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Magnetization plateaux and jumps in a class of frustrated ladders: A simple route to a complex behaviour

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Abstract

We study the occurrence of plateaux and jumps in the magnetization curves of a class of frustrated ladders for which the Hamiltonian can be written in terms of the total spin of a rung. We argue on the basis of exact diagonalization of finite clusters that the ground state energy as a function of magnetization can be obtained as the minimum - with Maxwell constructions if necessary - of the energies of a small set of spin chains with mixed spins. This allows us to predict with very elementary methods the existence of plateaux and jumps in the magnetization curves in a large parameter range, and to provide very accurate estimates of these magnetization curves from exact or DMRG results for the relevant spin chains.

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I. INTRODUCTION

It is by now well established that the magnetization curve of a low-dimensional magnet does not always correspond to a smooth increase between zero magnetization and saturation but can exhibit plateaux at some rational values of the magnetization (see e.g. [1–8]). The experimental investigation of this effect has attracted a lot of attention recently (see e.g. [9–12]), and frustrated systems emerge as prominent candidates. In fact, a number of papers have convincingly demonstrated that frustrated systems can indeed exhibit plateaux. However, in the analysis of any specific model, the proof of the existence of a plateau usually relies on quantum field theory methods, while the actual calculation of the magnetization curves is performed e.g. via exact diagonalizations of finite clusters. In that respect, models that allow for a simpler and unified analysis would be welcome.

In this paper, we analyze a class of models for which precise calculations can be performed, and for which the occurrence of plateaux and jumps can be explained in very simple terms and, to a certain extent, proved. These models are a class of N-leg $S = 1/2$ ladders in an external magnetic field h described by the Hamiltonians:

$$H = J \sum_{x=1}^{L} \left(\sum_{i=1}^{N} \vec{S}_{i,x} \right) \cdot \left(\sum_{j=1}^{N} \vec{S}_{j,x+1} \right) + J' \sum_{x=1}^{L} \frac{1}{2} \left(\left(\sum_{i=1}^{N} \vec{S}_{i,x} \right)^2 - \frac{3N}{4} \right) - h \sum_{x=1}^{L} \sum_{i=1}^{N} S^z_{i,x} . \quad (1.1)$$

The particularity of these ladders is that the Hamiltonian depends only on the total spin of each rung $\vec{T}_x = \sum_{i=1}^{N} \vec{S}_{i,x}$. As a consequence, the total spin of a rung is a good quantum number, and the eigenvalues of H can be classified according to the value T_x of the total spin of each rung. In other words, the diagonalization of H is equivalent to diagonalizing the family of Hamiltonians $H(\{T_x\})$

$$H(\{T_x\}) = J \sum_{x=1}^{L} \vec{T}_x \cdot \vec{T}_{x+1} + J' \sum_{x=1}^{L} \frac{1}{2} \left(\vec{T}_x^2 - \frac{3N}{4} \right) - h \sum_{x=1}^{L} T^z_x . \quad (1.2)$$

where $\vec{T}_x^2 = T_x(T_x + 1)$, and $T_x = N/2, N/2 - 1, \ldots$. So the problem is equivalent to spin chains in a magnetic field with different values of the spin at each site.

Although the main ideas of the analysis could be extended to the general case, we have decided for the sake of simplicity to consider only the cases $N = 2$ and 3 in this paper. For $N = 2$, this model can be considered as the $J = J_\times$ special case of a two-leg ladder with an additional diagonal coupling $J_\times$ (see Fig. 1a), *i.e.*

$$\begin{aligned} H = J \sum_{x=1}^{L} \left(\vec{S}_{1,x} \cdot \vec{S}_{1,x+1} + \vec{S}_{2,x} \cdot \vec{S}_{2,x+1} \right) + J' \sum_{x=1}^{L} \vec{S}_{1,x} \cdot \vec{S}_{2+1,x} \\ + J_\times \sum_{x=1}^{L} \left(\vec{S}_{1,x} \cdot \vec{S}_{2,x+1} + \vec{S}_{2,x} \cdot \vec{S}_{1,x+1} \right) - h \sum_{x=1}^{L} \sum_{i=1}^{2} S^z_{i,x} . \quad (1.3) \end{aligned}$$

The ground state phase diagram of the Hamiltonian (1.3) has been studied extensively using DMRG [13–15], series expansions [16], matrix product states [17] and bosonization [18,19].

