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Magnetic excitations in the stripe phase of high-T_c superconductors

G.S. Uhrig[a,*], K.P. Schmidt[a], M. Grüninger[b]

[a]Institut für Theoretische Physik, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany
[b]II. Physikalisches Institut, Universität zu Köln, Zülpicher Str. 77, 50937 Köln, Germany

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Abstract

The magnetic excitations in the stripe phase of high-T_c superconductors are investigated in a model of spin ladders which are effectively coupled via charged stripes. Starting from the effective single-triplon model for the isolated spin ladder, the quasi-one-dimensional spin system can be described straightforwardly. Very good agreement is obtained with recent neutron scattering data on $La_{15/8}Ba_{1/8}CuO_4$ (no spin gap) and $YBa_2Cu_3O_{6.6}$ (gapped). The signature of quasi-one-dimensional spin physics in a single-domain stripe phase is predicted.

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The role of magnetic excitations in the mechanism of high-T_c superconductivity is still an unsettled issue, for a review see e.g. Ref. [1]. Experimentally, a direct probe of these magnetic excitations is inelastic neutron scattering (INS) which provides information resolved both in energy and in momentum, see e.g. Ref. [2]. Three main features have to be understood: (i) the so-called resonance peak [1,2], which appears in the superconducting phase at the antiferromagnetic wave vector $\mathbf{Q}_{AF} = (\frac{1}{2}, \frac{1}{2})$; (ii) the appearance of superstructure satellites, which are usually attributed to stripes [1,3–5]; (iii) incommensurate excitations which lie energetically both below and above the resonance mode [6–9]. There is growing evidence that these phenomena [8–10] are linked. Two recent papers show the momentum dependence of the magnetic excitations in the superconducting [11] and in the stripe-ordered [12] phase over a broad energy range. The data show stunning similarities and allow a quantitative comparison with theory.

In the case of static stripes, the hole-poor regions are described by spin ladders [5]. But the number of legs of these spin ladders is not yet unambiguously determined. Recent ab initio results suggest that two-leg spin ladders are particularly stable [13]. This is appealing since two-leg ladders are very well understood [14–16]. We have shown recently that a model of weakly coupled spin ladders allows to describe the momentum and the energy dependence of the neutron scattering intensity of stripe-ordered $La_{15/8}Ba_{1/8}CuO_4$ (LBCO) [12] *quantitatively* [17]. Qualitatively similar results are obtained by considering coupled dimers [18] or by starting from a Néel state [19,20]. Approaches breaking the spin symmetry imply optical branches [19–21].

We consider a spin-only model of undoped two-leg $S = \frac{1}{2}$ ladders separated from each other by hole-rich

*Corresponding author. Tel.: +49 221 470 3481; fax: +49 221 470 5159.
E-mail address: gu@thp.uni-koeln.de (G.S. Uhrig).

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bond-centered stripes (cf. Fig. 1a in Ref. [17]). Such a spin-only model certainly provides a useful description if the charge excitations are gapped. In the metallic stripe phase, the charge degrees of freedom will cause a certain damping of the magnetic excitations, but recent results indicate that this damping does not change the main physics [21]. The Hamiltonian for a single ladder reads

$$H = \sum_i \left[J_\perp \mathbf{S}_i^{\mathrm{L}} \cdot \mathbf{S}_i^{\mathrm{R}} + J_\parallel \left(\mathbf{S}_i^{\mathrm{L}} \cdot \mathbf{S}_{i+1}^{\mathrm{L}} + \mathbf{S}_i^{\mathrm{R}} \cdot \mathbf{S}_{i+1}^{\mathrm{R}} \right) \right] + H_{\mathrm{cyc}},$$

where i labels the rungs and R, L the legs. We use $J = J_\parallel = J_\perp$ since the system is derived from a square lattice. Inclusion of the cyclic exchange

