{1/2},\ \pi)$$

and symmetry related points. For $0>\mu>4t'$, depending on temperature, frequency, and interaction, the shift $\delta$ will either be zero or at the position of the cusp. Sufficiently close to the ISDW instability, however, the shift will always be[13] $\delta=0$. We expect that the cusps would be difficult to observe experimentally because of the finite experimental resolution and the small difference in intensity between the cusp and the other structure. Assuming a doping-independent value of $t'$ then, it does not appear possible to shift the peaks in the right direction for both of the experimentally studied dopings. Realistic values[14] of $t'$ are in the range $=-0.20<t'<-0.10$. Hence, taking for example $t'=-0.10$, $\delta$ is increased slightly to 0.1254 if $x=0.14$, but $\delta$ is equal to zero if $x=0.075$. For $t'=-0.20$, $\delta$ is equal to zero for both concentrations.

The difficulty to accurately reproduce the peak positions within the one-band Hubbard model does not appear fundamental, however, since these positions are clearly a manifestation of details of the band structure.[15] On the other hand, it appears important to obtain at least the correct order of magnitude for the energy scale. When $t'=0$, the energy scale of the bare structure factor, $2|\mu|$, is set by the value of the bare chemical potential,[16] which is equivalent in our units to the difference between the Fermi energy at a given filling, and the Fermi energy at half-filling. Since the bare chemical potential is $-0.12t$ for hole doping of 0.07 and $-0.27t$ for hole doping of 0.14, this suggests, for $t\approx 5000$ K that the energy scale coming from band-structure effects only is 5 to 10 times too large. Second-neighbor hopping $t'$ could also add another small energy scale of the right order of magnitude, $-2(\mu-4t')/[1+(2t'/t)]$, $(\mu<4t'<0)$ when the system is close to the Van Hove singularity ($\mu=4t'$) which now appear away from half-filling. We feel, however, this is an unlikely explanation since the shift $\delta$ for the lower doping case[2,3] would then be zero.

An overdamped mode (analogous to antiparamagnons) which becomes soft at the incommensurate magnetic transition provides a mechanism to obtain a small energy scale in the paramagnetic phase. This is illustrated in Fig. 2 which plots the imaginary part of the susceptibility as a function of frequency $\omega$ (in units $t=1$) and $q_x$ for $q_y=\pi$. In Fig. 2(a) one can see the well-known[8,17,18] "spin gap" or "kinetic gap" around $(\pi,\pi)$ whose energy dependence remains on the scale of $2|\mu|$ despite the fact that $U/U_c=0.75$. At $U/U_c=0.975$, which is close to the ISDW instability occurring at $U_c\approx 2.0t$ ($U_0\approx 3.2t$) for dopings $x=0.14$, one can clearly identify a much smaller energy scale. This small energy scale may be present for a wide range of dopings and interactions when one adds the long wavelength fluctuations which remove the finite-temperature mean-field transition in two dimensions. However, if one remains strictly within our approach, one needs to be very close to the instability to see the decrease in frequency of the magnetic structure factor. This is in agreement with previous analysis of NMR experiments which also showed that it was necessary to be close to the ISDW instability to reproduce the temperature dependence of the Cu relaxation rate.[7]

To decide whether the small energy scale comes from proximity to a magnetic instability, as in the one-band Hubbard model, or from large MFL self-energy effects without magnetic fluctuations, we suggest experiments which would detect the presence of peaks located symmetrically around $Q=0$. Figure 3 shows the magnetic susceptibility $\chi_0''$ computed along the three high-symmetry directions of the Brillouin zone within the one-band nearest-neighbor Hubbard model. In the $U=0$ case, $\chi_0''$

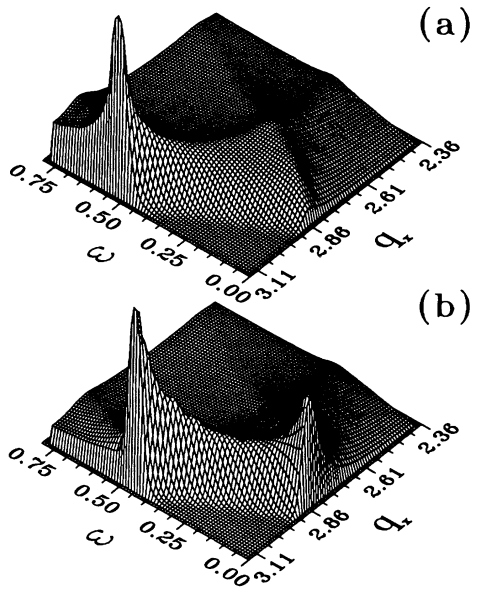


FIG. 2. The imaginary part of the susceptibility at finite $U$ for $x=0.14$, $t'=0$; (a) $U/U_c=0.75$ and (b) $U/U_c=0.975$ for a $4000\times 4000$ lattice. The overdamped mode softens as $U$ approaches the ISDW instability at a renormalized value of $U_c=2$. The peak in the intensity as a function of wave vector decreases as the frequency $\omega$ increases, as long as $\omega$ is larger than the resonance frequency.