Similarly for $N = 3$, the model (1.1) arises as the $J = J_\times$ special case of the cylindrical three-leg ladder with additional diagonal couplings shown in Fig. 1b) whose Hamiltonian is given by

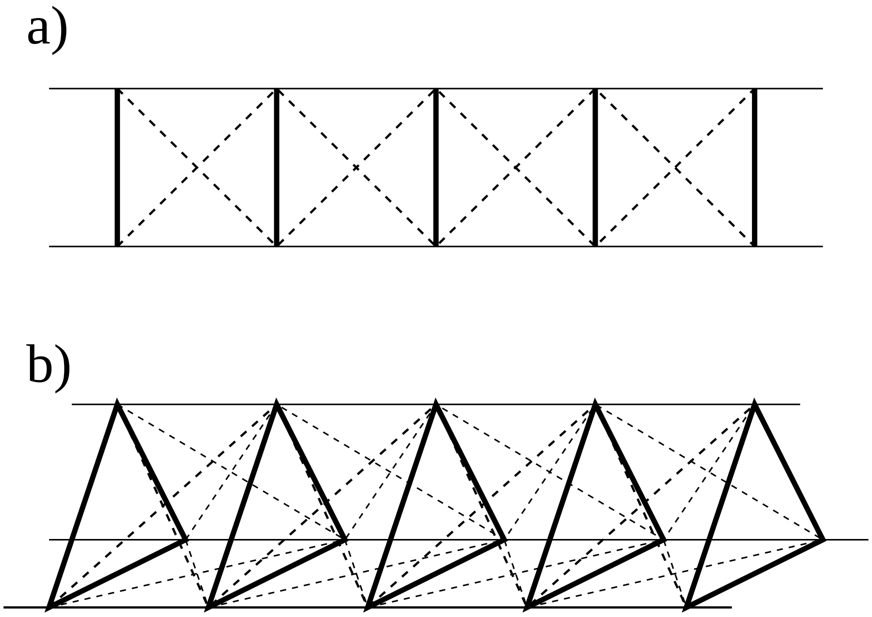

FIG. 1. Geometry of the a) two-leg and b) three-leg ladders considered in the present paper. The thick full lines denote coupling J', the thin full lines coupling J and the dashed lines coupling $J_\times$. Throughout this paper we use $J = J_\times$.

$$H = J \sum_{x=1}^{L} \sum_{i=1}^{3} \vec{S}_{i,x} \cdot \vec{S}_{i,x+1} + J' \sum_{x=1}^{L} \sum_{i=1}^{3} \vec{S}_{i,x} \cdot \vec{S}_{i+1,x} + J_\times \sum_{x=1}^{L} \sum_{i=1}^{3} \vec{S}_{i,x} \cdot \left(\vec{S}_{i-1,x+1} + \vec{S}_{i+1,x+1} \right) - h \sum_{x=1}^{L} \sum_{i=1}^{3} S^z_{i,x} \,. \tag{1.4}$$

Ground state properties of similar three- (and four-) leg ladders have been investigated recently in [20,21].

To understand why it is much simpler to study these specific frustrated ladders, we first note that one way to calculate the magnetization as a function of the field consists in first calculating the ground state energy as a function of magnetization $\langle M \rangle = 2T^z_{\text{tot}}/(LN)$ (where $T^z_{\text{tot}} = \sum_{x=1}^{L} T^z_x$) for zero field. The magnetization curves can then be constructed from this using the identity $h = \partial E / \partial T^z_{\text{tot}}$ [1]. It turns out that, for the present model, the ground state energy as a function of magnetization does *not* require a calculation of the ground state energy in all sectors $\{T_x\}$ but can be deduced from a few simple sectors only. Of course, this is useful numerically because these sectors are simpler to study than the original model, but the main advantage is qualitative since it leads to a simple interpretation of the accidents - plateaux and jumps - of the magnetization curve, which are all related to level crossings between different sectors.

