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Magnetic Structure of Electronic Inhomogeneities in Cuprates: Competition between Stripes and Spirals

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It is shown that the magnetic structure of high-T_c superconductors is strongly influenced by the next-nearest neighbor hopping parameter t' which distinguishes different families of cuprates. Our investigations indicate that uniform spirals get favored by a large t'/t ratio but are unstable at small doping towards stripes with spin canting. For large $|t'/t|$ spirals can be stabilized under certain conditions in the overdoped regime which may explain the elastic incommensurate magnetic response recently observed in iron-co-doped Bi2201 materials.

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1. Introduction

In recent years the origin and consequences of electronic inhomogeneities has been intensively investigated for a large variety of transition metal oxides, like manganites, nickelates and cuprate superconductors. Concerning the latter compounds, the question whether static or slowly fluctuating electronic order is an intrinsic property remains a strongly debated issue. The first firm evidence for the existence for a self-organized electronic state came from elastic neutron scattering (NS) on Nd-co-doped lanthanum cuprates [1]. In this experiment it was concluded from the splitting of both lattice and magnetic Bragg scattering peaks that doped holes arrange themselves in quasi one-dimensional stripes which simultaneously act as antiphase domain walls for the antiferromagnetic (AF) order. More recently the direct observation of an associated charge modulation has been achieved by resonant inelastic X-ray scattering (RIXS) spectroscopy [2, 3].

In the past years two of us have performed detailed investigations of stripes within the Gutzwiller approximation (GA) supplemented with Gaussian fluctuations which allowed for the explanation of the doping dependent incommensurability and various transport properties [4, 5], the optical conductivity [6] and magnetic excitations [7, 8] on the basis of striped ground states.

In other cuprate materials than lanthanum cuprates evidence for stripe-like electronic inhomogeneities is less evident from NS experiments due to the lack of large single crystals. Therefore it is remarkable that a recent study has revealed elastic incommensurate magnetic peaks in an overdoped $Bi_{1.75}Pb_{0.35}Sr_{1.9}CuO_{6+z}$ sample [(Bi,Pb)2201] co-doped with iron [9]. Within the error bars the doping $\delta \approx 0.23$ and the measured incommensurability $\varepsilon \approx 0.21$ seem to extend the relation $\varepsilon \approx \delta$ (which holds for underdoped lanthanum cuprates [10]) to large doping without saturation at $\delta \approx 0.12$.

Since the formation of stripes involves a modulation of the longitudinal spin component it couples to an associated charge modulation. Alternatively one could envisage the situation where the transverse spin component is spatially modulated leading to the concept of spirals. These textures are characterized by a homogeneous periodic and planar rotation of the Cu moments with no associated charge modulation and have also been proposed as an explanation for the incommensurate magnetic ground state of cuprate superconductors [11–13]. Based on Hubbard-type models spiral solutions have been investigated on the basis of the Hartree–Fock (HF) [14–16], slave-boson (or GA) [14, 15, 17–19] and dynamical mean-field [20] calculations.

In this paper we show that in some parameter regime relevant for cuprates spirals have in fact a lower ground state energy than homogeneous stripes. However, since at small doping the former are unstable with regard to phase separation this results in a new type of spin and charge structure which is characterized by substantial spin canting.

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2. Model and parameters

Our investigations are based on the extended single-band Hubbard model. Expectation values are evaluated with the Gutzwiller variational wave function $|\Psi_{\rm g}\rangle = P_{\rm g}|{\rm SD}\rangle$ where $P_{\rm g}$ is the Gutzwiller projector and $|{\rm SD}\rangle$ a Slater determinant. For $|{\rm SD}\rangle$ we use a state with arbitrary charge and spin order, e.g. stripe, spirals or solutions with spin canting. The energy of a given solution with $N_{\rm h}$ holes ($E_{N_{\rm h}}$) is evaluated with respect to the energy of the undoped antiferromagnet ($E_{\rm AF}$), according to

$$e_{\rm h} = \frac{E_{N_{\rm h}} - E_{\rm AF}}{N_{\rm h}}. \qquad (1)$$

In order to fix the value for the onsite repulsion U we refer to a previous paper [8] where we have shown that a time-dependent extension of the GA with $U/t = 8$ can accurately reproduce the magnon excitations of undoped lanthanum copper oxide (LCO) as revealed by neutron scattering [21]. Since U/t should not vary among the cuprate materials we restrict to $U/t = 8$ but investigate the dependence on the next-nearest neighbor hopping t'/t which from local density approximation (LDA) computations has been shown to specify the various high-$T_{\rm c}$ families [22] since it provides a direct relation to $T_{\rm c}^{\rm max}$ within a BCS-type scenario [23].

