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# Spin dynamics of the S = 1/2 antiferromagnetic zig-zag ladder with anisotropy

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## Abstract

We use exact diagonalization and the modified Lanczos method to study the finite-energy and finite-momentum spectral weight of the longitudinal and transverse spin excitations of the anisotropic zig-zag ladder. We find that the spin excitations form continua of gapless or gapped spinons in the different regions of the phase diagram. The results obtained are consistent with a picture previously proposed that in the anisotropic case there is a transition from a gapped regime to a gapless regime, for small interchain coupling. In the gapless regime we find a sharp low-energy peak in the structure function for the transverse spin excitations, consistent with a finite stiffness.

(Some figures in this article are in colour only in the electronic version)

#### 1. Introduction

Recently [1] it has been suggested that a two-dimensional spin system,  $Cs_2CuCl_4$ , has an excitation spectrum that can be described, similarly to the one-dimensional case [2], by a continuum originated from pairs of spin-1/2 spinons. The standard one-dimensional Heisenberg model is known to have fractional states where the usual spin-1 magnons are replaced by pairs of deconfined spin-1/2 topological excitations called spinons [3]. The characteristic low-excitation-energy coherent peaks that appear in the dynamical susceptibility are in this case replaced by a continuum. This property has been verified experimentally for several quasi-one-dimensional spin-1/2 systems such as CPC [4],  $KCuF_3$  [5,6] and copper benzoate [7], where a description in terms of a nearest-neighbour Heisenberg model is assumed to apply.

Real materials are, however, neither strictly one dimensional nor are the interactions of the simple Heisenberg nearest-neighbour form. Originally  $Cs_2CuCl_4$  was taken as a quasione-dimensional system [8] but a more careful estimate of the inter-chain parameters revealed that they are of the same order as the intrachain interactions [1]. The interlayer coupling is estimated to be two orders of magnitude smaller, implying that the system is essentially two dimensional. It forms a triangular lattice in the copper (Cu<sup>2+</sup>, S = 1/2) planes and constitutes therefore a frustrated system.

Frustrated systems have attracted considerable interest. Using a large-N bosonic expansion it has been predicted [9] that the presence of frustration may counteract the staggered fields responsible for confinement [10] and lead to deconfinement of the spinons. In a non-frustrated system it is known that the low-energy modes are spin-1 magnons. The presence of frustration leads to a non-collinear order parameter [11], which can be parametrized by three real scalar numbers. The representation of the spin operators in terms of bosonic operators contains a hidden internal gauge symmetry under which the scalar link fields transform either as charge +2 or charge +1 scalars [9]. It was predicted a long time ago that if the charge +2 scalars condense into a Higgs phase [12] then the unit charges are not confined and the spinons remain free [11]. However the Higgs phase is just one of the possible phases predicted to occur in the frustrated two-dimensional lattice. The Cs<sub>2</sub>CuCl<sub>4</sub> system provides a first experimental example of a two-dimensional system with a spectrum consistent with the existence of spinons.

One may think of a simpler system such as the zig-zag ladder, where only two chains are coupled, and study the excitation spectrum of this system as a first step towards understanding the two-dimensional triangular lattice obtained in the limit when several ladders are coupled to each other. In usual spin ladders an infinitesimal coupling between chains leads to a behaviour qualitatively different from the one-dimensional case. Therefore it is interesting to see whether in the case of the zig-zag ladder there is a qualitative difference from the single-chain case. It has been found before that if the next-nearest-neighbour (nnn) interaction is small enough the system still behaves qualitatively as the single-chain case. Therefore it seems reasonable that for small couplings we might find similar features characteristic of the single chain, in particular a spinon-originated spectrum. The main question to be answered is what happens for large couplings where the role of the nnn coupling is important. We shall show that indeed for all couplings a spinon description holds. A direct comparison with the experimental results for Cs<sub>2</sub>CuCl<sub>4</sub> would require a full two-dimensional calculation but our results for the zig-zag ladder give a first indication that the nnn coupling does not lead to a coherent energy spectrum.