[1]Since the magnetic field is coupled to a conserved quantity in (1.1) and (1.2), one has $E(T^z_{\text{tot}}, h) = E(T^z_{\text{tot}}, 0) - hT^z_{\text{tot}}$. From this one obtains a finite-size formula for the transition between ground states in T^z_{tot} and $T^z_{\text{tot}} + 1$: $h = E(T^z_{\text{tot}} + 1, 0) - E(T^z_{\text{tot}}, 0)$.

II. THE TWO-LEG CASE

First we consider the case of two legs. This case is particularly simple because a large number of eigenstates can be constructed exactly. The basic idea is the following: The total spin of each rung can be 0 or 1 in that case. If it is 0, then there is no coupling with the neighbouring rungs (for the present model this appears to have been noticed first in [22]). So any state with N_t spatially separated triplets on the rungs in a sea of singlets is an eigenstate of the Hamiltonian (1.1) with energy

$$E_{st}(N_t) = -\frac{3}{4}J'L + J'N_t\,, \tag{2.1}$$

($N_t \leq L/2$ due to the condition of spatial separation). The lowest energy among (2.1) for a given magnetization $\langle M\rangle$ is found when all triplets are polarized, *i.e.* for the smallest possible N_t. Then one has $\langle M\rangle = N_t/L$. With fully polarized triplets one can also construct exact eigenstates of the Hamiltonian (1.1) for $L/2 \leq N_t \leq L$. Namely one puts one fully polarized triplet every second rung and fills the remaining polarized triplets in the remaining rungs. The energy of such a state is $E_{st}(N_t) = -\frac{3}{4}J'L + J'N_t + (2N_t - L)J$. To summarize, we give the formula for the lowest energy among these exact eigenstates for a given magnetization $\langle M\rangle$

$$E_{st}(\langle M\rangle) = \begin{cases} \left(-\frac{3}{4} + \langle M\rangle\right) J'L & \text{for } 0 \leq \langle M\rangle \leq \frac{1}{2}, \\ \left(-\frac{3}{4} + \langle M\rangle\right) J'L + 2\left(\langle M\rangle - \frac{1}{2}\right) JL & \text{for } \frac{1}{2} \leq \langle M\rangle \leq 1. \end{cases} \tag{2.2}$$

In the limit where $J' \gg J$ the ground state is expected to be found among these states for any magnetization since this is the only way to minimize the number of triplets. However if J' is small enough - and certainly if it were negative and large - it will be more favourable to put triplets everywhere because the energy gain due to fluctuations between neighbouring triplets will dominate. The energy obtained by putting triplets (not necessarily polarized) on *each* rung is given by

$$E_{tt} = \frac{1}{4}J'L + JE^{S=1}(L, S^z)\,, \tag{2.3}$$

where $E^{S=1}(L, S^z)$ is the energy of an $S = 1$ chain with coupling constant 1, length L and a given S^z-sector.

We have checked for finite ladders using exact diagonalizations for up to 24 sites in total ($L = 12$ in (1.3)) that the states corresponding to (2.2) and (2.3) are in fact the only ground states which arise in an external magnetic field h for antiferromagnetic $J, J' > 0$, apart from special values of the magnetic field for which there seems to be a jump in the magnetization. Then assuming that this remains true in the thermodynamic limit, a very simple discussion of the magnetization curve can be given. The starting point is the energy as a function of magnetization for the relevant states, namely E_{st} and E_{tt}. For E_{st} (Eq. (2.2)) we have analytic expressions. For E_{tt} (Eq. (2.3)), we need the magnetization curve of a spin-1 chain. Since values were only quoted in the literature for rather small systems [23,24], we have computed it for periodic boundary conditions and $L \leq 60$ using

