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Ladders in a magnetic field: a strong coupling approach

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Abstract. We show that non-frustrated and frustrated ladders in a magnetic field can be systematically mapped onto an XXZ Heisenberg model in a longitudinal magnetic field in the limit where the rung coupling is the dominant one. This mapping is valid in the critical region where the magnetization goes from zero to saturation. It allows one to relate the properties of the critical phase (H_c^1, H_c^2, the critical exponents) to the exchange integrals and provide quantitative estimates of the frustration needed to create a plateau at half the saturation value for different models of frustration.

PACS. 75.10.Jm Quantized spin models – 75.40.Cx Static properties (order parameter, static susceptibility, heat capacities, critical exponents, etc.) – 75.50.Ee Antiferromagnetics

1 Introduction

Intermediate between 1D and 2D, ladders have been the subject of an impressive amount of work over the past few years [1]. Thanks to an intensive experimental [2–5] and theoretical [6–8] effort, quite a lot is understood concerning the properties of $S = 1/2$ ladders in a magnetic field. In particular, the magnetization starts to increase above a magnetic field H_c^1 and saturates above a magnetic field H_c^2, and the phase realized for intermediate magnetic fields is believed to be a Luttinger liquid with gapless excitations and a power law decay of the correlation functions. As usual, it is difficult however starting from a microscopic description in terms of exchange integrals to calculate the parameters of the low energy theory in the Luttinger liquid phase, and this description is to a certain extent phenomenological.

In parallel, it has been shown by various authors that more general ladders can exhibit a new phenomena, namely plateaus in the magnetization for intermediate magnetic fields. This has been shown for ladders with more than two rungs by Cabra *et al.* [9] on the basis of a strong coupling expansion in the limit of strong rung couplings. This has also been shown for frustrated, two-leg ladders by Totsuka [10] and by Tonegawa *et al.* [11]. In that case, the existence of plateaus was predicted using bosonization [10], confirmed with exact digonalizations [11], and a description of the intermediate phase inside the plateau was given in terms of a Heisenberg XXZ model again starting from the limit of strong rungs [10].

In this paper, we show that all the physics of the general problem of frustrated and non–frustated ladders in a magnetic field can be understood within a unified framework in the limit of strong rung couplings. This is based on a mapping of the original model onto the XXZ model in a longitudinal magnetic field. The picture developped by Totsuka [10] for the intermediate phase inside the plateau is a particular case of this mapping, and the approach of Cabra *et al.* [9] is the analog of this calculation for non–frustrated, N-leg ladders. However the unifying power of this mapping to understand all the aspects of the problem was not recognized so far. Besides, the limit of strong rungs is not unphysical. In fact, this is actually the relevant one for $Cu_2(C_5H_{12}N_2)_2Cl_4$, the ladder system on which most results under strong magnetic fields have been obtained so far [2–5].

The paper is organized as follows. In the next section, we derive the effective Hamiltonian in the general case. In Section 3, we discuss the Luttinger liquid phase that appears for non- and weakly-frustrated ladders. In Section 4, we discuss the strongly-frustrated case where a plateau shows up for intermediate fields. Finally a summary is given in Section 5.

2 The effective Hamiltonian

The mapping presented in this section can be performed for any type of coupling between the rungs. To be both specific and general, we will study the following Hamiltonian (see Fig. 1)

$$\mathcal{H} = J_\perp \sum_{i=1}^{N} \mathbf{S}_{i,1}\mathbf{S}_{i,2} + J_1 \sum_{i=1}^{N}\sum_{\alpha=1}^{2} \mathbf{S}_{i,\alpha}\mathbf{S}_{i+1,\alpha} + J_2' \sum_{i=1}^{N} \mathbf{S}_{i,1}\mathbf{S}_{i+1,2} + J_2'' \sum_{i=1}^{N} \mathbf{S}_{i,2}\mathbf{S}_{i+1,1} - H \sum_{i=1}^{N}\sum_{\alpha=1}^{2} S_{i,\alpha}^z. \quad (1)$$