In the context of a frustrated two-leg ladder similar to the zig-zag ladder [13], it has been shown that the spinons survive as the elementary excitations in a spontaneously dimerized ground state but become massive. A local  $Z_2$  symmetry related to independent translations by one lattice spacing on each chain is spontaneously broken and leads to a non-vanishing dimerization for strong enough frustration. This symmetry breaking leads to kinks as elementary excitations which are massive. These kinks have been shown to have S = 1/2 and therefore at least two must be created.

In general if a term removes explicitly the  $Z_2$  degeneracy between the two dimerized ground states this leads to soliton confinement. An example is to introduce explicit dimerization in the Hamiltonian. The role of explicit dimerization has also been addressed in the context of spin–Peierls systems such as CuGeO<sub>3</sub> [14], NaV<sub>2</sub>O<sub>3</sub> [15] or Cu(NO<sub>3</sub>)<sub>2</sub>2.5D<sub>2</sub>O [16]. The excitation spectrum of these systems is however considerably different from the chains without dimerization. The spectrum is gapped and the lowest-energy excitations are coherent spin-1 magnon peaks [17] that separate from the continuum that appears at higher energies. The spectrum of these systems is actually closer to integer spin chains [18] or to spin ladders [19]. The effects of explicit dimerization have received renewed attention recently [20].

Another source of interest in the zig-zag ladder is that it has been proposed that in the anisotropic case incommensurate quasi-long-range spin correlations should be observed. Also a gapless chiral phase has been predicted to occur [21]. In this work we focus our attention on the combined effects of an nnn frustrating interaction and of anisotropy. In a two-dimensional non-frustrating system the spectrum is coherent and composed of magnons. The addition of

frustrating terms may lead to deconfined spinons. In the zig-zag ladder when the nnn frustrating coupling is absent the system has a spectrum determined by gapless spinons (this is the case of the simple Heisenberg chain). Adding frustration it is expected that the spinons will remain deconfined. In the isotropic case where the effect of the nnn coupling is to dimerize the spinons are massive at sufficiently strong nnn coupling. In the anisotropic case at strong enough nnn couplings we expect the system to have a transition from the intermediate dimer phase to a gapless phase where we expect the deconfined spinons to be massless.

## 2. Hamiltonian

The anisotropic zigzag ladder is defined by the Hamiltonian

$$H = \frac{1}{2}J_1^{XY} \sum_i \left(S_i^+ S_{i+1}^- + S_i^- S_{i+1}^+\right) + J_1^z \sum_i S_i^z S_{i+1}^z + \frac{1}{2}J_2^{XY} \sum_i \left(S_i^+ S_{i+2}^- + S_i^- S_{i+2}^+\right) + J_2^z \sum_i S_i^z S_{i+2}^z.$$
(1)

The spin operators refer to spin S = 1/2 states, while the summation i = 1, ..., N runs along the 'rib' of the zig-zag ladder. We shall parametrize the interactions by the coupling parameter  $j = J_2^{XY}/J_1^{XY}$  and by the anisotropy parameter  $J_1^z/J_1^{XY} = \Delta = J_2^z/J_2^{XY}$ . (The isotropic case reduces to  $j = J_2/J_1$  and  $\Delta = 1$ .) We shall set  $J_1^{XY} = 1$  henceforth. The nearest-neighbour Heisenberg chain with anisotropy corresponds to both the weak-coupling  $(J_1 = 0)$  and the strong-coupling  $(J_2 = 0)$  limits of the zig-zag ladder. The spectrum is gapless for the case of XY anisotropy,  $|\Delta| \leq 1$ , as shown by the Bethe ansatz [22]. The excitation spectrum consists of spin-1/2 particles dubbed spinons. Since flipping one spin represents a spin-1 excitation, the spinons can only be created in pairs. Therefore the conventional spin-1 magnons are deconfined into spin-1/2 spinons that propagate incoherently.

