Resonant magnetic mode in superconducting 2-leg ladders

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The spin dynamics of a doped 2-leg spin ladder is investigated by numerical techniques. We show that a hole pair-magnon boundstate evolves at finite hole doping into a sharp magnetic excitation below the two-particle continuum. This is supported by a field theory argument based on a SO(6)-symmetric ladder. Similarities and differences with the resonant mode of the high-Tc cuprates are discussed.

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Spin ladders materials are built from weakly coupled ladder units consisting of chain sub-units of spins S=1/2 (so-called “legs”) connected via some “rung” couplings and exhibit numerous fascinating and intriguing properties [1]. Among them, the role of the parity of the number of legs is remarkable: only ladders with an even number of legs exhibit a spin gap (ie a finite energy scale for triplet excitations) as seen from different characteristic behaviors of the spin susceptibility observed in SrCu$_2$O$_3$ and SrCu$_2$O$_5$ [2], typical 2-leg and 3-leg compounds respectively.

Besides exotic experimental properties, spin ladders are of special interest for theorists as well, especially the simple 2-leg ladder: indeed, it is believed that its ground state (GS) is a close realization of the Resonating Valence Bond (RVB) state proposed by Anderson [3] in the context of high-Tc superconductivity. The striking difference between “even” and “odd” ladders mentioned above can naturally be explained in this simple picture since pairing nearest neighbor (NN) spins into spin singlets is more easily realized on rungs with an even number of sites. While the generic two dimensional (2D) Mott insulator (for one electron per site) is antiferromagnetic (AF) and may evolve into an RVB state only at finite doping, the 2-leg spin ladder exhibits a finite spin correlation length. It is therefore an ideal system to investigate doping into the RVB-like spin liquid [4] leading to d_{x^2-y^2}-like pairing [5]. As a matter of fact, pressure was shown to induced superconductivity in the intrinsically doped Sr$_2$Ca$_{12}$Cu$_{24}$O$_{41+\delta}$ ladder material [6] hence bridging the apparent gap between 2-leg ladder and layer-based cuprates.

In this Letter, we investigate the spin dynamics of a 2-leg spin ladder doped with mobile holes. In 2D superconducting cuprates, a resonant mode at an energy around 40 meV was observed by Inelastic Neutron Scattering (INS) [7, 8]. This mode was shown to be quite sharp both in energy and in momentum space (centered around the AF wavevector) and its observation seems to be directly linked to the appearance of superconductivity. Anomalous spectral lineshape in photoemission experiments was also interpreted as the effect of a coupling of the quasiparticles to a collective mode [9] related to the pairing interaction. On the other hand, in ladders, the spin dynamics remains largely to be explored. We believe that a closer inspection, both experimentally and theoretically, of the low energy spin excitations in such a basic system will provide insights into the mechanism of pairing mediated by spin fluctuations in the 2D high-Tc analogs. In this study, combining different techniques, we provide evidences of a new magnetic mode in the two ladder system and discuss similarities and differences with the resonant mode of the 2D cuprates.

We shall consider here a generic 2-leg t-J ladder,

$$\mathcal{H} = J_{\text{leg}} \sum_{i,a} \mathbf{S}_{i,a} \cdot \mathbf{S}_{i+1,a} + J_{\text{rung}} \sum_{i} \mathbf{S}_{i,1} \cdot \mathbf{S}_{i,2} + t_{\text{leg}} \sum_{i,a} c_{i,a}^{\dagger} c_{i+1,a} + t_{\text{rung}} \sum_{i,a} c_{i,a}^{\dagger} c_{i,a}^{\dagger+1} + H.C.,$$

where $c_{i,a}$ are projected hole operators and $a (=1, 2)$
labels the two legs of the ladder. Isotropic couplings, \( t_{\text{leg}} = t_{\text{rung}} = t \) and \( J_{\text{leg}} = J_{\text{rung}} = J \), will be of interest here. A value like \( J = 0.4 \) (in set to 1) and dopings between 0.1 and 0.2 are typical of the above-mentioned superconducting ladder materials. In this regime, the ladder belongs to the Luther-Emery class with a single zero-energy charge mode \[11\] and the dominant superconducting correlations exhibit power-law decay \[12\].

Prior to the investigation of the spin dynamics at finite doping it is very instructive to first consider a simpler case consisting of two holes (forming a hole pair) immersed into an infinite (or very large) ladder. Following previous investigations \[11\] and using finite size extrapolations \[13\], we have tentatively sketched the triplet excitation spectrum in Fig. 1. Apart from the two expected types of excitations associated with (i) the dissociation of a hole pair into two separate holes leading to a two-hole continuum and to (ii) magnon-hole pair scattering states, a boundstate of the hole pair with a magnon state (see \[13\] for details about the boundstate wavefunction) can also be clearly identified. How this remarkable feature evolves at finite doping is the crucial issue we would like to address hereafter.