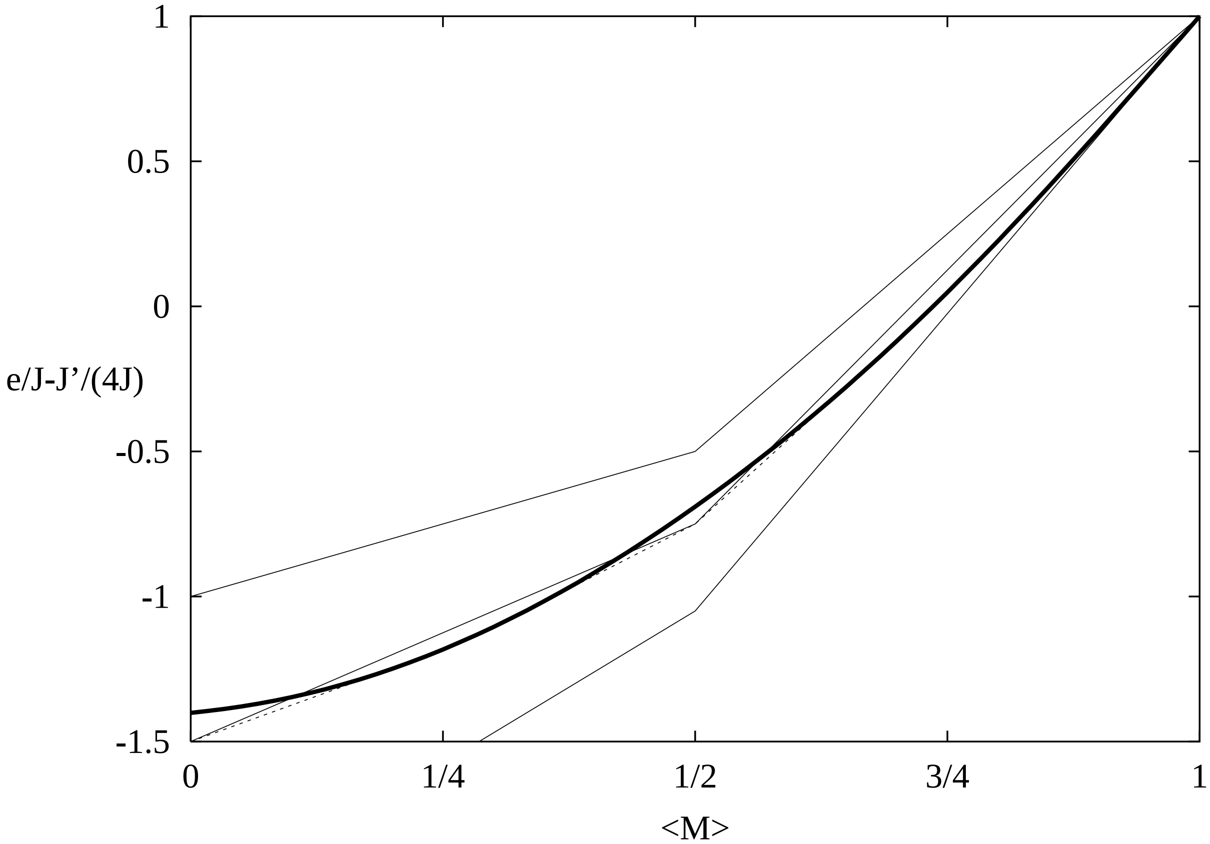

FIG. 2. Ground state energy per site versus magnetization. Bold line: Spin-1 chain Eq. (2.3). Thin lines: Eq. (2.2) for $J'/J = 1$, 1.5 and 2.1 (from top to bottom). Dashed lines: Maxwell constructions required for $J'/J = 1.5$.