The isotropic case has been studied before [23-28] as a function of the coupling parameter,  $j = J_2/J_1$ . As j increases, the system goes from gapless (single chain) to a dimer phase and then to a spiral phase, where the structure factor has a maximum at a momentum  $\pi/2 < q < \pi$ . The system has a spin gap in these last two phases, and it therefore only displays shortrange order. In the limit where the intra-chain interaction is much larger than the interchain interaction  $(i \rightarrow \infty)$  the two chains decouple and a gapless single-chain behaviour is recovered. It has been argued that this only happens, strictly speaking, at  $i = \infty$ : the spin gap becomes exponentially small as j grows, but it remains non-vanishing [27]. Recently, on the other hand, it has been proposed that incommensurate quasi-long-range spin correlations should be observed if easy-plane (XY) anisotropy is included in the zigzag ladder [21]. This is argued to be due to the presence of a 'twist' term that results from the inter-chain interaction. It has been proposed that there is one gapless mode and one mode with a gap in the regime of strong XY anisotropy in the inter-chain coupling. Another prediction of this work is the existence of spontaneous local spin currents. This, however, has been refuted in [29]. Also, other recent numerical work [30] has failed to confirm the gapless nature of the ground state in the anisotropic XY case at weak interchain coupling. Recent density matrix renormalization group (DMRG) results [31] suggest, however, that the zig-zag ladder does indeed show a gapless chiral phase as predicted in [21].

Also, recently an analysis of the exact properties of such finite systems was carried out, looking at various correlation functions and the structure of the spectrum in both the isotropic and the anisotropic cases [32]. The spin stiffness of the zig-zag ladder was calculated, and evidence was found for a gapless regime at weak coupling that survives the thermodynamic limit in the case of *XY* anisotropy. This was also concluded looking at the level crossings

to detect the phase transition between the two regimes [32], using a previously proposed procedure to detect the dimer transition at strong interchain coupling [23]. The same method was also recently used in [33].

In this work we shall study the structure function and the spectral weight of the spin excitations both for the longitudinal and the transverse correlations. Our results are consistent with previous conclusions that there is a transition to a gapless regime at weak coupling if anisotropy is present. The results indicate a continuum of gapless excitations in the transverse correlations in the *XY* case, and a continuum of gapped excitations in the isotropic case.

#### 3. Spectral weight

The structure function is defined by the overlap of two states coupled either by the longitudinal or the transverse spin operator [3],

$$S_{\mu\nu}(q,\omega) = \frac{1}{N} \sum_{l,R} e^{iqR} \int_{-\infty}^{\infty} dt \, e^{i\omega t} \langle S_l^{\mu}(t) S_{l+R}^{\nu}(0) \rangle \tag{2}$$

where  $\mu$  and  $\nu$  are Cartesian components. At zero temperature we obtain therefore

$$S_{\mu\mu}(q,\omega) = \sum_{\lambda} M^{\mu}_{\lambda} \delta(\omega + E_{\rm G} - E_{\lambda}) \delta(q + k_0 - k_{\lambda})$$
(3)

where  $E_G$  is the ground-state energy,  $E_{\lambda}$  is the energy of an excited state,  $\omega$  is the excitation energy (energy difference to the ground state) and q is its momentum (momentum difference to the momentum of the ground state  $k_0$ ) and the spectral weight is defined by

$$M^{\mu}_{\lambda} = 2\pi \left| \langle G | S^{\mu}(q) | \lambda \rangle \right|^2 \tag{4}$$

where  $S^{\mu}(q)$  is the Fourier transform of the spin operator. We shall calculate the structure functions  $S_{+-}(q, \omega)$  and  $S_{zz}(q, \omega)$  which probe the transverse and the longitudinal spin excitations, respectively.