$$H_{\mathrm{cyc}} = J_{\mathrm{cyc}} \sum_i \left[\left(\mathbf{S}_i^{\mathrm{L}} \cdot \mathbf{S}_i^{\mathrm{R}} \right) \left(\mathbf{S}_{i+1}^{\mathrm{L}} \cdot \mathbf{S}_{i+1}^{\mathrm{R}} \right) + \left(\mathbf{S}_i^{\mathrm{L}} \cdot \mathbf{S}_{i+1}^{\mathrm{L}} \right) \left(\mathbf{S}_i^{\mathrm{R}} \cdot \mathbf{S}_{i+1}^{\mathrm{R}} \right) - \left(\mathbf{S}_i^{\mathrm{L}} \cdot \mathbf{S}_{i+1}^{\mathrm{R}} \right) \left(\mathbf{S}_{i+1}^{\mathrm{L}} \cdot \mathbf{S}_i^{\mathrm{R}} \right) \right]$$

is justified both from first principles, e.g. Ref. [22], and phenomenologically, e.g. Ref. [23]. The established size is $x_{\mathrm{cyc}} = J_{\mathrm{cyc}}/J = 0.20$–$0.25$, which is important for quantitative agreement [17]. The ladders are coupled *ferromagnetically* between one another by $J' < 0$ because the effective superexchange via a strongly doped stripe prefers parallel alignment. This ferromagnetic coupling shifts the minima of the dispersion away from $\mathbf{Q}_{\mathrm{AF}}$ thus leading to incommensurate satellites [17].

The effective model for isolated ladders has been obtained previously [16] by a continuous unitary transformation. The elementary $S = 1$ excitations are called triplons [24]. The ladders are coupled among themselves by J' via a Bogoliubov transformation. It is only at this last step that the hard-core repulsion is neglected [17].

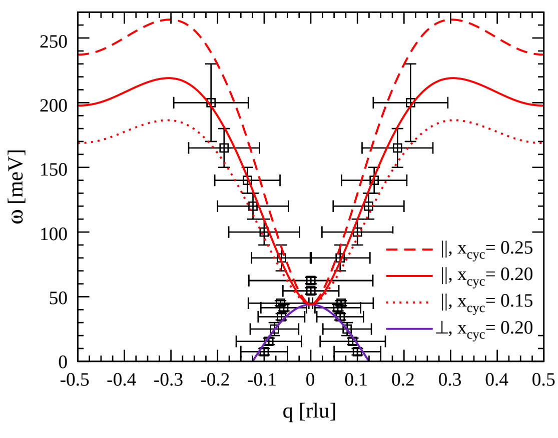

Fig. 1. Triplon dispersion; q is the distance from $\mathbf{Q}_{\mathrm{AF}}$. Symbols with error bars are INS data for LBCO [12]. Theoretical curves for $(x_{\mathrm{cyc}}, J[\mathrm{meV}], J'/J) = (0.15, 102, -0.098)$; $(0.20, 127, -0.072)$ and $(0.25, 162, -0.051)$ [17]. Dispersion parallel (perpendicular) to the ladders is denoted $\parallel$ ($\perp$). Below the resonance mode curves for different x_{cyc} are indistinguishable.

In Ref. [17] we compared the momentum dependence in constant energy slices and the frequency dependence of the momentum-integrated structure factor $S(\omega)$ with the INS data of stripe-ordered LBCO [12]. In Fig. 1 we show that the same parameters determined before [17] to describe $S(\omega)$ yield also an excellent description of the dispersion. In particular the data for $x_{\mathrm{cyc}} = 0.2$ agree very well over the full energy range. This strongly supports coupled ladders as model for the magnetic excitations in the stripe phase. The relatively large experimental error bars, however, still leave room for possible other features like a local 'roton'-minimum [21]. Certainly, further progress in experiment will settle this question.

An essential issue is how far the magnetic excitations of the stripe phase and of the superconducting state are related to each other. The main features observed in the superconducting phase—the resonance mode, the downward dispersion below the resonance and the upward dispersion above [6–9,11]—are generic features of our model [17]. In underdoped $YBa_2Cu_3O_{7-\delta}$ ($YBCO_{7-\delta}$), the observation of incommensurate scattering below the resonance has been interpreted as a signature of stripe formation [8–10]. The new experimental results for underdoped $YBCO_{6.6}$ [11] are stunningly similar to the data of stripe-ordered LBCO [12] over a broad energy range.