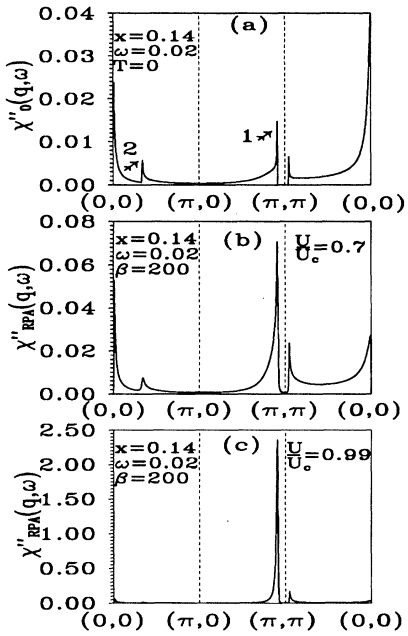


FIG. 3. Imaginary part of the spin susceptibility for the nearest-neighbor one-band Hubbard model. (a) Exact result for the Lindhard function. (b) and (c) were computed for the parameters indicated in the figure on $1000\times1000$ lattices with Lorentzian energy-level broadening $\eta=0.02t$.

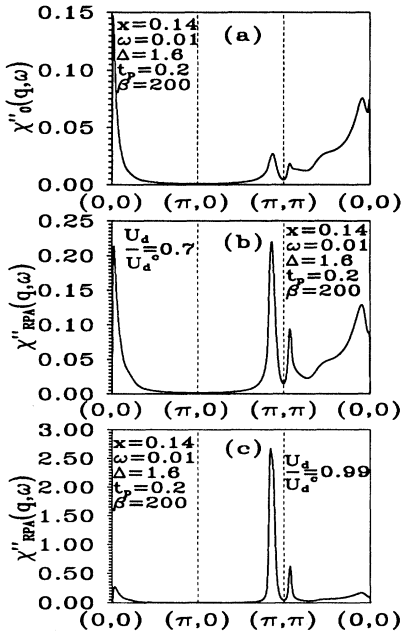


FIG. 4. Imaginary part of the spin susceptibility using the three-band model of the MFL approach in the low-frequency limit (no self-energy effects). Form factors are included and vertex corrections at finite $U$ are computed in the generalized RPA approach. $U_d$ indicates repulsion on the Cu $d$ site alone. $t_p$ is the $O(p_x)-O(p_y)$ hopping, and $\Delta=(\varepsilon_p-\varepsilon_d)$ is the bare charge-transfer energy. Lattice size is $500\times500$ and $\eta=0.01t$.

was computed analytically[19] and plotted in Fig. 3(a). The feature already detected by experiment is indicated by arrow No. 1. Arrow No. 2 at $2\cos^{-1}(1-|\mu|/2t)$ indicates a feature which is absent for a spherical Fermi surface. It originates from *umklapp* scattering between two of the rounded corners of the diamond-shape Fermi surface. Figure 3 clearly shows that the new peak is comparable in magnitude to the one already observed, until one increases $U$ to a value very close to the magnetic instability.

Analogous results also hold true within the MFL approach,[10] as illustrated in Fig. 4 in the low-frequency limit. In this case, the largest new incommensurate features near the origin are in the diagonal direction. This comes from effective second-neighbor hopping which leads to sign changes in the curvature of the corresponding Fermi surface. In fact, the one-band Hubbard model with $t'\approx-0.10$ (Fig. 5) behaves in a manner quite analogous to the MFL result[20] in Fig. 4. The main point to notice in the MFL result of Fig. 4 is that again one needs to be quite close to the magnetic instability to see only the incommensurate features near $(\pi,\pi)$. As seen in all the cases just discussed (Figs. 3 to 5), $\chi''$ has a rich momentum structure in two dimensions, even without strict nesting or interactions. This structure gives information on the Fermi surface since, as can be shown, the position of the peaks is negligibly affected by interactions in the low-frequency limit. However, very close to a magnetic instability $\chi''$ becomes dominated by a single feature.

