Magnetic Properties of Quantum Spin Ladders at Strong Coupling

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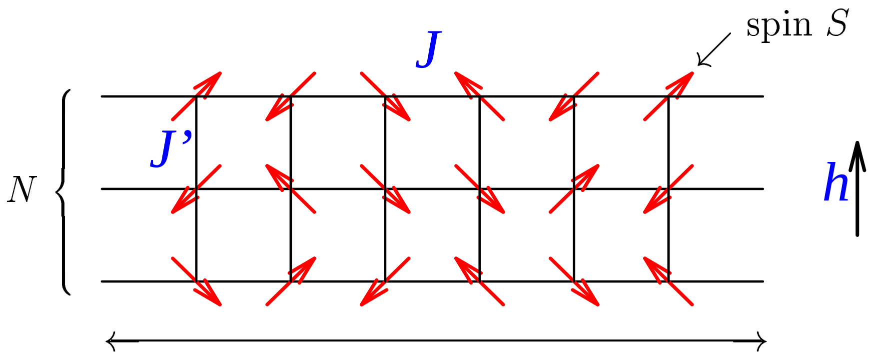
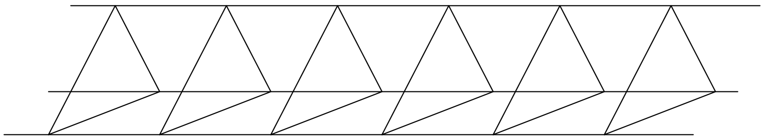
Introduction

($N = 3$, open boundary conditions (OBC))



realized e.g. in $Sr_2Cu_3O_5$

(or periodic boundary conditions (PBC), $N = 3$)



Hamilton operator:

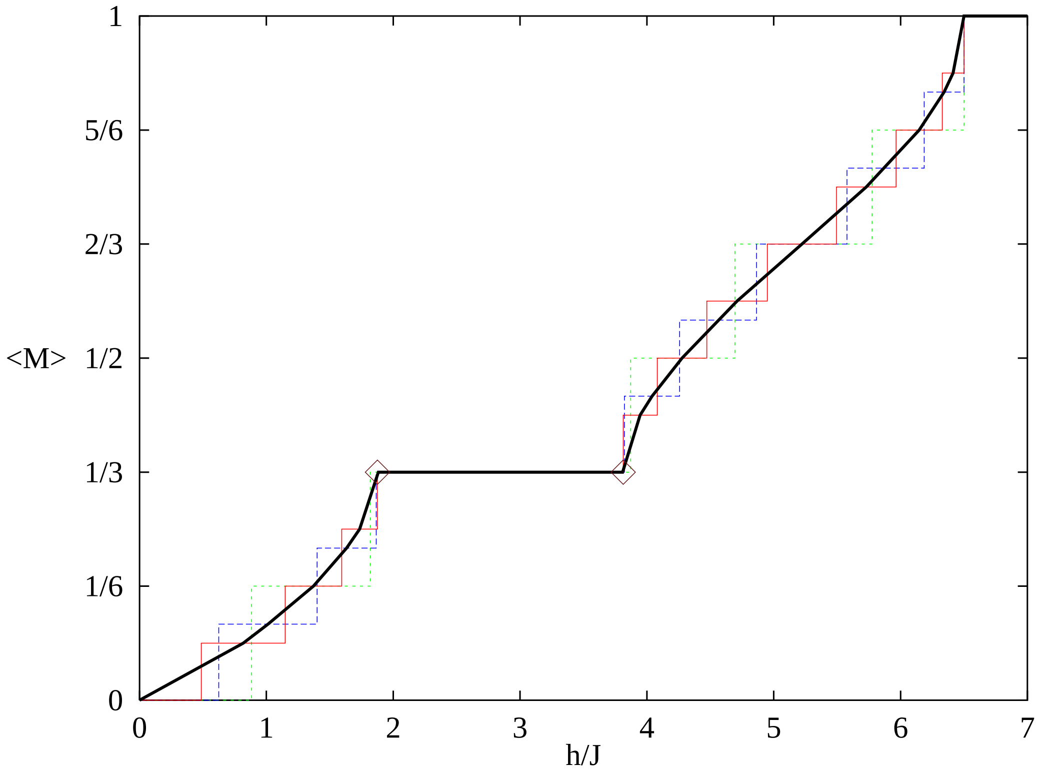
$$
\begin{aligned}
H^{(N)} &= J \sum_{i=1}^{N} \sum_{x=1}^{L} \left\{ \Delta S^z_{i,x} S^z_{i,x+1} + \frac{1}{2} \left(S^+_{i,x} S^-_{i,x+1} + S^-_{i,x} S^+_{i,x+1} \right) \right\} \\
&+ J' \sum_{i,j} \sum_{x=1}^{L} \vec{S}_{i,x} \vec{S}_{j,x} \\
&- h \sum_{i,x} S^z_{i,x}
\end{aligned}
$$