The single-chain case was studied before by both the Bethe ansatz [2] and using numerical diagonalization of small systems [3]. The continuum of excitations is contained in the thermodynamic limit between two limiting functions of q: the bottom curve is the single-spinon dispersion,  $\epsilon_l(q)$ , and the upper one is the maximum energy resulting from the combined effect of two spinons,  $\epsilon_u(q)$ . In the isotropic case ( $\Delta = 1$ ) the lines are defined by

$$\frac{\epsilon_l(q)}{J_1} = \frac{\pi}{2} |\sin(q)|$$

$$\frac{\epsilon_u(q)}{J_1} = \pi \left| \sin\left(\frac{q}{2}\right) \right|$$
(5)

and in the *XY* case ( $\Delta = 0$ ) they are defined by

$$\frac{\epsilon_l(q)}{J_1^{XY}} = |\sin(q)|$$

$$\frac{\epsilon_u(q)}{J_1^{XY}} = 2\left|\sin\left(\frac{q}{2}\right)\right|.$$
(6)

In the *XY* case the longitudinal structure function can be calculated exactly [34] since this system is equivalent to free spinless fermions and it is given by [3]

$$S_{zz}(q,\omega) = 2 \frac{\Theta(\omega - \sin(q))\Theta(2\sin(q/2) - \omega)}{\sqrt{4\sin^2(q/2) - \omega^2}}.$$
(7)

In the isotropic case there is no exact solution but Müller *et al* [3] proposed an ansatz that fits very well both numerical results for small systems and various experimental results where a description in terms of a single chain is expected to hold. The Müller ansatz is

$$S_{zz}(q,\omega) = \frac{A}{\sqrt{\omega^2 - \epsilon_l^2(q)}} \Theta(\omega - \epsilon_l(q))\Theta(\epsilon_u(q) - \omega)$$
(8)

where  $\Theta$  is a step function and A a constant [35], [3]<sup>1</sup>. This function diverges at the lower boundary while in the XY case it diverges at the upper boundary<sup>2</sup>. At momentum  $\pi$  the divergence is stronger and it diverges as  $S_{zz} \sim \omega^{-1}$ .

In the thermodynamic limit the structure function equation (3) can be written as a product [3]

$$S_{\mu\mu}(q,\omega) = M^{\mu}(q,\omega)D(q,\omega)$$
<sup>(9)</sup>

where  $M^{\mu}(q, \omega)$  is the continuum limit of the spectral weight originating in the overlap equation (4) and  $D(q, \omega)$  is the density of states. In the isotropic and in the XY case the density of states is finite and nearly constant close to the low-energy threshold and it diverges at the upper threshold. On the other hand  $M^{\mu}(q, \omega)$  is constant in the XY case and it diverges at the lower threshold in the Heisenberg case. The structure function as a consequence diverges in the lower threshold for the Heisenberg chain and it diverges in the upper threshold in the XY case [3]. For any finite system the density of states is a set of delta functions at the excitation energies.

Using field theory it is also possible to determine the dependence of the transverse structure function close to the lower threshold. In the single-chain case the transverse function is given by [37]

$$S_{+-}(q,\omega) \sim \frac{1}{\left(\omega^2 - \epsilon_l^2(q)\right)^{3/4}} \qquad j = 0 \quad \Delta = 0$$
 (10)

and therefore

$$S_{+-}(\pi,\omega) \sim \omega^{-3/2}.$$
 (11)

However the finite-energy structure function is not known analytically.

The ladder case is more involved. We shall use exact diagonalization of finite systems together with the modified Lanczos method [36].

#### 4. Numerical results

Let us begin by recalling the quantum numbers of the ground state as a function of the size N for the S = 1/2 zig-zag antiferromagnet. Periodic boundary conditions are imposed throughout. The ground state is a spin singlet in general due to the antiferromagnetic interactions. The system has three well defined regimes, (a) strong coupling, (b) intermediate coupling and (c) weak coupling. Consider the isotropic case first. For strong enough coupling between chains,  $j = J_2/J_1 < 1/2$ , it has either momentum  $\pi$  for N = 4n + 2 or momentum 0 for N = 4n. For intermediate couplings (j > 1/2), on the other hand, the momentum oscillates between 0 and  $\pi$  as a function of the coupling parameter j and of the system size N [38]. There are several points along j in this regime where the corresponding energy levels for these two momentum

<sup>&</sup>lt;sup>1</sup> See also [35] where the exponent of the structure function for the Heisenberg chain was obtained using the Luttinger model analogy.