In conclusion, neutron scattering could settle the important question of the proximity to an incommensurate magnetic instability as raised in particular in the MFL

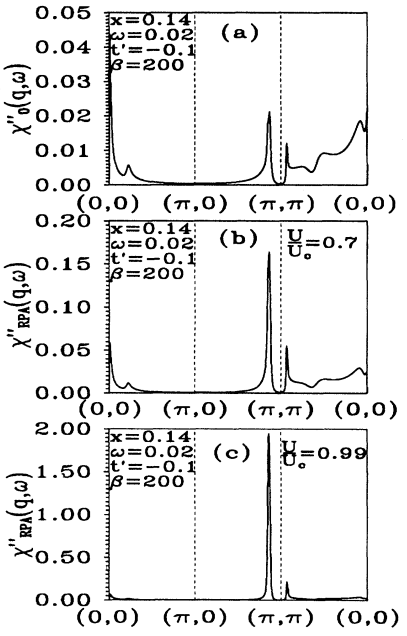


FIG. 5. Imaginary part of the one-band spin susceptibility including next-nearest-neighbor hopping.

approach.[10] It would suffice to measure, in the normal state, the relative size of the incommensurate structures near (0,0) and near $(\pi,\pi)$. These features should be displaced from these two points in comparable amounts and they should be of comparable intensity unless one is indeed extremely close to the magnetic instability. In other words, the intermediate-coupling Hubbard scenario corresponds to Fig. 3(c), while the MFL scenario typically corresponds to Fig. 4(b). These two results are so qualitatively different that the experiment should clearly be able to differentiate between the two scenarios. Already, the known experimental results near $(\pi,\pi)$ give larger intensity in the diagonal direction than predicted by Fig. 3(c), but experimental resolution at present prevents an unambiguous interpretation of the data.

We would like to thank T. Mason and especially P. Littlewood for providing copies of their work before publication and for most useful discussions. We would also like to thank R. J. Gooding, T. Li, and R Coté for discussions. We acknowledge the support of the Natural Sciences and Engineering Research Council of Canada (NSERC), the Fonds pour la formation de chercheurs et l'aide á la recherche from the Government of Québec (FCAR), and (A.-M. S. T.) the Canadian Institute of Advanced Research (CIAR).

[1]R. J. Birgeneau *et al.*, Phys. Rev. B **38**, 6614 (1988); T. R. Thurston *et al.*, *ibid.* **40**, 4585 (1989); S. M. Hayden *et al.*, Phys. Rev. Lett. **66**, 821 (1991).

[2]S. W. Cheong *et al.*, Phys. Rev. Lett. **67**, 1791 (1991).

[3]T. E. Mason, G. Aeppli, and H. A. Mook, Phys. Rev. Lett. **68**, 1414 (1992).

[4]H. Chou *et al.*, Phys. Rev. B **43**, 5554 (1991), and references therein.

[5]L. Chen, C. Bourbonnais, T. C. Li, and A.-M. S. Tremblay, Phys. Rev. Lett. **66**, 369 (1991); N. Bulut, in *Dynamics of Magnetic Fluctuations in High Temperature Superconductors,* edited by G. Reiter *et al.*, NATO Advanced Study Institute (Plenum, New York, 1991).

[6]J. R. Schrieffer, X. G. Wen, and S. C. Zhang, Phys. Rev. B **39**, 11 663 (1989).

[7]N. Bulut, D. Hone, D. J. Scalapino, and N. E. Bickers, Phys. Rev. B **41**, 1797 (1990); Phys. Rev. Lett. **64**, 2723 (1990).

[8]N. Bulut and D. J. Scalapino (unpublished).

[9]J. P. Lu, Q. Si, J. H. Kim, and K. Levin, Phys. Rev. Lett. **65**, 2466 (1990); Physica C **179**, 191 (1991).

[10]P. B. Littlewood, J. Zaanen, and G. Aeppli (unpublished).

[11]C. M. Varma *et al.*, Phys. Rev. Lett. **63**, 1996 (1989); **64**, 497 (1990).

[12]H. J. Shulz, Phys. Rev. Lett. **64**, 1445 (1990).

[13]In fact the real part of the susceptibility has a broad maximum of half-width $2\cos^{-1}(-\mu/2t)$ centered on $(\pi,\pi)$, which implies that sufficiently close to the spin-density-wave instability the maximum will always be at $(\pi,\pi)$.

[14]M. S. Hybertsen, E. B. Setchel, M. Schluter, and D. R. Jennison, Phys. Rev. B **41**, 11 068 (1990).

[15]It is a different matter in the strong-coupling limit. Results of R. R. P. Singh and R. L. Glenister do suggest a displacement of the peaks.

[16]For temperatures higher than $2|\mu|$, the incommensurate peaks move to $(\pi,\pi)$ and the nested Fermi-liquid theory of J. Ruvalds and A. Virosztek, Phys. Rev. B **42**, 4064 (1990) describes the behavior of the structure factor.

[17]S. Wermbter and L. Tewordt, Phys. Rev. B **43**, 10 530 (1991).

[18]J. Rossat-Mignot *et al.*, Physica B **169**, 58 (1991); P. M. Gehring *et al.*, Phys. Rev. B **44**, 2811 (1991).

[19]D. R. Grempel and M. Lavagna, Solid State Commun. **83**, 595 (1992) studied the diagonal direction but our result differs from theirs.

[20]In the MFL model, but at fillings other than $x=0.14$, the new peak seen in Fig. 3 for the $t'=0$ case also appears but is smaller.