For that purpose, the dynamic spin structure factor

\[
S(q, \omega) = -\frac{1}{\pi} \text{Im}[\langle \Psi_0 | S^\alpha_q \omega + E_0 + i \eta - H S^\alpha_q | \Psi_0 \rangle],
\]

is computed by Lanczos Exact Diagonalisations (ED) of \( 2 \times L \) periodic ladders of size \( L = 12 \) supplemented by a continued-fraction technique. Typical results shown in Fig. 2 bear similarities with the case of 2 holes in Fig. 1. First, in the vicinity of momentum \((\pi, \pi)\) a strong low energy incommensurate peak is observed well separated from the higher energy excitations. Its energy rises when \( q \rightarrow (\pi, \pi) \) where it becomes damped. Assuming single-particle excitations \[11\] at momenta \( \pm k_{F,b} \) \((b = 1, 2\) for bonding and anti-bonding branches, \( k_{F,b} \sim \pi/2\)), this feature can naturally be assigned to a \( k_{F_1} + k_{F_2} = \pi(1 - n_h) \) spin density wave (SDW) type of excitations. For vanishing doping, \( k_{F_1} + k_{F_2} \rightarrow \pi \), corresponding to the momentum of the hole-pair magnon boundstate. Note also that the boundstate in Fig. 1 has a minimum energy of 0.34J \( \simeq 0.14 \) close to the energy of the incommensurate peak in the right panel of Fig. 2. Furthermore, the lowest triplet excitations at \( q_y = 0 \) might be interpreted as the sum of two single-particle excitations with momenta around \( \pm (k_{F,1}, 0) \) or around \( \pm (k_{F,2}, \pi) \) giving excitations with total longitudinal momentum 0 or \( 2k_{F,1} \simeq 2k_{F,2} \). In that case, the peaks in the left panel of Fig. 2 would signal the edge of this 2-particle continuum (or a new boundstate with small binding energy). Note that the lowest excitation energy at \( q_y = 0 \) is indeed close to that of Fig. 1.

From the similarities between Figs. 1 and 2 it is tempting to interpret the \( q_y = \pi \) feature as a collective mode emerging below the continuum. However, the ED data do not provide enough energy (and momentum) resolution to investigate the shape of the spectral weight in more details. For this purpose, the bosonized ladder model with SO(6)~SU(4) symmetry \[16\] \[17\] is of special interest. Schulz \[10\] first pointed out the existence in this model of kink boundstates (Majorana fermions) related to \((2k_F, \pi)\) spin density waves. Calling \( M \) the mass of elementary kinks \[15\], the mass of these boundstates is \( M' = M\sqrt{2} \) and the continuum starts at \( 2M \). We believe that the boundstate is, in fact, robust and more generic and that the above feature seen in the numerics of the t-J ladder (with lower symmetry than SO(6)) is a signature of it. This conjecture is partially supported by the fact that the renormalization group flow of the bosonized ladder model is attracted to the direction of SO(6) symmetry \[16\]. Let us briefly summarize the derivation of the low energy spin dynamics within the SO(6) field-theoretic scheme. In bosonisation, the SDW operator at \( q_x \sim 2k_F \) \((= k_{F,1} + k_{F,2}) \) and \( q_y = \pi \) is written as \( O_{\text{SDW}} = e^{i\phi_{+}(x)}N(x) \). The correlation function \( \langle N(x, \tau)N(x) \rangle \) can be decomposed into \[19\] \[20\]:

\[
\int d\theta \langle 0 | N | B(\theta) \rangle^2 \exp(M'(i \frac{x}{v} \sin \theta - \tau \cosh \theta) + \int d\theta_1 d\theta_2 \langle 0 | N | A(\theta_1)A(\theta_2) \rangle^2 \exp(i \frac{Mx}{v} (\sin \theta_1 + \sin \theta_2) - M\tau(\cosh \theta_1 + \cosh \theta_2)) + ...
\]