3. Results and discussion

Figure 1 compares the doping dependence of the binding energies per hole for the various textures investigated in the present paper. Let us note that for fixed stripe or spiral periodicity, $e_{\rm h}(\delta)$ aquires a minimum at a specific doping δ which determines the optimum filling $\nu_{\rm opt}$ for the texture under consideration. The $e_{\rm h}$ curves for spirals and stripes shown in Fig. 1 correspond to the optimum filling for different periodicities, i.e. the wave vector of the textures varies along the curves. For the spin-canted solutions (cf. below) we also show the doping dependence of $e_{\rm h}$ for various periodicities at $t'/t = -0.4$.

It is found that for all dopings only vertical or diagonal spiral textures correspond to minima of the energy landscape and the corresponding $e_{\rm h}$ curves are shown in Fig. 1 as dashed and solid lines, respectively. The occurrence of two stable symmetry directions can be understood from the analysis of the instabilities of the large Fermi surface paramagnetic metal found at smaller values of U/t. As discussed in Ref. [24] the dominant instabilities occur for those wave vectors which correspond to a crossing of two nesting curves ("double nesting"). These double nesting points determine the maximum susceptibilities and are always found to lie along high-symmetry directions.

For both, diagonal and vertical spirals, $e_{\rm h}$ has a minimum at $\delta_{\rm s}$ which means that for doping smaller than $\delta_{\rm s}$ spiral ground states are unstable with respect to phase separation. The resulting energy of the phase separated solutions calculated from a Maxwell construction is shown as a thin horizontal solid line in Fig. 1.

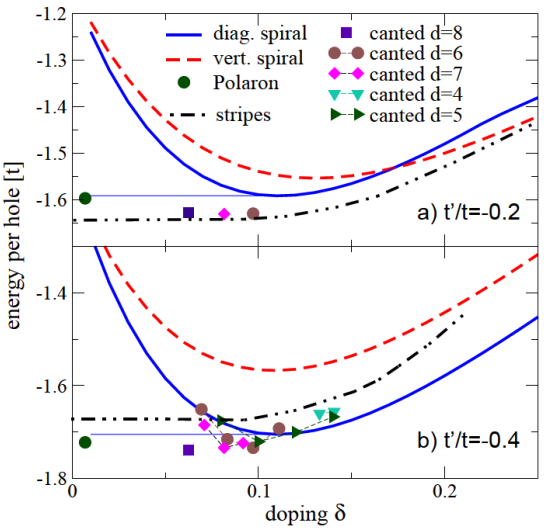

Fig. 1. Comparison of diagonal (blue solid) and vertical (red dashed) spirals with the energy of vertical stripes (dash-dotted). Let us note that in the regime of non-interacting stripes (where the dash-dotted line is flat) diagonal and vertical stripes are almost degenerate in energy. The thin horizontal line corresponds to the energy of the phase separated state for diagonal spirals. The full circle reports the energy of a single polaron state. Other symbols refer to $e_{\rm h}$ of the diagonal spin canted solution with different periodicities as indicated by the labels. Let us note that the energies which are reported by symbols are obtained on smaller clusters ($\approx 20 \times 20$) than spirals and stripes (100×100). The resulting error is of the order of the symbol size.

The dashed-dotted line in Fig. 1 represents the doping evolution of the minimum energy for vertical stripes. At low doping the separation between the charge stripes is large and thus the interaction between them becomes negligible. For this reason the corresponding $e_{\rm h}$ curves are "flat" up to $\delta \approx 0.1$ where the energy per hole starts to increase due to the repulsion between stripes. It should be noted that at low doping diagonal stripes become energetically more favorable [5], however, the energy difference with respect to vertical textures is small and of the order of the line width in Fig. 1. Therefore other mechanisms like long-range Coulomb interactions and lattice distortions are decisive in determining the exact stripe state in the very underdoped regime.

