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 ($H^1_c$, $H^2_c$, 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.

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I. 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 $H_1^c$ and saturates above a magnetic field $H_2^c$, 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 this paper, we show explicitly how this problem can be mapped onto the XXZ model in a longitudinal magnetic field if the rung coupling is the dominant one. This is actually the case of Cu$_2$(C$_5$H$_{12}$N$_2$)$_2$Cl$_4$, the ladder system on which most results under strong magnetic fields have been obtained so far [2–5]. Such a mapping can actually be performed for any type of coupling between the rungs, and we will study the following Hamiltonian (see Fig. 1)

$$H = J_1 \sum_{i=1}^{N} \vec{S}_{i,1} \vec{S}_{i,2} + J_1 \sum_{i=1}^{N} \sum_{\alpha=1}^{2} \vec{S}_{i,\alpha} \vec{S}_{i+1,\alpha} + J'_2 \sum_{i=1}^{N} \vec{S}_{i,1} \vec{S}_{i+1,2}$$
$$+ J''_2 \sum_{i=1}^{N} \vec{S}_{i,2} \vec{S}_{i+1,1} - H \sum_{i=1}^{N} \sum_{\alpha=1}^{2} S_{i,\alpha}^z$$

(1)

In this expression, $\alpha$ (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. 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 $|S> = (|\uparrow\downarrow>-|\downarrow\uparrow>)/\sqrt{2}$, $|T_1> = |\uparrow\uparrow>$, $|T_0> = (|\uparrow\downarrow>+|\downarrow\uparrow>)/\sqrt{2}$ and $|T_{-1}> = |\downarrow\downarrow>$. In a configuration $|\sigma_1 \sigma_2>$, $\sigma_1$ (resp. $\sigma_2$) 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 $|S>$ and the triplet $|T_1>$ 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 \( H^1_c \) and \( H^2_c \), \( H^2_c - H^1_c \) 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 \( H^1_c \leq H \leq H^2_c \) are best understood by splitting the Hamiltonian into two parts:

\[
\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_1,
\]

\[
\mathcal{H}_0 = J_\perp \sum_{i=1}^{N} \vec{S}_{i,1} \vec{S}_{i,2} - H_c \sum_{i=1}^{N} \sum_{\alpha=1}^{2} S_{i,\alpha}^z,
\]

\[
\mathcal{H}_1 = J_1 \sum_{i=1}^{N} \sum_{\alpha=1}^{2} \vec{S}_{i,\alpha} \vec{S}_{i+1,\alpha} + J'_2 \sum_{i=1}^{N} \vec{S}_{i,1} \vec{S}_{i+1,2} + J''_2 \sum_{i=1}^{N} \vec{S}_{i,2} \vec{S}_{i+1,1} - (H - H_c) \sum_{i=1}^{N} \sum_{\alpha=1}^{2} S_{i,\alpha}^z \quad (2)
\]

The ground state 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 perturbation theory. Let us start by introducing pseudo-spin \( S=1/2 \) operators \( \vec{\sigma}_i \) that act on the states \(|S\rangle_i\) and \(|T_1\rangle_i\) of rung \( i \) according to

\[
\sigma_i^z |S\rangle_i = -\frac{1}{2} |S\rangle_i, \quad \sigma_i^z |T_1\rangle_i = \frac{1}{2} |T_1\rangle_i
\]

\[
\sigma_i^+ |S\rangle_i = |T_1\rangle_i, \quad \sigma_i^+ |T_1\rangle_i = 0
\]

\[
\sigma_i^- |S\rangle_i = 0, \quad \sigma_i^- |T_1\rangle_i = |S\rangle_i
\]

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

\[
\mathcal{H}_{\text{eff}} = \sum_{i=1}^{N} [J_{xy}^\text{eff}(\sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y) + J_z^\text{eff} \sigma_i^z \sigma_{i+1}^z] - H_{\text{eff}} \sum_{i=1}^{N} \sigma_i^z \quad (4)
\]

The parameters of \( H_{\text{eff}} \) are given by

\[
J_{xy}^\text{eff} = J_1 - \frac{J'_2}{2} - \frac{J''_2}{2}
\]

\[
J_z^\text{eff} = \frac{J_1}{2} + \frac{J'_2}{4} + \frac{J''_2}{4}
\]

\[
H_{\text{eff}} = H - H_c - \frac{J_1}{2} - \frac{J'_2}{4} - \frac{J''_2}{4} \quad (5)
\]