where \( | B(\theta) \rangle \) is a state which contains a single Ma-
jorana fermion of rapidity \( \theta \), \( |A(\theta_1)A(\theta_2)| \) a state with 2 kinks of rapidity \( \theta_1, \theta_2 \). Since Lorentz invariance \( [9] \) makes \( \langle 0|N|B(\theta) \rangle \) independent of \( \theta \), the contribution of the Majorana fermion to the correlation function \( [21] \) becomes \( \langle N(x, \tau)N(x) \rangle _{\text{fermion}} = K_0(M'r/v) \) with \( r = \sqrt{x^2 + (v \tau)^2} \). In real space, the correlation function \( \langle O_{SDW}(x, \tau)O_{SDW}(0,0) \rangle \) is given by \( (1/r)^{K_{\rho+}/2} K_0(M'r/v) \) where \( K_{\rho+} \) is a non-universal constant whose inverse is the exponent of the power law decay of the superconducting correlations. The Fourier transform of this correlator involves a Weber Schaefflin integral \( [22] \) and, eventually, one gets for the dynamic susceptibility: \( \chi_{SDW}(q, \omega) \sim F_1(1 - K_{\rho+}/4, 1 - K_{\rho+}/4; 1; (\omega^2 - (vq)^2)/(M')^2 + ...) \), where \( F_1 \) is the usual hypergeometric function and \( q = q_x - 2k_F \). At the onset, the imaginary part of \( \chi_{SDW}(q, \omega) \sim S(q, \omega) \) for \( q = (2k_F + q, \pi) \), exhibits a power-law singularity instead of a \( \delta \)-function as seen in Fig. 3. In the vicinity of the onset one gets, \( \chi_{SDW}(q, \omega) \sim 1/(\omega^2 - (vq)^2 - M^2)^{1-K_{\rho+}/2} \). Physically, it means that, in e.g. an inelastic neutron scattering (INS) experiment, holons can be excited together with the triplet boundstate, the initial neutron momentum being distributed among all the constituents. A complete characterization of such a singularity is beyond the ability of present day numerical techniques but the results of Fig. 2 shown also in Fig. 3 revealing a low energy pole with a large fraction of the spectral weight accompanied by a few tiny peaks are consistent with such a scenario.

To complete our study of the spin dynamics, we have combined complementary Density Matrix Renormalisation group (DMRG) and Contractor Renormalisation (CORE) methods \( [14] \) supplemented by finite size analysis to extract the collective mode energy. In the CORE method the ladder is decomposed into plaquette units and an effective interaction between adjacent plaquettes is constructed. In the bosonic version (B), on each plaquette, only the lowest energy undoped singlet (vacuum), triplet state (mapped as a triplet boson) and hole pair GS (mapped as a pair boson) are retained while in the more involved boson-fermion (BF) version the lowest one-hole doped plaquette states are also included. Typically, the effective B-hamiltonian is simply written as a sum of a simple bilinear kinetic term for the bosons and a quartic interaction. DMRG and CORE computations involving open and periodic boundary conditions respectively give rise to different types of finite size corrections as seen in Fig. 4(a). The resulting extrapolations of the lowest triplet excitation are shown in Fig. 4(b) as the function of the hole doping. All extrapolations with a fixed number of 2 holes agree very well with each other and, as mentioned in Refs. \$13 \$14, the spin excitation in the limit of vanishing doping is not continuous due to the binding of the magnon with a hole pair. The main result shown by Fig. 4(b) is that the energy of the magnon-hole pair state evolves continuously, at finite doping, into the magnetic mode energy previously studied. Note that the CORE approaches (both B & BF versions) remain very accurate for hole doping below 10% but the bosonic version fails for larger doping. Physically, this signals that the pair size becomes too large for the spin-singlet and spin-triplet pair wavefunctions to be correctly captured by the small subset of states kept here (unless longer range effective interactions are included).

Apart from singularities in \( S(q, \omega) \), the spin-triplet mode is expected to have effects on the spectral functions \( \chi \). We have re-examined the tunnelling density
of states first reported in Ref. [11, 15] looking closely at the low energy region. As expected, the data shown in Fig. 4 fulfill sum rules and show a quasiparticle gap $\Delta_{QP}$ which should correspond to the kink energy $M$ of the SO(6) model. After enlarging the low energy region one can see two sub-peaks at an energy $\Omega \sim 0.1$ from the gap edge. This could signal scattering of the hole or electron quasiparticle by a collective mode. Note that the characteristic energy $\Omega$ is indeed close to the lowest spin-triplet energy reported before (see Fig. 2).

It is interesting to compare our results to the behavior of the resonant spin excitation observed in the 2D copper oxide superconductors by Inelastic Neutron Scattering [10, 11, 12]. Remarkably, this mode was observed both in under-, optimally and over-doped materials and only below the superconducting transition temperature, $T_C$ and approximately scales with $T_C$. While the excitation in the 2D cuprates occurs with wavevector $(\pi, \pi)$, an incommensurate mode is found in the ladder. Although in 2D the mode could be interpreted as a soft mode signaling the proximity of a magnetic instability [20], its nature should be different in the ladder which originates from a different class of “parent compound”, namely a spin liquid rather than a 2D ordered AF. Note however that, in 2D, lower energy incommensurate spin fluctuations have also been seen experimentally pointing towards the existence of a dispersive spin 1-collective mode [21], a feature that might well be related to our finding in the ladder.

To conclude, by investigating the spin dynamics of a doped 2-leg spin ladder, we have shown that a hole pair-magnon boundstate evolves into a sharp magnetic excitation at finite hole doping. Such a feature is reproduced by a SO(6) field theory which gives a power-law singularity at the mode energy. Analogies with the resonant mode of the high-$T_c$ cuprates have been discussed.

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