White's DMRG method [25,26]. In all computations we have performed around 30 sweeps at the target system size increasing the number of kept states up to $m = 400$ during the final sweeps. The large number of sweeps was necessary because of the choice of periodic boundary conditions for the chains. To test the reliability of our calculation, we have compared our estimates of the ground state energy per site e_∞ and of the gap to magnetic excitations Δ_∞ with available results. An estimate for these two quantities is obtained by applying a Shanks transformation to our data for $L = 20$, 40 and 60: $e_\infty = -1.401484(5)$ and $\Delta_\infty = 0.4106(2)$. Although we did not try to push the calculation as far as possible since it had to be repeated for all magnetizations, these estimates compare well with the estimates obtained in earlier works which were aiming at as high accuracy as possible: Ref. [27] obtained $e_\infty = -1.401484038971(4)$, $\Delta_\infty = 0.41050(2)$ using DMRG and ref. [28] estimated $e_\infty = -1.401485(2)$, $\Delta_\infty = 0.41049(2)$ by exact diagonalization of chains with length up to $L = 22$ sites. In the following, we will use the results for 60 sites without any extrapolation. This gives an approximation of the ground state energy of an infinite chain with an accuracy of 10^{-4}, which is more than enough for the present discussion.

The results for the energy as a function of magnetization are plotted in Fig. 2 for different values of J'/J. To make the comparison between the different cases easier, we have shifted the energies by $J'/(4J)$ so that E_{tt} is independent of J'. Then the result depends only on

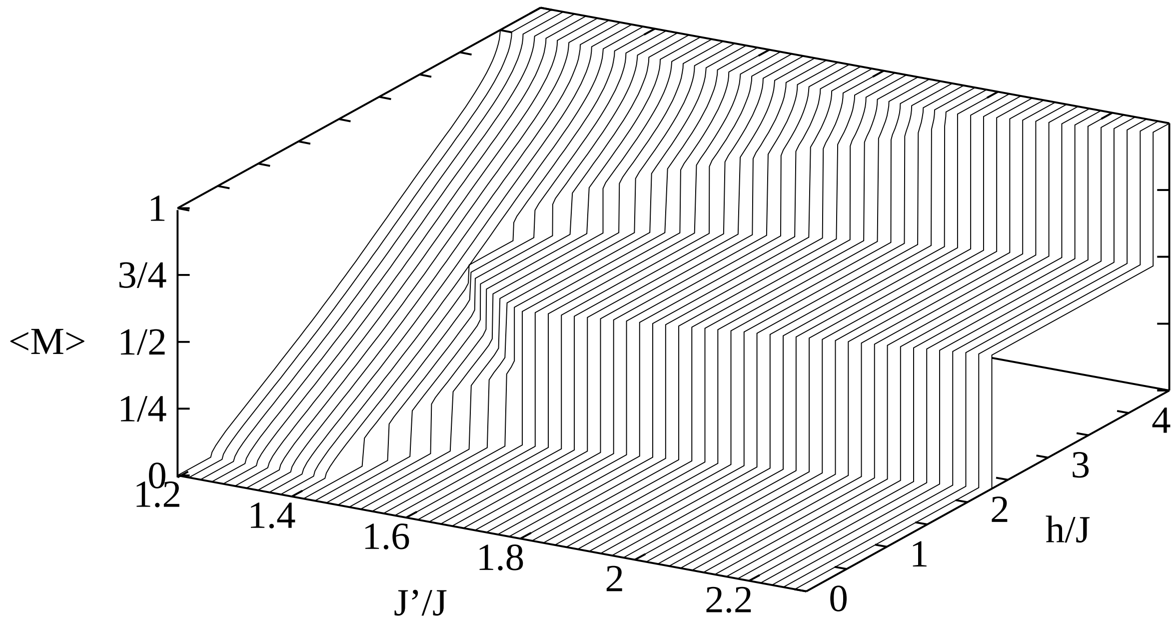

FIG. 3. Magnetization curves of the two-leg ladder Eq. (1.1).

the position of E_{st} with respect to E_{tt}.