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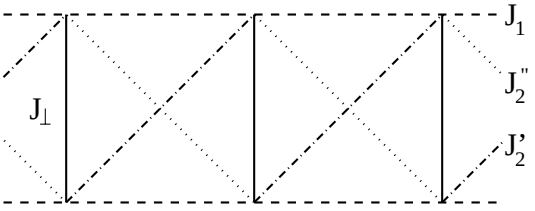

Fig. 1. Sketch of the ladder considered in this paper.

In this expression, α (resp. i) is a chain (resp. rung) index, N is the total number of rungs, and periodic boundary conditions along the chain direction are implicit. The frustration comes from the competition between J_1, J_2' and J_2'': the models with $J_2' = J_2'' = 0$ (resp. $J_1 = 0$) are not frustrated. Besides, in the following approach, J_1 and $(J_2' + J_2'')/2$ play the same role. So we will limit our discussion to the case $J_1 \geq (J_2' + J_2'')/2$ without loss of generality. If all the couplings except $J_\perp$ are set to zero, the system is a collection of independent rungs. The states of a given rung are denoted by $|S\rangle = (|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle)/\sqrt{2}$, $|T_1\rangle = |\uparrow\uparrow\rangle$, $|T_0\rangle = (|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle)/\sqrt{2}$ and $|T_{-1}\rangle = |\downarrow\downarrow\rangle$. In a configuration $|\sigma_1\sigma_2\rangle$, σ_1 (resp. σ_2) refers to chain 1 (resp. 2). Their energies are $E(S) = -3J_\perp/4$, $E(T_1) = J_\perp/4 - H$, $E(T_0) = J_\perp/4$ and $E(T_{-1}) = J_\perp/4 + H$. So upon increasing the magnetic field the groundstate of a given rung undergoes a transition between the singlet $|S\rangle$ and the triplet $|T_1\rangle$ at $H_c = J_\perp$, and the total magnetization of the system jumps discontinuously from zero to saturation.

If the other couplings are non-zero but small, this abrupt transition is expected to broaden between H_c^1 and H_c^2, $H_c^2 - H_c^1$ being of the order of the largest of the couplings J_1, J_2' and J_2''. In this limit, the properties of the system for $H_c^1 \leq H \leq H_c^2$ are best understood by splitting the Hamiltonian into two parts:

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_1, \\
\mathcal{H}_0 &= J_\perp \sum_{i=1}^{N} \mathbf{S}_{i,1}\mathbf{S}_{i,2} - H_c \sum_{i=1}^{N}\sum_{\alpha=1}^{2} S^z_{i,\alpha}, \\
\mathcal{H}_1 &= J_1 \sum_{i=1}^{N}\sum_{\alpha=1}^{2} \mathbf{S}_{i,\alpha}\mathbf{S}_{i+1,\alpha} + J_2' \sum_{i=1}^{N} \mathbf{S}_{i,1}\mathbf{S}_{i+1,2} \\
&\quad + J_2'' \sum_{i=1}^{N} \mathbf{S}_{i,2}\mathbf{S}_{i+1,1} - (H - H_c) \sum_{i=1}^{N}\sum_{\alpha=1}^{2} S^z_{i,\alpha}. \quad (2)
\end{aligned}$$