 $<sup>^{2}</sup>$  Note however that in the case of the *XY* chain the high-energy behaviour is not well described by the Luttinger model [35].

values cross. The ground state is degenerate at these points, and this is reflected by peaks in the dimer correlation function [32, 39]. Such level crossings grow in number as the system size grows, and this indicates that the two singlet states in question are in fact degenerate in the thermodynamic limit. By the Lieb–Schultz–Mattis theorem [40], this is consistent with a spin gap in the excitation spectrum that survives the thermodynamic limit in the weak-coupling regime j > 1/2.

The spectrum of the anisotropic S = 1/2 XXZ zig-zag ladder has also been studied previously in the strong-coupling regime up to the Majumdar–Ghosh line (0 < j < 1/2) [41]. A gapless regime occurs for XY anisotropy  $\Delta \leq 1$  and strong coupling  $j < j_{c1}(\Delta)$ ; an Ising antiferromagnet along the rib of the zig-zag that shows a spin gap in the excitation spectrum occurs for  $\Delta > 1$  and  $j < j_{c1}(\Delta)$ , and a dimer phase regime that also has a spin gap exists at  $j > j_{c1}(\Delta)$  and any  $\Delta$ . The line  $j = j_{c1}(\Delta)$  separates the gapless phase from the dimer phase for  $\Delta \leq 1$ , while it separates the dimer phase from the (Ising) Néel phase for  $\Delta > 1$ . The line at  $\Delta = 1$  and  $j < j_{c1}$  separates the XY gapless phase from the Ising phase.

It was found [32] that there is a transition from the gapped intermediate-coupling regime to a weak-coupling gapless regime. In the intermediate-coupling regime the two lowest states are two states with  $S_z = 0$ , of momenta  $k = 0, \pi$ . There is a line,  $j_{c2}(\Delta)$ , where the first excited state becomes a  $S_z = \pm 1, k = \pi/2$  state, signalling the doubling of the periodicity and leading to a gapless regime as confirmed from the spin stiffness tensor highest eigenvalue [32]. The curve  $j_{c2}(\Delta)$  shown in figure 4 of [32] separates a spin-gap (dimer) phase from a gapless phase at small interchain couplings. As expected, the value of  $j_{c2}$  grows near the isotropic point. (It should tend to  $j = \infty$  at  $\Delta = 1$  according to White and Affleck [27], but finite-size effects give a finite value.)

Let us now analyse the spectral weight equation (4) at various points in the phase diagram parametrized by j and  $\Delta$ . We shall focus our attention on two classes of parameters. We shall consider the isotropic case ( $\Delta = 1$ ) and the XY case ( $\Delta = 0$ ), varying in both cases the interchain coupling, j.

Let us begin with the single-chain case for both values of  $\Delta$  and let us consider the particular case N = 16. In figure 1 we show the lowest energy levels (taking the ground state as the zero of energy) for  $S_z = 0$  and 1 and a given momentum for the Heisenberg chain and the XY chain. In the Heisenberg case the states are organized into spin multiplets due to the SU(2) spin invariance. The ground state is a spin singlet with momentum zero. The first excited state is a spin triplet with momentum  $k = \pi$  and the next state is another spin singlet but with momentum  $k = \pi$ . In the  $\Delta = 0$  case the first excited state is now a state with  $S_z = 1$  and momentum  $k = \pi$  and the next state is fourfold degenerate with  $S_z = 0$  and momentum  $k = \pi/N$  or momentum  $k = \pi$ , or  $S_z = 2$  and the same momentum values [32].

The structure function  $S_{zz}$  only couples the ground state to states with  $S_z = 0$  and  $S_T = 1$ . On the other hand  $S_{+-}$  only couples the ground state to states with  $S_z = 1$  and  $S_T = 1$  ( $S_T$  is the total spin). In the isotropic case  $S_{+-}$  couples to a subset of the states probed by  $S_{zz}$  while in the anisotropic case the two functions probe different sets of states.