If $J' > 2J$, E_{st} is always below E_{tt}. The energy is then a piece–wise linear function, and the reconstruction of the magnetization curve is straightforward. The slopes of the two pieces correspond to the two critical fields h_{c_1} and h_{c_2}. Below h_{c_1}, the magnetization is identically zero ($\langle M \rangle = 0$), it jumps at h_{c_1} to half the saturation value ($\langle M \rangle = 1/2$), remains constant up to h_{c_2} and then jumps again to the saturation value ($\langle M \rangle = 1$). This behaviour has already been predicted in Ref. [6] on the basis of a strong coupling analysis. The corresponding transition fields h_{c_1} and h_{c_2} are computed easily from Eq. (2.2). One finds that

$$h_{c_1} = J' \,, \qquad\qquad h_{c_2} = 2J + J' \,. \tag{2.4}$$

If on the contrary J' is small enough, E_{tt} is always below E_{st}, and the magnetization curve is identical to that of a spin-1 chain. In particular, it raises smoothly between h_{c_1} and h_{c_2} and has no discontinuity at these points.

In the intermediate region, the situation is far more complicated because the two curves intersect several times. Increasing J' from small values, E_{st} first touches E_{tt} at $\langle M \rangle = 1/2$ for $J'/J = 1.3807(5)$. Beyond but close enough to that value, there will thus be two intersections below and above $\langle M \rangle = 1/2$. However this is not the end of the story since the energy given by $\min(E_{tt}, E_{st})$ is no longer convex. So one has to perform Maxwell constructions on each side of the point $\langle M \rangle = 1/2$. They are shown as dashed lines in Fig. 2. The slopes of the energy on each side of $\langle M \rangle = 1/2$ then give the two critical fields between which a plateau $\langle M \rangle = 1/2$ exists. At both critical fields there will be a discontinuity in the magnetization since the slope of the energy is constant over a finite range of magnetization.

Increasing J' further, another transition occurs where E_{st} touches E_{tt} at $\langle M \rangle = 0$, *i.e.*