The groundstate of $\mathcal{H}_0$ is 2^N times degenerate since each rung can be in the state $|S\rangle$ or $|T_1\rangle$, and the first excited state has an energy equal to $J_\perp$. $\mathcal{H}_1$ will lift the degeneracy in the groundstate manifold, leading to an effective Hamiltonian that can be derived by standard many-body perturbation theory [12]. Let us start by introducing pseudo-spin $S = 1/2$ operators $\boldsymbol{\sigma}_i$ that act on the states $|S\rangle_i$ and $|T_1\rangle_i$ of rung i according to

$$\begin{aligned}
\sigma_i^z|S\rangle_i = -\frac{1}{2}|S\rangle_i \qquad & \sigma_i^z|T_1\rangle_i = \frac{1}{2}|T_1\rangle_i \\
\sigma_i^+|S\rangle_i = |T_1\rangle_i \qquad & \sigma_i^+|T_1\rangle_i = 0 \\
\sigma_i^-|S\rangle_i = 0 \qquad & \sigma_i^-|T_1\rangle_i = |S\rangle_i. \quad (3)
\end{aligned}$$

Then, to first order, and up to a constant, the effective Hamiltonian reads:

$$\begin{aligned}
\mathcal{H}_{\mathit{eff}} &= \sum_{i=1}^{N} [J_{xy}^{\mathit{eff}} (\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + J_z^{\mathit{eff}} \sigma_i^z \sigma_{i+1}^z] \\
&\quad - H^{\mathit{eff}} \sum_{i=1}^{N} \sigma_i^z. \quad (4)
\end{aligned}$$

The parameters of H_{eff} are given by

$$\begin{aligned}
J_{xy}^{\mathit{eff}} &= J_1 - \frac{J_2'}{2} - \frac{J_2''}{2} \\
J_z^{\mathit{eff}} &= \frac{J_1}{2} + \frac{J_2'}{4} + \frac{J_2''}{4} \\
H^{\mathit{eff}} &= H - H_c - \frac{J_1}{2} - \frac{J_2'}{4} - \frac{J_2''}{4}. \quad (5)
\end{aligned}$$

The Hamiltonian of equation (4) is nothing but the XXZ model in a longitudinal magnetic field. The calculation can actually be pushed to higher orders. The simplicity of the effective model is already lost however at second order: In addition to second-order corrections to the effective couplings of the XXZ Hamiltonian, there appears a 3-site term involving next-nearest neighbours. So we will limit ourselves to the first-order effective Hamiltonian of equation (4).

This problem has been studied by several authors over the years, and most of the relevant information concerning the properties of the model is available in the literature (see below). To translate these results into the language of the original Hamiltonian of equation (1), one just has to express the original operators $S^+_{i,\alpha}$, $S^-_{i,\alpha}$ and $S^z_{i,\alpha}$ in terms of the pseudo-spin operators. This can be done by inspection, and the results are:

$$\begin{aligned}
S_{i,1}^+ = -\frac{1}{\sqrt{2}}\sigma_i^+ \qquad & S_{i,2}^+ = \frac{1}{\sqrt{2}}\sigma_i^+ \\
S_{i,1}^- = -\frac{1}{\sqrt{2}}\sigma_i^- \qquad & S_{i,2}^- = \frac{1}{\sqrt{2}}\sigma_i^- \\
S_{i,1}^z = \frac{1}{2}(\sigma_i^z + \frac{1}{2}) \qquad & S_{i,2}^z = \frac{1}{2}(\sigma_i^z + \frac{1}{2}). \quad (6)
\end{aligned}$$

We now discuss the implications of this mapping in different cases. Two situations have to be discussed separately: $J_z^{\mathit{eff}} < J_{xy}^{\mathit{eff}}$, which corresponds to weak frustration and includes the non–frustrated case, and $J_z^{\mathit{eff}} > J_{xy}^{\mathit{eff}}$, which corresponds to strongly frustrated ladders.