In figure 2(a) we show the spin excitations that contribute to  $S_{zz}(q, \omega)$  for N = 16 and for  $\Delta = 1$ . As mentioned above the spectral weight of the spin excitations decreases as we move away from the lower threshold. The states contained in the region defined by  $\epsilon_l(q)$  and  $\epsilon_u(q)$  have a considerable weight while those at higher energies have a much smaller weight [3]. The spectral weight of these higher states will vanish in the thermodynamic limit. Also other states contained in the continuum have very small weights. The continuum is therefore well defined by the set of states with highest spectral weight. In figure 2(b) we show the structure function for the Heisenberg chain. The delta functions at the excitation energies have been given a finite width in both frequency and momentum for better visualization.



Figure 1. Excitation energies from the exact diagonalization of an N = 16 chain as a function of momentum for  $S_z = 0$  and 1 for the Heisenberg chain and the *XY* chain.

In figure 3 we show the states with non-vanishing spectral weight for the longitudinal and the transverse structure functions for the XY chain. The longitudinal spectral weight is uniform inside the continuum defined by equations (6). The spectrum of the transverse excitations is however different. The lower spinon dispersion is well described by the single-spinon dispersion; particularly close to  $q = \pi$  the gap is already rather small for such a small system. At higher energies the spectral weight is considerably spread.

As we introduce the nnn interaction the spectrum remains gapless for all  $\Delta$  if *j* is small. In the intermediate-coupling regime ( $j \sim 1$ ) the system becomes gapped. In figure 4 we show (a) the spectral weight and (b) the structure function for j = 1 in the isotropic case. The states with  $S_z = 0$  and momenta  $k = 0, \pi$  are nearly degenerate [32]. The next excited state is a spin triplet with momentum  $k = \pi/2$ , which in the thermodynamic limit will have a gap to the ground state. Accordingly the spectral weight shows a gap with a continuum above it indicative of massive spinons. In the anisotropic case the two lowest states are the same as in the isotropic case but the next excited state is an  $S_z = 1$ ,  $k = \pi/2$  state [32]. The next state



**Figure 2.** (a) Excitation energies of the states that contribute to the longitudinal spectral weight for the Heisenberg chain. The solid lines are the exact Bethe ansatz results for the thermodynamic limit. The numerical results are obtained via exact diagonalization of a N = 16 system. The points correspond to states with a spectral weight that is (i)  $M(q, \omega) > 1$  (full circles), (ii)  $1 > M(q, \omega) > 0.1$  (full squares) and (iii)  $0.1 > M(q, \omega) > 0.01$  (open diamonds). The same colour code is used in the remaining figures. In (b) we show the structure function. The momentum is shown in units of  $\pi$ . The vertical scale is in arbitrary units.

is an  $S_z = 0$ ,  $k = \pi$  singlet. The low value of the gap signals the near level crossing that for N = 16 occurs around j = 1.2 leading to a gapless regime [32]. In figure 5 we show the spectral weights and the structure functions for the longitudinal and the transverse spin excitations. In the case of  $S_{zz}$  the lowest gap is at  $k = \pi$ , while for  $S_{+-}$  the lowest gap is at  $k = \pi/2$ . It is also clear that the spectrum is quite sharp at  $k = \pi/2$  in the transverse spin function.

As we increase j further the sharpness of the gapless transverse mode at  $k = \pi/2$  becomes stronger. In figure 6 we show the structure function for the isotropic case and in figure 7 the same function for the anisotropic case at j = 2. The Goldstone mode predicted to occur in the anisotropic case for the transverse spin excitations is clearly singled out.

We also consider the finite-size dependence of the low-energy excitations for the longitudinal and the transverse spectral functions as a function of the system size using results from exact diagonalizations and the modified Lanczos method. We consider system sizes up to N = 24. The results extrapolate to the single-spinon dispersion curve for the various values of  $\Delta$  and *j*. In particular we consider the anisotropic case.

