Incommensurate spin fluctuations in the two-dimensional t-t′-U model

Adolfo Avella, Ferdinando Mancini and Dario Villani
Dipartimento di Scienze Fisiche "E.R. Caianiello" - Unità INFN di Salerno
Università degli Studi di Salerno, 84081 Baronissi (SA), Italy
(July 24, 1997)

Magnetic properties of the two-dimensional t-t′-U model are investigated by studying the static spin magnetic susceptibility as a function of momentum for various temperatures. The calculations are performed by means of the Composite Operator Method in the static approximation. By increasing the value of the t′ parameter the magnetic scattering in the reciprocal space evolves to an isotropic structure. It is shown that the results are in qualitative agreement with the experimental situation observed in LSCO and YBCO compounds.

74.72.-h; 75.10.-b; 71.10.Fd.

The persistence of antiferromagnetic fluctuations in the superconducting state of high-Tc cuprates is one of the most striking features in these materials. Indeed, it is widely accepted that in cuprate materials there is a close relation between the unusual magnetic properties and the occurrence of high temperature superconductivity, and that a comprehension of the magnetic correlations in the normal state may be an important step in the understanding of the microscopic mechanism of pairing.

The knowledge of the wave-vector and energy dependencies of the spin excitation spectrum is of the most importance in the attempt to build up an appropriate theory for high-Tc superconductivity [1]. The dynamical spin susceptibility for cuprate materials has been investigated by inelastic neutron scattering and NMR techniques. Neutron scattering data on La2−x(Ba, Sr)xCuO4 have shown [2, 3, 4] that away from half-filling the magnetic Bragg peak in the dynamical structure factor S(k, ω) broadens and develops a structure with four peaks located at [(1 ± δ)p, p] and [p, (1 ± δ)p]. Also, very recent neutron scattering experiments [6–10] have solved the commensurate peak structure issue in YBa2Cu3O6+y. P. Dai et al. [10] have shown that the magnetic response in YBa2Cu3O6.6 is complex with incommensurate fluctuations at low temperatures for energies below the commensurate resonance [11]. The low frequency spin fluctuations change from commensurate to incommensurate on cooling with the incommensuration first appearing at temperatures somewhat above Tc. The same behavior has been observed in BiiSr2CaCu2O8−δ [12].

In a previous paper [12], in the context of a single-band Hubbard model, we advanced a theoretical prediction; namely, it was claimed a close relation between superconductivity and incommensurate magnetism in some high-Tc cuprates due to the reported proportionality between the calculated amplitude of incommensurability and the experimental superconducting critical temperature for La2−xSrxCuO4 over the whole phase diagram. In the present experimental context, where the incommensurability seems to be a common feature for all cuprate superconductors, it results natural to revisit the analysis of the spin fluctuations spectrum by adding a finite diagonal hopping term t′ to the original Hubbard Hamiltonian. Infact, the addition of a t′ bare parameter has often been suggested to handle the complexity of the experimental situation for the cuprates [13, 14]. Moreover, the next nearest neighbor hopping parameter t′ emerges from various reduction procedures as the single parameter, which carries, at the level of the single-band description, the information about the crystal structure outside the CuO2 planes and thus differentiates between the various cuprates [15, 16].

In this letter, we focus the attention on the momentum dependence of the static spin magnetic susceptibility χ(k), because this quantity provides strict information about the spatial range of the magnetic correlations. We show that the t-t′-U model presents an incommensurate phase at finite doping that disappears by increasing temperature. In addition, the next-nearest neighbor hopping term drives the evolution of the magnetic scattering to an isotropic structure in the reciprocal space.