The Hamiltonian of Eq.(4) is nothing but the XXZ model in a longitudinal magnetic field. 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 \[7\]. In particular, the exponents of the spin-spin correlation functions have been obtained analytically when the model is integrable and numerically otherwise. To translate these results into the language of the original Hamiltonian of Eq.(4), 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:

$$
\begin{align*}
S^+_{i,1} &= -\frac{1}{\sqrt{2}}\sigma^+_i \\
S^+_{i,2} &= \frac{1}{\sqrt{2}}\sigma^+_i \\
S^-_{i,1} &= -\frac{1}{\sqrt{2}}\sigma^-_i \\
S^-_{i,2} &= \frac{1}{\sqrt{2}}\sigma^-_i \\
S^z_{i,1} &= \frac{1}{2}(\sigma^z_i + \frac{1}{2}) \\
S^z_{i,2} &= \frac{1}{2}(\sigma^z_i + \frac{1}{2})
\end{align*}
$$

(6)

A detailed discussion of the correlation functions measured in NMR experiments can be found in Ref. [7]. We now discuss the implications of this mapping in different cases.

### II. THE REGULAR LADDER: $J_2' = J_2'' = 0$

In that case $J_{xy}^\text{eff} = J_1$ is twice as large as $J_z^\text{eff}$: We are in the XY universality class of the anisotropic Heisenberg model. The system is gapless, and it behaves as a Luttinger liquid. Having explicit expressions of the coupling constants in terms of the microscopic parameters, one can calculate everything in terms of these parameters. For instance, we can express $H^1_c$ and $H^2_c$ in terms of $J_\perp$ and $J_1$. This is most easily done by first performing a Jordan-Wigner transformation to map the problem onto a problem of interacting, spinless fermions:

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

(7)

The parameters of this Hamiltonian are given in terms of those of Eq.(4) by $t = J_{xy}^\text{eff}/2$, $V = J_z^\text{eff}$ and $\mu = H_z^\text{eff} + J_z^\text{eff}$. $H^1_c$ 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 $H^1_c$ is given by $\mu = -2t$. This leads to the result $H^1_c = J_\perp - J_1$. To estimate $H^2_c$, 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 Eq.(7): $c_i^\dagger \rightarrow d_i$. Up to a constant, the new Hamiltonian reads

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

(8)

where the hole chemical potential $\mu_h$ 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 Eq.(7) since $V$ appears in the expression of $\mu_h$. The chemical potential corresponding to $H_c^2$ is thus given by $\mu_h = -2t$, leading to $H_c^2 = J_\perp + 2J_1$. These expressions of $H_c^1$ and $H_c^2$ agree with those of Ref. [3] obtained along different lines, and they compare well with the experimental values for Cu$_2$(C$_5$H$_{12}$N$_2$)$_2$Cl$_4$ [3].

The same argument actually apply if $J'_2$ and $J''_2$ are not equal to zero. To first order, $H_c^2$ is unaffected, and $H_c^1$ is given by $H_c^1 = J_\perp - J_1 + (J'_2 + J''_2)/2$.

### III. THE FRUSTRATED LADDER: $J'_2 = J''_2 = J_2$

When $J_2 \neq 0$, the effective Hamiltonian is in the universality class of the XY model only if $J_2$ is not too large: There is a transition to the Ising universality class when $J'_{xy}^\text{eff} = J_z^\text{eff}$, i.e. $J_2 = J_1/3$ to first order. In terms of spinless fermions, the Ising limit means that $V$ is large enough to make the half-filled system insulating [10]. 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. Note that similar conclusions have been obtained along different lines by several authors [11-13] concerning the case $J''_2 = 0$ (see next section). In the plateau region, there is an order parameter corresponding to alternating singlets and triplets on neighbouring rungs. For $J_2 = J_1$, the effective Hamiltonian becomes purely Ising: $J_z^\text{eff} = J_1$, $J_{xy}^\text{eff} = 0$. This result, clearly valid up to first order after Eq.(3), 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 $H^1_c$ and $H^2_c$, which are given by $H^1_c = J_{\perp}$ and $H^2_c = J_{\perp} + 2J_1$ in the present case. So the plateau will extend over all the intermediate region between zero and saturated magnetization.

**IV. THE ZIGZAG LADDER: $J''_2 = 0$**

This case is very similar to the previous one. There will be a transition to an Ising phase when $J'_2$ is large enough, a conclusion already reached by other authors using different arguments [11,12,14]. To first order the critical value is given by $J'_2 = 2J_1/3$. The only difference is that there is no pure Ising phase in that case since 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$_5$H$_{12}$N$_2$)$_2$Cl$_4$. 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$_5$H$_{12}$N$_2$)$_2$Cl$_4$ 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.

**V. 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 $H_{c1}$, $H_{c2}$ and the critical exponents of the spin-spin correlation functions to the exchange integrals. Reported values for $H_{c1}$ and $H_{c2}$ in Cu$_2$(C$_5$H$_{12}$N$_2$)$_2$Cl$_4$ are well reproduced by this approach. It will be interesting to analyze the critical exponents along the same lines when experimental data are available. 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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FIG. 1. Sketch of the ladder considered in this paper.
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