In figure 8 we show the lowest-energy states for (a)  $S_z = 0$  and (b)  $S_z = 1$  as a function of momentum for the XY case for j = 2. The spectrum clearly shows the doubling of the lattice cell with a significant low-energy mode at  $q = \pi/2$ , particularly in the transverse correlations ( $S_z = 1$ ), where once again as the system size increases the gapless nature of the spectrum is evident as j grows (weak interchain couplings).



**Figure 3.** Excitation energies of the states that contribute to the (a) longitudinal and (c) transverse spectral weight of the XY chain. The solid curves in (a) are the exact Bethe ansatz results. We also show the structure function for the (b) longitudinal and (d) transverse excitations.

In the single-chain case the longitudinal spectrum can be obtained considering the twospinon curves (assuming non-interacting spinons) via the usual procedure  $E(q) = \epsilon(k_1) + \epsilon(k_2)$ 



Figure 4. (a) Excitation energies obtained from the exact diagonalization of an N = 16 ladder in the isotropic case and j = 1 that contribute to the spectral weight and (b) the structure function.

where  $q = k_1 + k_2$ , E(q) is the two-spinon curve and  $\epsilon(k)$  is the single-spinon dispersion curve. These two limiting curves define the region of the continuum spectrum. The transverse excitations in the anisotropic case probe however a different set of states as can be seen for example from the single-chain XY case shown in figure 3(c). The high-energy part of the spectrum shows that the interactions between the spinons cannot be ignored (remember that in the Jordan–Wigner transformation from an XY chain to spinless fermions, the transverse correlations involve the presence of strings). Therefore the two-spinon rule requires a proper treatment of the spinon interactions. The zig-zag ladder case is still more involved, particularly for the transverse excitations. In any case the continuum is clearly visible.

# 5. Conclusions

The finite-energy and finite-momentum structure function provides a direct way of analysing the excitation spectrum. Previously the structure factor was analysed in the isotropic case [26, 27, 32]. The structure factor is obtained integrating the structure function over frequency at a fixed momentum. In the isotropic case the peak in the structure factor shifts from  $q = \pi \text{ to } \pi/2$  when the spiral phase is reached as the Majumdar–Ghosh point is crossed. In the anisotropic case on the other hand it has been predicted that in the limit of very weak interchain coupling an incommensurate gapless chiral phase should be observed [21]. However, for finite systems it is difficult to detect the incommensurability since the shift from commensurability is very small [30].

In this work we have analysed the structure function itself for the zig-zag ladder as a function of anisotropy ( $\Delta$ ) and the interchain coupling (*j*). The results show that in general



**Figure 5.** Excitation energies of the states that contribute to the (a) longitudinal and (c) transverse spectral weight in the anisotropic case and j = 1. We also show the structure function for the (b) longitudinal and (d) transverse excitations.

the excitations are gapless or gapped spinons that have to be created in pairs as for the singlechain case. In the XY case ( $\Delta = 0$ ) as j grows it is clear that a gapless mode in the transverse



Figure 6. Structure function of an N = 16 ladder in the isotropic case and j = 2.



Figure 7. Structure function for the (a) longitudinal and (b) transverse excitations in the anisotropic case and j = 2.

excitations arises in agreement with previous results from field theory [21] and with previous numerical results [32] obtained analysing the stiffness and the level crossings. In the isotropic case ( $\Delta = 1$ ) the spectrum is a continuum of massive spinons. These results may be relevant to understand the ladder limit in the context of the recent experimental results on the two-dimensional system Cs<sub>2</sub>CuCl<sub>4</sub> [1].

After this work was completed we became aware of a preprint [42] where using Möbius boundary conditions it is shown that in the isotropic case for strong and intermediate coupling the spectrum may be described by a continuum resulting from two-spinon scattering, in agreement with the general conclusions of our paper.



**Figure 8.** Lowest-energy branch for  $\Delta = 0$  and j = 2 for (a)  $S_z = 0$  and (b)  $S_z = 1$  for different system sizes.

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