The t-t′-U model is described by the Hamiltonian

\[ H = \sum_{ij} t_{ij} c_i^\dagger c_j + U \sum_i n_{i\uparrow} (i) n_{i\downarrow} (i) - \mu \sum_i n (i) \]

where we use a standard notation. In the hopping matrix t_{ij} we have retained the terms up to the next-nearest neighbors situated along the plaquette diagonals. In the static approximation [17], the k-dependent susceptibility \( \chi(k) \) can be written as

\[ \chi(k) = \sum_{i,j=1}^{2} \chi_{ij}(k) \]

where

\[ \chi_{ij}(k) = \int \frac{dp}{(2\pi)^2} \frac{f[E_i(k+p)] - f[E_j(p)]}{E_i(k+p) - E_j(p)} K_{ij}(k,p) \]

(3)
FIG. 1. The static susceptibility $\chi (\mathbf{k})$ for various temperatures. $U = 4$, $t' = 0$ and $n = 0.97$. In panels (a) and (b) are reported the lines $\mathbf{k} = (\pi, k)$ and $\mathbf{k} = (k, k)$, respectively.

FIG. 2. Surface plot in reciprocal space of $\chi (\mathbf{k})$ for $U = 4$, $t' = 0$, $n = 0.97$ and $T = 0.01$

$E_1 (\mathbf{k})$ and $E_2 (\mathbf{k})$ are the upper and the lower Hubbard subbands, $K_{ij} (\mathbf{k}, p)$ are expressed in terms of the spectral intensities. The explicit expressions for these quantities have been computed in the framework of the COM [17, 18]. The term $\chi_{\text{inter}} = \chi_{12} + \chi_{21}$ describes the propagation of a spin accompanied by a spin excitation between the two bands $E_1 (\mathbf{k})$ and $E_2 (\mathbf{k})$; while the two terms $\chi_{11}$ and $\chi_{22}$ describe the propagation with a subsequent intraband spin excitation.

In Fig. 3 we present the static susceptibility $\chi (\mathbf{k})$ for various temperatures. The choice for the parameters is $U = 4$, $t' = 0$ and the particle filling has been fixed as $n = 0.97$. In this letter the energies are expressed in unity of $t$. In panels (a) and (b) $\chi (\mathbf{k})$ is reported along the line $\mathbf{k} = (\pi, k)$ and the line $\mathbf{k} = (k, k)$, respectively. In both cases by increasing the temperature the incommensurate double-peak structure becomes a broad maximum centered at $(\pi, \pi)$. Along the $(k, k)$ line the intensity at incommensurate positions is lower than the one along $(\pi, k)$. This can be clearly observed in Figs. 2 and 3 where four well-resolved incommensurate peaks are located at $[(1 \pm \delta) \pi, \pi]$ and $[\pi, (1 \pm \delta) \pi]$. The important features of the data are:

1. the overall square symmetry of the scattering with the sides of the square parallel to the $(k, k)$ and to the $(k, -k)$ lines;
2. the accumulation of intensity near the corners of the square.

These features reproduce the experimental situation for $La_{2-x} (Ba, Sr)_x CuO_4$ [17, 18].

In Figs. 4 and 5 we report the results for $t' = -0.1$. In this case incommensurate magnetic resonance modes are isotropically distributed around the $(\pi, \pi)$ point. The occurrence of such an evolution of the magnetic fluctuations can be related to the spreading of the nesting vector in the momentum space. That is, the evolution from a pseudo-nested to a roughly circular hole-like Fermi surface. Infact, the shape and, in particular, the bending of the Fermi surface are strongly dependent on the value of the $t'$ parameter, which leads for fixed values of filling $n$ and of the $U$ parameter to a real rotation of the Fermi surface [18].

Besides, the intensity of the incommensurate peaks along the $(k, k)$ line is now comparable to that along $(\pi, k)$ (Fig. 4). In this case the structure along the diagonals is not related to a saddle point topology as in $LSCO$, but to a really increased scattering as it has been observed in $YBa_2Cu_3O_{6.6}$ [19]. Again, by increasing temperature the commensurability is recovered. An isotropic magnetic scattering, as we have found for $t'$ different from zero, should be detected for $YBCO$ once extended scans over the whole Brillouin zone will be made. Indeed, this prediction is supported by ARPES data for $YBCO$ [20], which seem to exclude an underlying symmetry for the in-plane magnetic scattering identical to that of $LSCO$, but $\pi/4$ rotated [11].

Performed theoretical calculations show that by increasing further $t'$ the magnetic scattering processes are suppressed at all wave vectors so that we have a featureless susceptibility with no clearly detectable peaks over all the Brillouin zone.