3 The weakly-frustrated ladder

Let us first discuss the situation where $J_z^{\mathit{eff}} < J_{xy}^{\mathit{eff}}$. This corresponds to the case $J_1 > 3(J_2' + J_2'')/2$. Then the effective Hamiltonian is in the universality class of the XY

model when the effective field H^{eff} vanishes, and the system behaves as a Luttinger liquid for all the values of the magnetic field between H_c^1 and H_c^2. Having explicit expressions of the effective coupling constants in terms of the microscopic parameters, one can calculate everything in terms of these parameters. For instance, we can express H_c^1 and H_c^2 in terms of $J_\perp$, J_1 J_2' and J_2''. This can actually be done without calculating the excitation spectrum by performing a Jordan-Wigner transformation to map the problem onto a problem of interacting, spinless fermions:

$$\mathcal{H}_{SF} = t\sum_i^N (c_i^\dagger c_{i+1} + \text{h.c.}) + V\sum_i^N n_i n_{i+1} - \mu\sum_i^N n_i. \tag{7}$$

The parameters of this Hamiltonian are given in terms of those of equation (4) by $t = J_{xy}^{eff}/2$, $V = J_z^{eff}$ and $\mu = H^{eff} + J_z^{eff}$. H_c^1 corresponds to the chemical potential at which the band of spinless fermions starts to fill up. In that limit the repulsion term is irrelevant because the density of spinless fermions vanishes, so that the chemical potential corresponding to H_c^1 is given by $\mu = -2t$. This leads to the result $H_c^1 = J_\perp - J_1 + (J_2' + J_2'')/2$. This result can also be obtained by a first order calculation of the gap of the original Hamiltonian, H_c^1 being equal to this gap [3]. To estimate H_c^2, one cannot neglect the repulsion term because the band is completely filled. The simplest way to take it into account is to perform a particle-hole transformation on the Hamiltonian of equation (7): $c_i^\dagger \rightarrow d_i$. Up to a constant, the new Hamiltonian reads

$$\mathcal{H}_{hole} = -t\sum_i^N (d_i^\dagger d_{i+1} + \text{h.c.}) + V\sum_i^N n_i^d n_{i+1}^d - \mu_h\sum_i^N n_i^d \tag{8}$$

where the hole chemical potential μ_h is given by $\mu_h = -\mu + 2V$. In terms of holes, H_c^2 corresponds to the chemical potential where the band starts to fill up, and one can again neglect the repulsion term. Note however that this is not equivalent to neglecting the repulsion in equation (7) since V appears in the expression of μ_h. The chemical potential corresponding to H_c^2 is thus given by $\mu_h = -2t$, leading to $H_c^2 = J_\perp + 2J_1$. This value agrees with the value one would deduce from the instatiblity of the spin-wave spectrum in the ferromagnetic phase [3]. Let us note however that the present calculation is more rigorous: the instability of the spin-wave spectrum gives a lower bound of H_c^2 since it only detects an instability towards states with a total spin reduced by one with respect to the saturation value and does not exclude a transition to a lower spin state at a higher value of the magnetic field. Such a possibility is indeed excluded by the present calculation. These expressions of H_c^1 and H_c^2 compare well with the experimental values for $Cu_2(C_5H_{12}N_2)_2Cl_4$ [3] for reasonable values of the parameters.

A lot more is known about the physical properties of the *XXZ* Hamiltonian in a magnetic field, especially concerning the spin-spin correlation functions thanks to the work of many people [13–18]. In particular, the exponent controlling the decay at large distances have been obtained analytically in zero magnetic field and numerically otherwise [14]. Experimentally, these exponents are in principle accessible *via* the temperature dependence of the relaxation rate measured in NMR experiments. Equation (6) shows that the spin-spin correlation functions of the original model are closely related to those of the effective model. In particular, the exponents describing the long-distance decay or the low temperature relaxation rate will be the same. This problem has been recently addressed by Chitra and Giamarchi [7] who showed that the relaxation rate is expected to behave like $1/T_1 \propto T^{-\alpha}$ at low temperature in a variety of models. More precisely, $1/T_1$ is the sum of contributions coming from parallel and perpendicular fluctuations respectively with $(1/T_1)_\parallel \propto T^{2K-1}$ and $(1/T_1)_\perp \propto T^{1/2K-1}$ at low temperature, where K is a model-dependent constant. One of the contributions will dominate at low temperature, and $\alpha = \max(1-2K, 1-1/2K)$. In the present case, K is never smaller than 1/2 [13,14], and the relaxation is always dominated by the perpendicular term. Exact results for the exponent α can be obtained in two limits: when $H \rightarrow H_c^1$ or H_c^2, the system becomes effectively non interacting in terms of spinless fermions, $K \rightarrow 1$ and $\alpha \rightarrow 1/2$. The other soluble case corresponds to $H^{eff} = 0$ *i.e.* $H = H_c + J_1/2 + (J_2' + J_2'')/4$. In that case the Bethe ansatz solution leads to $K = \pi/(2\cos^{-1}(-J_z^{eff}/J_{xy}^{eff}))$, *i.e.*