Magnetization:

$$\langle M \rangle = \frac{1}{SLN} \left\langle \sum_{i,x} S^z_{i,x} \right\rangle$$

Magnetization curve of an $N = 3$ leg ladder with open boundary conditions

$(J'/J = 3$, zero temperature$)$



The red full line is for $L = 8$, the blue dashed line for $L = 6$ and the green dashed line for $L = 4$. The **black** full line indicates the expected form in the thermodynamic limit. The two grey diamonds denote fourth order series results for the boundaries of the plateau.

The quantization condition

On a plateau the magnetization $\langle M \rangle$ satisfies

$$lNS(1 - \langle M \rangle) \in \mathbb{Z} \,. \qquad (*)$$

l : Period in lattice sites of a groundstate with broken translational invariance

N : Number of chains

S : Spin, e.g. $S = 1/2$

(compare Haldane's conjecture: $l = N = 1$, $\langle M \rangle = 0$,
or its generlization to spin ladders: $l = 1$, $\langle M \rangle = 0$)

This condition appears

- in a generalized Lieb-Schultz-Mattis theorem

  Lieb, Schultz, Mattis, Ann. Phys. **16** (1961) 407
  Affleck, Phys. Rev. **B37** (1988) 5186
  Rojo, Phys. Rev. **B53** (1996) 9172
  Oshikawa, Yamanaka, Affleck, Phys. Rev. Lett. **78**, (1997) 1984

  Problem: Apart from subtleties in the statement, the gapless excitation which is constructed in the theorem is *non-magnetic*, but we wish to know something about a gap to magnetic excitations.

- as a commensurability condition for certain operators that can be radiatively generated in the field theoretical description of the weak-coupling regime $J' \ll J$.

  compare Affleck et.al., Totsuka

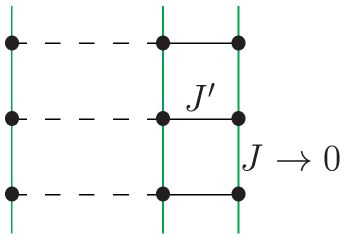
- by a counting argument at the strong-coupling point $J = 0$.

  At $J = 0$, clusters of volume $V = N$ decouple and thus magnetize independently. The condition $(*)$ then simply counts the number of possible S^z-values of spin-S spins in a cluster.

  Note: This argument is applicable whenever there is a point at which the system decouples into finite clusters. It works extremely well also for polymerized spin chains (*i.e.* $N = 1$, but with x-dependent coupling constants subject to a period l – Cabra, Grynberg, cond-mat/9803368; A. Honecker, in preparation).

The strong-coupling limit in more detail

Consider the limit $J' \gg J$.



In zeroth order ($J = 0$), the rungs are decoupled:

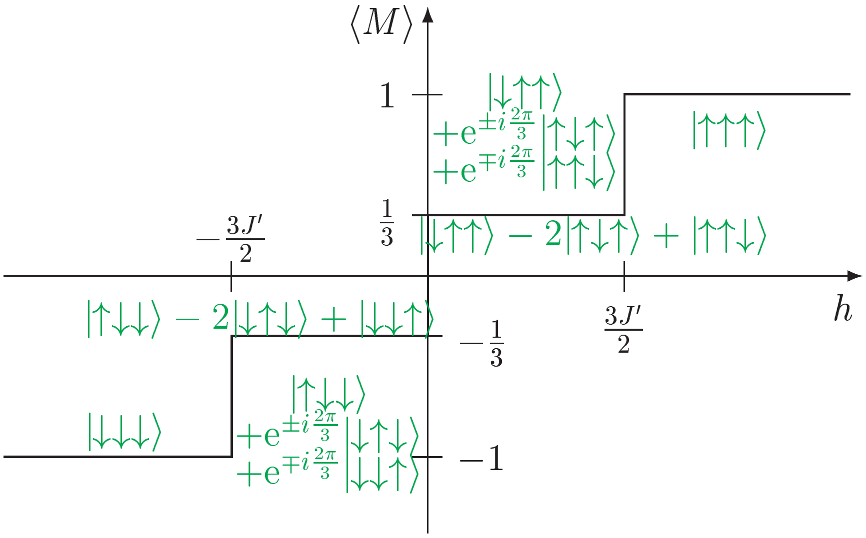
$$H_{\text{eff.}} = J' \sum_{i=1}^{N(-1)} \vec{S}_i \vec{S}_{i+1} - h \sum_{i=1}^{N} S_i^z \,.$$

In this limit, one has N spin-1/2 spins. Thus, the only possible values of the magnetization are:

$$\langle M \rangle \in \left\{ -1, -1 + \frac{2}{N}, \ldots, 1 - \frac{2}{N}, 1 \right\}$$

$\longrightarrow$ plateaux at the solutions of $(*)$ with $l = 1$, $S = 1/2$.