Fig. 2 displays the results of our model for parameters pertaining to $YBCO_{6.6}$ [11]. We stick to $x_{\mathrm{cyc}} = 0.2$ and determine $J = 114\,\mathrm{meV}$ and $J'/J = -0.035$ via the experimental values for the energy of the saddle point (i.e. the resonance) $\omega_{\mathrm{r}} = 34\,\mathrm{meV}$ and the spin gap $\Delta = 20\,\mathrm{meV}$ [25]. We neglect the bilayer structure of YBCO, since the small bilayer coupling of $\approx 0.1J$ [26] will not change the result for the acoustic (odd) modes qualitatively.

On the one hand, neglecting the charge degrees of freedom appears to be a much more severe shortcoming in superconducting YBCO than in stripe-ordered LBCO. On the other hand, the use of the Bogoliubov transformation for the interladder hopping and the concomitant omission of the hard-core constraint is even better justified in YBCO because of the finite spin gap and the smaller value of $J'/J = -0.035$. It is not astounding that J' varies from system to system. It is an effective parameter which depends on the properties of the charges like the doping level, the size of the charge gap and the nature of the charge order.

Fig. 2 agrees surprisingly well with the INS data of $YBCO_{6.6}$ [11]. The resonance mode at ω_{r} and the positions of the four incommensurate peaks below and above ω_{r} are reproduced very well. The general agreement strongly supports the underlying assumption

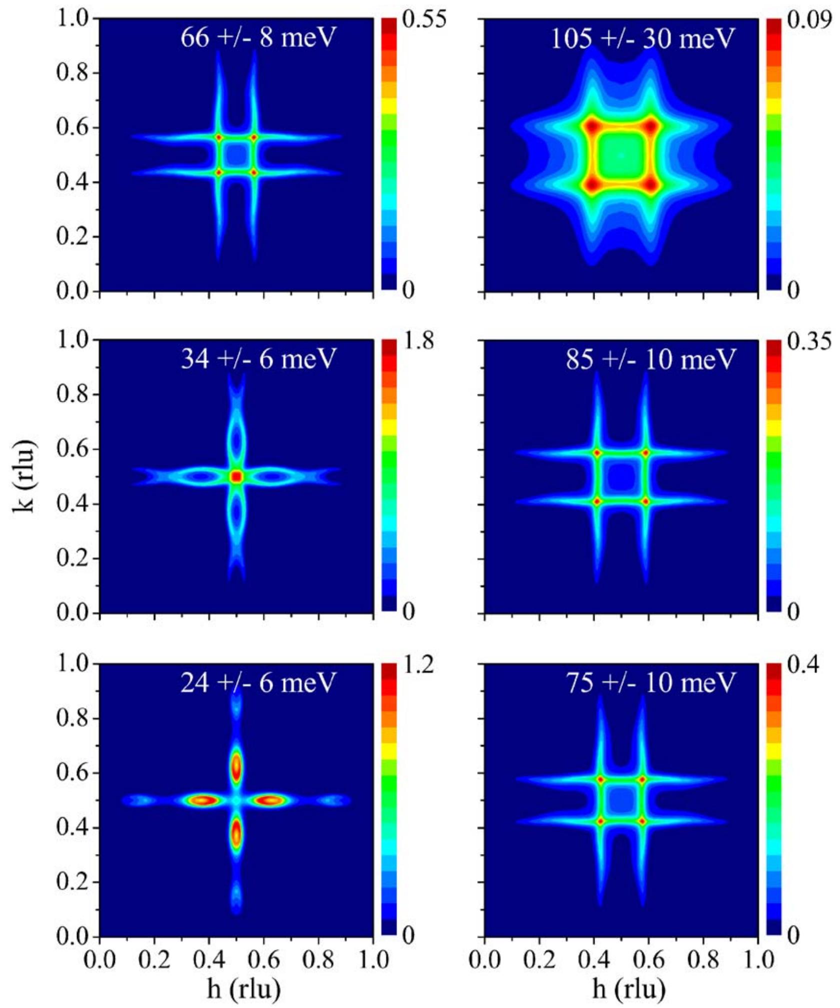

Fig. 2. Constant-energy slices for the indicated energies and resolutions from coupled ladders (superposition of vertical and horizontal stripes) for $x_{\mathrm{cyc}} = 0.2, J = 114\,\mathrm{meV}, J' = -0.035J$ [17]; to be compared with INS data of $\mathrm{YBCO}_{6.6}$ [11].

that the magnetic excitations can be described by coupled two-leg spin ladders.