The above finding that low doping spirals are unstable towards phase separation suggests that there should exist a solution with even lower energy. One could envisage e.g. an elliptical spiral [25] which has an eccentricity proportional to certain amount of charge order. We have therefore performed an unconstrained minimization of the spin-rotational GA energy functional [26] on finite clusters. It is found that the low doping solutions are diagonal stripes with significant spin canting. An example is shown in Fig. 2 and the corresponding energy is indicated for different periodicities in Fig. 1. This textures is

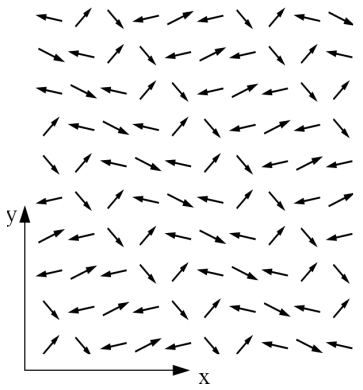

Fig. 2. Diagonal stripe solution with spin canting. The (hole) charge is accumulated on the lines with ferromagnetically aligned spins. The planar spin structure has been chosen to lie in the xy-plane. 10×10 system with 10 holes corresponding to doping $x = 1/10$. $U/t = 8$, $t'/t = -0.4$.

characterized by a domain wall of the antiferromagnetic order which has a fractional phase change of the AF order parameter $\Delta\theta < \pi$ (with θ the angle between the staggered magnetization and the quantization axis) contrary to collinear stripes which have $\Delta\theta = \pi$. Thus instead of building up a macroscopic phase separation between undoped AF and doped spiral regions the system prefers to separate these textures at the nanoscale, corresponding to the modulated structure shown in Fig. 2.

The structure of the (planar) texture shown in Fig. 2 can be decomposed in harmonics as

$$S_i^x = \sum_n S_n^x \cos(\boldsymbol{Q}^{(n)} \cdot \boldsymbol{R}_i),$$
$$S_i^y = \sum_n S_n^y \cos(\boldsymbol{Q}^{(n)} \cdot \boldsymbol{R}_i) \qquad (2)$$

with $\boldsymbol{q} = \left(\frac{2\pi}{10}, \frac{2\pi}{10}\right)$ and we have set $\boldsymbol{Q}^{(n)} = \boldsymbol{Q}_{\mathrm{AF}} - n\boldsymbol{q}$. The solution breaks spin rotational symmetry, so the relative weights of the Fourier components on the x and y magnetization directions depend on the particular solution or quantization axis. For the choice shown in Fig. 2 the amplitudes are zero in the y direction. The nonzero amplitudes are given by $S_1^x \approx 0.22$, $S_3^x \approx -0.04$, $S_0^y \approx 0.03$, and $S_2^y \approx -0.11$, i.e. the x-component shows "conventional" antiphase domain walls, whereas the y-component is "commensurate" with finite weight at the AF wave vector.

Let us note that for smaller values of $|t'/t|$ stripes do not profit from the transversal spin degrees of freedom and the energy of the spin canted solution is approximately that for the collinear solutions (cf. Fig. 1). Nevertheless, the finding that very different patterns are so close in energy suggests that stripes will be very susceptible to quenched disorder inducing charge-spin glass behavior and making difficult to obtain clear signatures of stripes.

In the overdoped regime and for sufficiently large $|t'/t|$ spirals do not phase separate and under certain conditions may constitute the ground state in cuprate superconductors. In fact, from Fig. 1 it turns out that for large doping even the diagonal spin canted solutions are energetically less favorable than spirals. In this regard, the recent elastic NS study [9] on (Bi,Pb)2201 co-doped with iron is interesting since it reveals incommensurate magnetic correlations at a doping concentration $\delta \approx 0.23$. The detected periodicity is compatible with vertical spirals [27] provided that the value of the next-nearest hopping for Bi2201 is in the range $-0.4 < t'/t < -0.2$. LDA calculations by Pavarini and co-workers [22] yield a value of $t'/t \approx -0.25$ for $Bi_2Sr_2CuO_6$ where our results (cf. Fig. 1) suggest that vertical spirals are still more favorable than diagonal ones and may even dominate over stripes. Naturally, our computations which are for perfectly modulated spirals, can only be qualitative since the measured coherence length of the magnetic modulation [9] is of the order of the iron distance. Therefore additional effects like the disorder and magnetic moment arising from the Fe dopants should also be taken into account.

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