Example: $N = 3$, $J' > 0$, $J = 0$:



Both OBC and PBC: Plateau with $\langle M \rangle = 1/3$.

Expectation: When switching on $J' > 0$, the transitions will broaden, but the plateaux will survive.
In fact, in some cases series expansions can be performed for the plateau boundaries, e.g. $N = 3$ (OBC) $\Delta = 1$:

$$\frac{h_{c_1}}{J'} = 2\frac{J}{J'} - \frac{2}{9}\left(\frac{J}{J'}\right)^2 - \frac{94}{243}\left(\frac{J}{J'}\right)^3 - \frac{1847}{8748}\left(\frac{J}{J'}\right)^4 + \mathcal{O}\left(\left(\frac{J}{J'}\right)^5\right),$$

$$\frac{h_{c_2}}{J'} = \frac{3}{2} - \frac{J}{J'} + \frac{3}{4}\left(\frac{J}{J'}\right)^2 + \frac{2065}{3888}\left(\frac{J}{J'}\right)^3 + \frac{38915}{326592}\left(\frac{J}{J'}\right)^4 + \mathcal{O}\left(\left(\frac{J}{J'}\right)^5\right).$$

Strong-coupling effective Hamiltonian of a frustrated ladder

1st order in J for N odd and PBC ($h = 0$):

$$H^{(N,p)}_{\text{eff.}} = \frac{J}{N} \sum_{x=1}^{L} \underbrace{\left(1 + \alpha_N \left(\sigma_x^+ \sigma_{x+1}^- + \sigma_x^- \sigma_{x+1}^+\right)\right)}_{\text{spatial degeneracy}} \times \left(\Delta S_x^z S_{x+1}^z + \frac{1}{2}\left(S_x^+ S_{x+1}^- + S_x^- S_{x+1}^+\right)\right)$$

with (for $\Delta = 1$ see Kawano, Takahashi, J. Phys. Soc. Jpn. **66** (1997) 4001)

$$\alpha_3 = 1\,, \quad \alpha_5 = \frac{16}{9}\,, \quad \alpha_7 = 2.6206859\ldots\,, \quad \alpha_9 = 3.5012083\ldots\,.$$

Remark: This effective Hamiltonian describes the magnetization process for $|\langle M\rangle| \leq 1/N$.

Numerical data for the spin gap at $4 \leq L \leq 14$ is nicely fitted by

$$\mathsf{E}_{\Sigma^z=0,S^z=1}(L) = \mathsf{E}_{\Sigma^z=0,S^z=1}(\infty) + \frac{a}{L}$$

Parameters for this fit for $N = 3$ and various values of Δ:

Δ	0	0.2	0.4	0.8	1.0	1.2
$\frac{\mathsf{E}_{\Sigma^z=0,S^z=1}(\infty)}{J}$	0.139(5)	0.134(8)	0.166(5)	0.200(1)	0.208(1)	0.214(2)
$\frac{a}{J}$	2.78(4)	3.35(6)	3.19(4)	3.079(7)	3.088(7)	3.13(2)

At $\Delta = 1$ agrees with the result of Kawano, Takahashi:

$$\mathsf{E}_{\Sigma^z=0,S^z=1}(\infty) = 0.27(7)J\,.$$

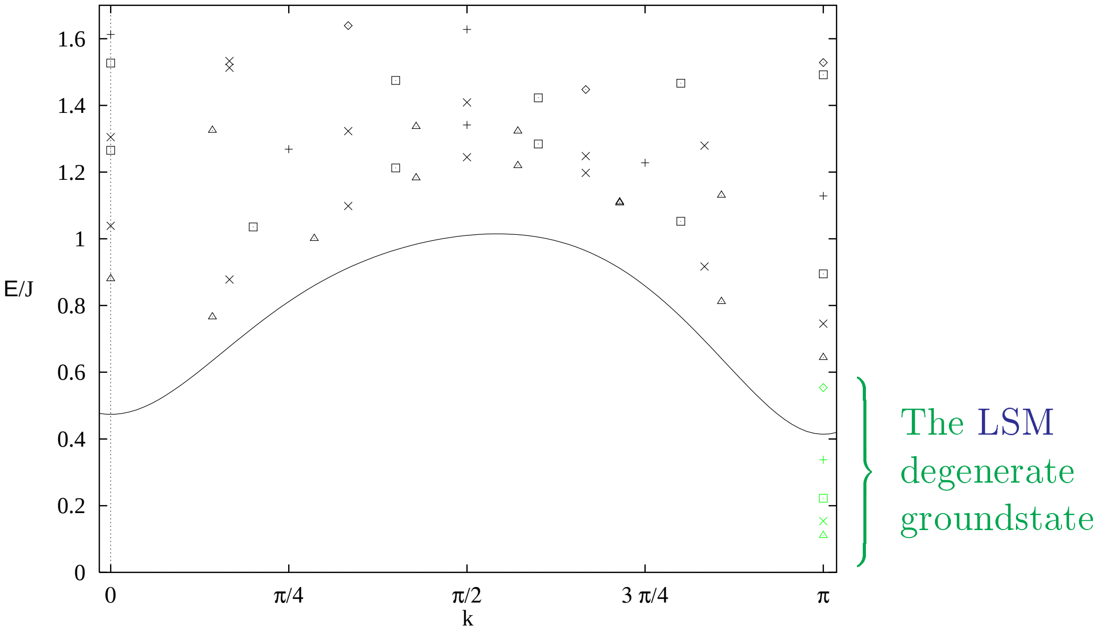
Take the limit $N \to \infty$ and formally set $\alpha_N/N \to 1$ (it actually behaves as $\alpha_N \approx 0.44N$)
$\longrightarrow$ at $\Delta = 1$:

$$\mathsf{E}_{\Sigma^z=0,S^z=1}(\infty) = 0.390(6)J\,, \qquad a = 5.72(4)J\,.$$

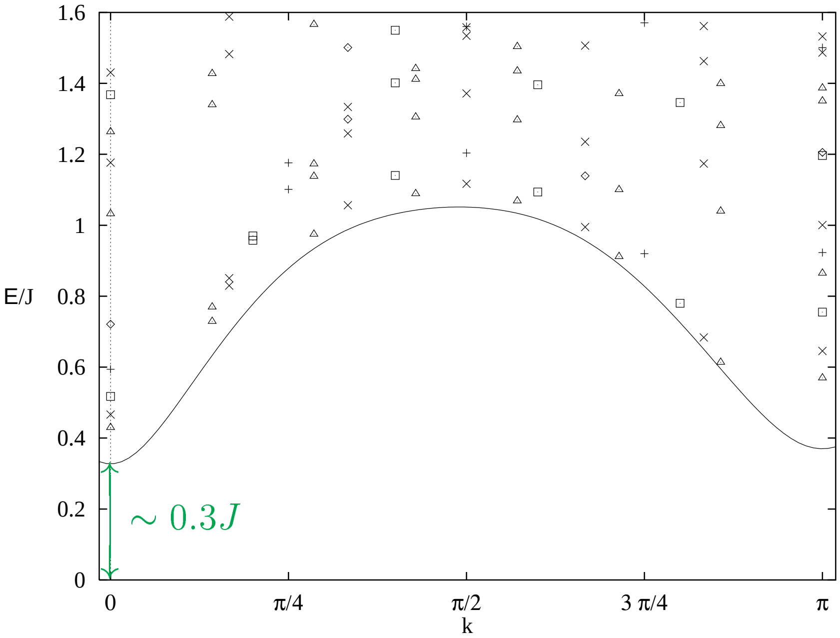
Note: After a crossover region, finite-size effects should become smaller than $1/L$. So, the above numbers should be regarded as lower bounds for rather than accurate estimates of the spin gap.

The low-lying spectrum for $N = 3$, $\Delta = 1$

$S = 0$:

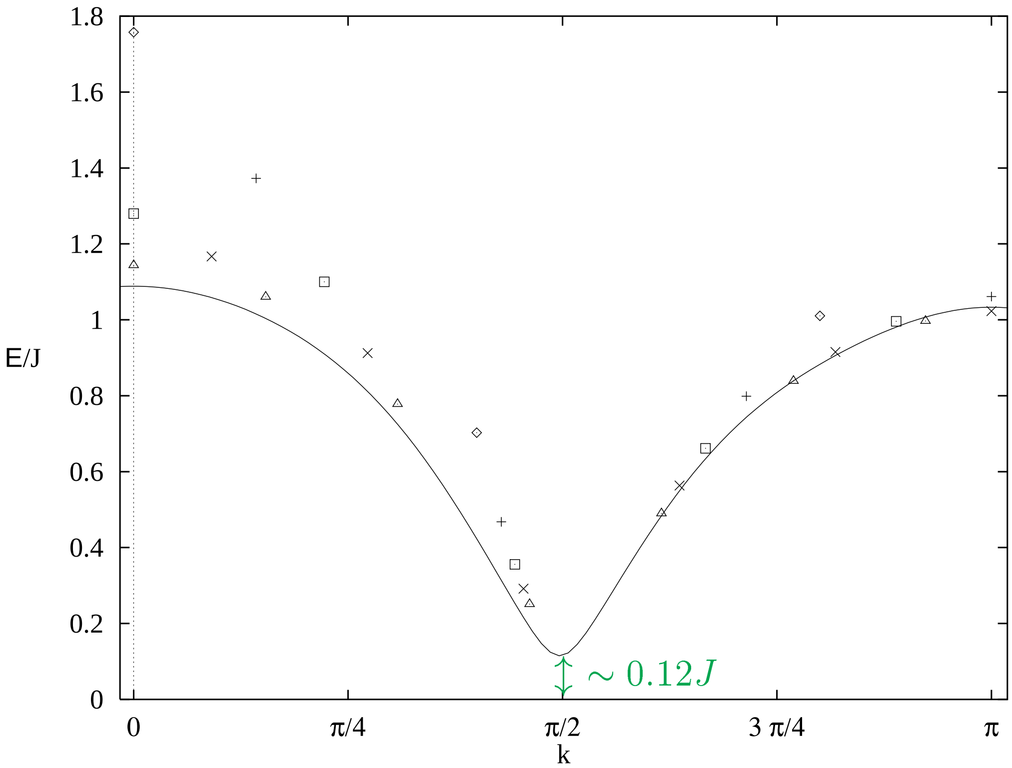


$S = 1$:



Symbols are for $L = 6$ ($\diamond$), $L = 8$ ($+$), $L = 10$ ($\boxdot$), $L = 12$ ($\times$) and $L = 14$ ($\triangle$), respectively. The lines denote extrapolations $L \to \infty$ of the lower boundary.

The spinon for $N = 3$, $\Delta = 1$



The 'spinon' of the strong-coupling effective Hamiltonian, *i.e.* lowest gaps in the sector with $\Sigma^z = 1/2$ and total spin $S = 1/2$. The symbols are for $L = 5$ ($\diamond$), $L = 7$ ($+$), $L = 9$ ($\boxdot$), $L = 11$ ($\times$) and $L = 13$ ($\triangle$), respectively. The line is an extrapolation of the dispersion curve to the thermodynamic limit.

Transitions between plateaux

If the groundstate for two neighbouring plateaux are unique for $J = 0$, the transition between them is described by an effective spin-1/2 XXZ-chain at first order in J.

(Totsuka, Phys. Rev. **B57** (1998) 3454,
Mila, cond-mat/9805029,
Tandon, Lal, Pati, Ramasesha, Sen, cond-mat/9806111)

The following properties therefore carry over from the XXZ-chain to transitions between plateaux:

- The magnetization close to a plateau boundary is of the Dzhaparidze-Nersesyan-Pokrovsky-Talapov type
$$\langle M \rangle - M_c \sim \sqrt{|h - h_c|} \, .$$
- The correlation exponents at plateau boundaries are given by
$$\eta_z = 2 \, , \qquad \eta_{xy} = \frac{1}{2} \, .$$

These results are in fact predicted to be universal !

Remark: If the effective XXZ-anisotropy turns out to be large enough ($\Delta_{\text{eff.}} > 1$), further plateaux appear between the two at $J = 0$. (This is one way to realize condition ($*$) with $l = 2$).

Summary

- The strong-coupling analysis provides an elementary way to understand the appearance of plateaux in magnetization curves and the related quantization condition of the magnetization.
- Frustated ladders (*i.e.* with PBC) are clearly gapped for $N = 3$ and probably for all N at strong coupling ($J' \gg J$).
- The transitions between plateaux are described by effective Hamiltonians at first order in J/J'.

Some open problems

- Does the gap of the $N = 3$ leg ladder system with PBC close for $J' > 0$?
  (At present, there seems to be no consensus about the prediction from a field-theoretical analysis of the weak-coupling limit $J' \ll J$ – see e.g. Arrigoni, Phys. Lett. **A215** (1996) 91 and Totsuka, Suzuki, J. Phys. A: Math. Gen. **29** (1996) 3559).

- What is the low-energy effective field theory corresponding to the strong-coupling Hamiltonian ?
  For example, is spinon-spinon scattering elastic ?