A central yet unresolved issue is the domain structure. A single-domain stripe phase gives rise to two low-energy satellites. The experimentally observed four peaks require the existence of different domains. On the one hand, INS data on a sample where one kind of domain dominates [27] support an interpretation in terms of one-dimensional (1D) stripes. Recent STM data [28], on the other hand, do not find 1D structures but checkerboard-like patterns at the surface. The clear prediction of our model for the signature of single-domain stripes and ladders is depicted in Fig. 3 for the same parameters as in Fig. 2. Below $\omega_{\mathrm{r}} = 34\,\mathrm{meV}$, only two satellite peaks are present. Above ω_{r}, there are two elongated features with the intensity peaking at their centers. The positions of the maximum intensity rotate by 90° around $\mathbf{Q}_{\mathrm{AF}}$ on sweeping through ω_{r}, in contrast to the rotation by 45° observed in multi-domain samples. The shape and orientation of the features above ω_{r} do not depend strongly on the energy, in contrast to the result for a spin-symmetry broken phase of the Hubbard model [21]. To find structures like the ones in Fig. 3 would be the 'smoking gun' of quasi-1D spin physics. Alternatively, for short-range stripe correlations one will observe patterns as in Fig. 2. At present, there is no theoretical prediction for INS how to distinguish short-range stripe correlations from the superposition of different domains of long-range stripes.

In conclusion, a model of coupled spin ladders with established coupling parameters leads to very good agreement with neutron data. The predictions made will

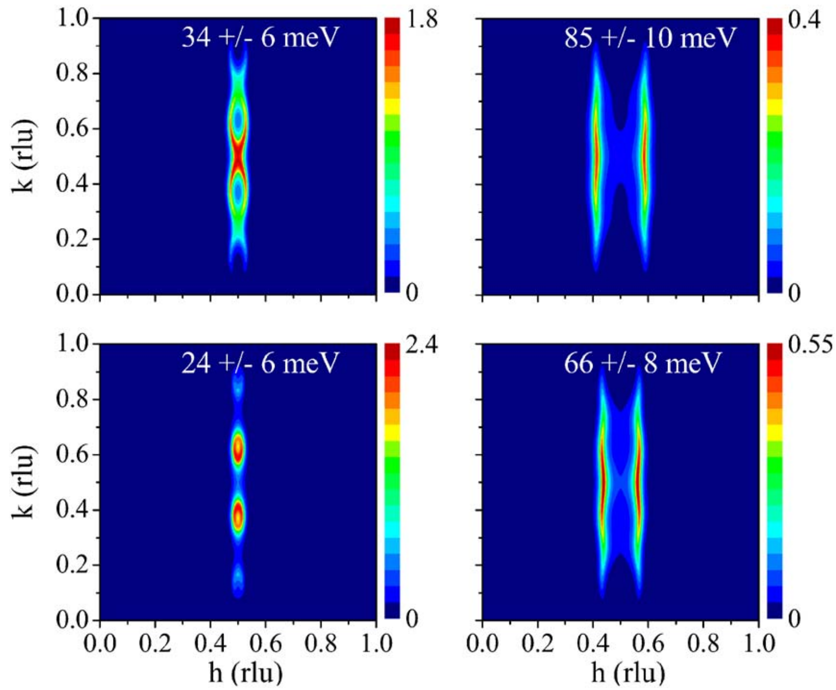

Fig. 3. Like Fig. 2 for a single-domain stripe phase.

help to distinguish stripes from checkerboard patterns or other scenarios.

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