In conclusion, we have shown that the $t'-U$ model presents an incommensurate phase at finite doping and that the magnetic scattering become isotropic as $t'$ is increased. The occurrence of such an evolution of the magnetic fluctuations can be related to the spreading of the nesting vector in the momentum space. That is, the evolution in the dynamical response of a spatially uniform electron liquid from a pseudo-nested to a roughly circular hole-like Fermi surface.

[1] C. Varma et al., Phys. Rev. Lett. 63, 1996 (1989).
[2] T. Thurston et al., Phys. Rev. B 40, 4585 (1989).
[3] G. Shirane et al., Phys. Rev. Lett. 63, 330 (1989).
[4] R. Birgenau et al., Phys. Rev. B 38, 6614 (1988).
[5] S. Cheong et al., Phys. Rev. Lett. 67, 1791 (1991).
[6] G. Shirane et al., Physica B 196, 158 (1994).
[7] K. Yamada et al., Phys. Rev. Lett. 75, 1626 (1995).
[8] K. Yamada et al., Doping dependence of the spatially modulate spin correlations and the superconducting transition temperature in $La_{2-x}Sr_x CuO_4$, Preprint 1996.
[9] S. Petit et al., Spin dynamics study of $La_{2-x}Sr_x CuO_4$ by inelastic neutron scattering, Preprint 1996.
[10] P. Dai, H. Mook, and F. Dogan, Incommensurate magnetic fluctuations in $YBa_2Cu_3O_{6.6}$, cond-mat/9707112, and references therein.

FIG. 3. Contour plot in reciprocal space of $\chi (\mathbf{k})$ for $U = 4$, $t' = 0$, $n = 0.97$ and $T = 0.01$

FIG. 4. Surface plot in reciprocal space of $\chi (\mathbf{k})$ for $U = 4$, $t' = -0.1$, $n = 0.97$ and $T = 0.01$

FIG. 5. Contour plot in reciprocal space of $\chi (\mathbf{k})$ for $U = 4$, $t' = -0.1$, $n = 0.97$ and $T = 0.01$

FIG. 6. The static susceptibility $\chi (\mathbf{k})$ for various temperatures. $U = 4$, $t' = -0.1$ and $n = 0.97$. In panels (a) and (b) are reported the lines $\mathbf{k} = (\pi, k)$ and $\mathbf{k} = (k, k)$, respectively.
[11] P. Dai et al., Phys. Rev. Lett. 77, 5425 (1996).

[12] F. Mancini, D. Villani, and H. Matsumoto, *Incommensurate magnetism in cuprate materials*, cond-mat/9703207.

[13] D. Duffy and A. Moreo, Phys. Rev. B 52, 15607 (1995).

[14] U. Trapper, D. Ihle, and H. Fehske, *Theory of magnetic short-range order for itinerant electron systems*, cond-mat/9609014.

[15] L. F. Feiner, J. H. Jefferson, and R. Raimondi, Phys. Rev. B 53, 8751 (1996).

[16] R. Raimondi, J. H. Jefferson, and L. F. Feiner, Phys. Rev. B 53, 8774 (1996).

[17] F. Mancini, S. Marra, and H. Matsumoto, Physica C 250, 184 (1995).

[18] A. Avella, F. Mancini, D. Villani, and H. Matsumoto, *The two-dimensional t-t’-U model as a minimal model for cuprate materials*, cond-mat/9707088.

[19] F. Mancini, S. Marra, and H. Matsumoto, Physica C 252, 361 (1995).

[20] Z.-X. Shen, and D. S. Dessau, Physics Reports 253, 1 (1995), and references therein.
This figure "fig2.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/9707266v1
This figure "fig3.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/9707266v1
This figure "fig4.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/9707266v1
This figure "fig5.jpg" is available in "jpg" format from:

http://arxiv.org/ps/cond-mat/9707266v1
\( \chi(k) \)

(a) \( U = 4 \), \( n = 0.97 \), \( t' = -0.1 \)

(b) \( T = 0.01 \), \( T = 0.05 \), \( T = 0.10 \), \( T = 0.15 \)