$$\alpha = 1 - \frac{1}{\pi}\cos^{-1}\left(-\frac{2J_1 + J_2' + J_2''}{4J_1 - 2J_2' - 2J_2''}\right). \tag{9}$$

When the magnetic field increases from H_c^1 to H_c^2, the exponent α is first expected to decrease from 1/2 down to its minimum when $H^{eff} = 0$ and then to increase back to 1/2. For the regular ladder ($J_2' = J_2'' = 0$), the minimum value of α is 1/3. The actual variation of this exponent between these limits can be deduced from the curves of reference [14]. More precise estimates might be obtained with *e.g.* exact diagonalizations using today's numerical facilities. Let us note that, in agreement with Chitra and Giamarchi's general analysis, the behaviour of the exponent α away from H_c^1 is not universal: it decreases in the present case, whereas it increases in the case of the $S = 1$ Haldane chain [19].

4 The strongly-frustrated ladder

4.1 The general case

Let us now turn to the situation where $J_z^{eff} > J_{xy}^{eff}$, *i.e.* when $J_1 < 3(J_2' + J_2'')/2$. Then the system is no longer in the XY universality class when $H^{eff} = 0$ but in the Ising universality class, and the spectrum is gapped. In terms of the mapping of equation (7) onto spinless fermions, the Ising limit means that V is large enough to make the half-filled system insulating [20–22]. The chemical potential

as a function of the band-filling will then have a jump. In the original spin language, this implies that there will be a plateau in the magnetization at half the saturated value as a function of magnetic field extending between two values denoted by H_p^1 and H_p^2. Note that similar conclusions have been obtained along different lines by several authors [9–11] concerning the case $J_2'' = 0$ (see Sect. 4.3). In the plateau region, there is an order parameter corresponding to alternating singlets and triplets on neighbouring rungs. Since $\mu = H^{\tilde{eff}} + J_{\tilde{z}}^{eff} = H - H_c$, the width of the plateau $\Delta H = H_p^2 - H_p^1$ is given by the jump of the chemical potential, *i.e.* by the charge gap in the spinless fermion language. This problem has been studied analytically with Bethe ansatz [20,21]. When J_z^{eff}/J_{xy}^{eff} is close to 1, *i.e.* when J_1 is close to $3(J_2' + J_2'')/2$ the Bethe ansatz results lead to

$$\Delta H = 4\pi(J_2' + J_2'') \times \exp\left[-\frac{\pi^2}{2\sqrt{2}}\left(\frac{2J_1 + J_2' + J_2''}{4J_1 - 2J_2' - 2J_2''} - 1\right)^{-1/2}\right]. \quad (10)$$

When J_{xy}^{eff} goes to zero, *i.e.* when $J_1 = (J_2' + J_2'')/2$, the spinless fermion model is in the atomic limit, and the gap is equal to $2V$, leading to $\Delta H = 2J_1$. In between, the gap can be obtained from the results of reference [21].

Outside the plateau, *i.e.* when the magnetic field is between H_c^1 and H_p^1 or between H_p^2 and H_c^2, the system behaves as a Luttinger liquid, and the exponents can be deduced from reference [14] as in the previous case. The only difference is that the parameter K entering the expression of the exponent α will now go from 1 at H_c^1 (resp. H_c^2) to 1/4 at H_p^1 (resp. H_p^2). As a consequence, there is now a competition between the parallel and perpendicular contributions to the relaxation rate. When K decreases between 1 and 1/2, the relaxtion rate is dominated by $(1/T_1)_\perp$, and α decreases from 1/2 to 0. Then the parallel contribution takes over, and α increases back to 1/2. So the main difference with the weakly-frustrated case is that the minimum value of α between H_c^1 and H_p^1 (resp. H_c^2 and H_p^2) is always 0, *i.e.* there is always a field for which the relaxation rate does not diverge at low temperature.

4.2 The $J_2' = J_2'' = J_2$ case

For this system [23], the Ising limit has a very simple interpretation. In that case, the effective Hamiltonian becomes purely Ising for $J_2 = J_1$. This result, clearly valid up to first order after equation (5), is actually exact including all order corrections. The simplest way to understand this is to realize that a singlet on a given rung is completely decoupled from the rest because all the exchange integrals starting from this singlet belong to a pair of equal exchange integrals connecting a spin to both ends of the singlet. So the perturbation cannot couple to the singlets, and the XY exchange integral must vanish. Besides, this argument shows that the state with alternating singlets and triplets is an eigenstate of the Hamiltonian. It is easy to prove that it is the groundstate for H between H_c^1 and H_c^2, which are given by $H_c^1 = J_\perp$ and $H_c^2 = J_\perp + 2J_1$ in the present case. So the plateau will extend over all the intermediate region between zero and saturated magnetization, and its width is equal to $2J_1$, in agreement with the general result.

4.3 The $J_2'' = 0$ case

This case is very similar to the previous one. The transition to the Ising phase occurs for $J_2' = 2J_1/3$. The only difference is that the results for the pure Ising phase cannot be extended beyond first order perturbation theory since in that case a singlet is only decoupled from neighbouring singlets, and not from neighbouring triplets. The reason for mentioning this particular case of frustration is that it corresponds in principle to the physical situation realized in $Cu_2(C_5H_{12}N_2)_2Cl_4$. Our estimate of the critical value of J_2' to enter the Ising phase can be used as an upper bound to this exchange integral in $Cu_2(C_5H_{12}N_2)_2Cl_4$ since no plateau at half the saturated value has been reported. With $J_1 = 2.4$ K, this means that J_2' cannot exceed 1.6 K. Although there is some discussion in the literature as to what the actual value of this parameter is, all the estimates reported so far appear to be smaller than this upper bound.

5 Conclusion

In conclusion, we have shown that a strong coupling approach starting from the limit of strong rungs provides a simple and unifying picture of the very rich physics that appears when ladders are put in a magnetic field. On one hand, it gives a simple explanation of how the Luttinger liquid physics emerges in the intermediate phase of unfrustrated ladders. On the other hand, this approach naturally leads to the presence of a plateau in the intermediate phase at half the saturation value when the coupling between the rungs is strongly frustrated. In systems where $J_\perp$ is effectively the largest coupling, this calculation allows one to relate measurable quantities like H_c^1, H_c^2 and the critical exponents of the spin-spin correlation functions to the exchange integrals. Reported values for H_c^1 and H_c^2 in $Cu_2(C_5H_{12}N_2)_2Cl_4$ are well reproduced by this approach. It will be interesting to analyze the critical exponents along the same lines when experimental data are available. It seems that currently available data on $Cu_2(C_5H_{12}N_2)_2Cl_4$ do not give access to these exponents because of a 3D ordering that controls the very low temperature behaviour of the relaxation rate. Finally, this approach provides quantitative estimates of the frustration needed to create a plateau at half the magnetization value for systems where the rung coupling is the largest one and should help in the search for systems exhibiting this remarkable property.

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