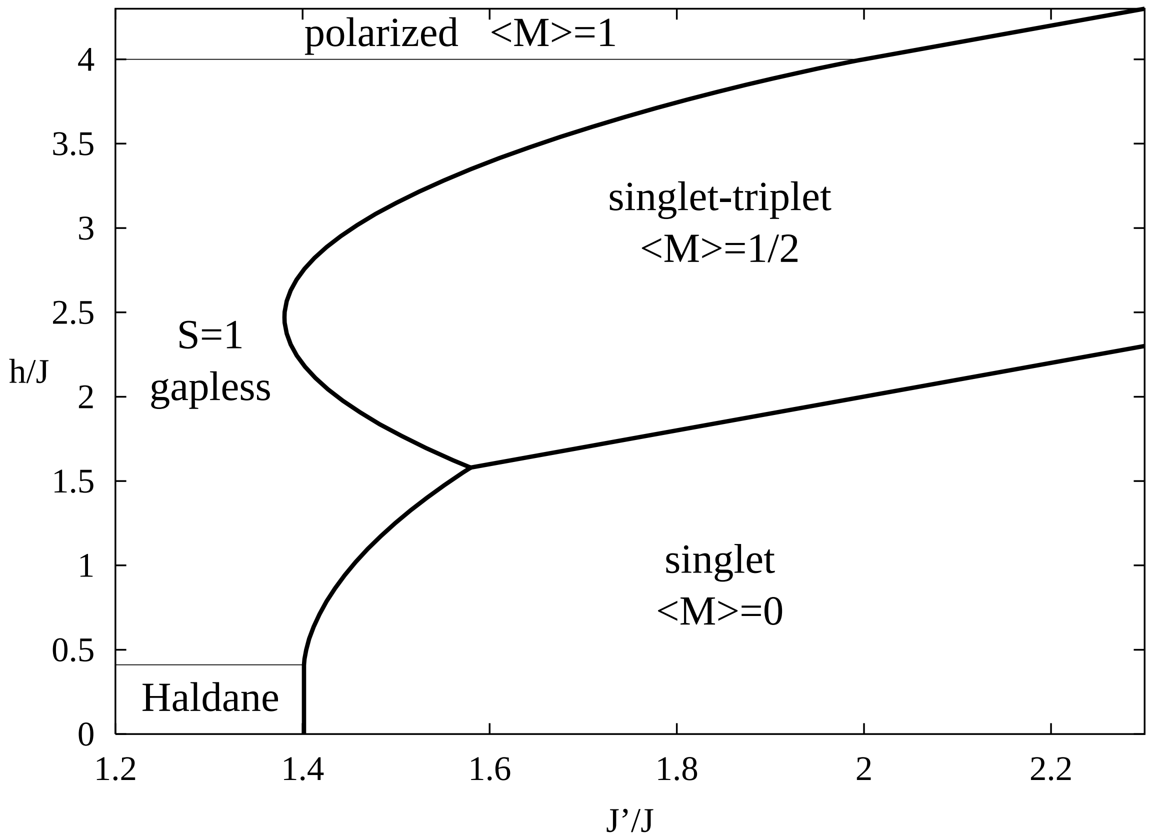

FIG. 4. Ground state phase diagram for the two-leg ladder. The heavy lines denote first order transitions, the thin ones second order transitions.

when $J'/J = -e_\infty = 1.401484...$ [2]. Beyond that value, a Maxwell construction is again necessary resulting in a discontinuity of the magnetization at the corresponding critical field.

The above conclusions are illustrated by Fig. 3 which shows the evolution of the magnetization curves with J' obtained from the DMRG data. It is also straightforward to construct the full ground state phase diagram of the two-leg ladder as a function of J'/J and h – see Fig. 4.

For $h/J < \Delta_\infty$ and $J'/J < -e_\infty$, the ground state is the Haldane gap ground state [29] with a gap to magnetic excitations. For larger magnetic fields one finds that the ground state is given by the corresponding one of the $S = 1$ chain. The magnetization curve in this region is smoothly varying demonstrating the presence of gapless magnetic excitations. In this phase, the $\langle M \rangle = 1/2$ plateau opens at $J'/J = 1.3807(5)$, $h/J = 2.4706(2)$. Typically, the opening of a plateau as a function of a coupling constant would have to occur via a Kosterlitz-Thouless transition. Here it is clearly of a different type due to the fact that the opening of the $\langle M \rangle = 1/2$ plateau occurs by a crossing of the energy levels Eq. (2.2) and

[2]The critical values of J' for $\langle M \rangle = 0$ and $\langle M \rangle = 1/2$ are surprising close but can be distinguished safely with our accuracy.

Eq. (2.3) at $S^z = L/2$.

The transitions between the $S = 1$ gapless phase and the $\langle M\rangle = 0$ and $1/2$ plateaux are first order transitions as a function of the external magnetic field. In the $(J'/J,\langle M\rangle)$–plane one would therefore find finite regions in the phase diagram where the system phase-separates into regions with finite $S = 1$ chains and regions which singlets on all rungs (for $\langle M\rangle < 1/2$) or alternating singlets and polarized triplets (for $\langle M\rangle > 1/2$).

The $S = 1$ gapless phase, the singlet $\langle M\rangle = 0$ phase and the $\langle M\rangle = 1/2$ plateau meet at $h/J = J'/J = 1.5796(4)$.

III. THREE LEGS

For the Hamiltonian of Eq. (1.1) with $N = 3$ the relevant eigenstates are:

1. Spin-3/2 states on all rungs with energy

$$E_{3/2} = \frac{3}{4}J'L + JE^{S=3/2}(L, S^z)\,, \tag{3.1}$$

2. alternating spin-1/2 and -3/2 on the rungs with corresponding energy

$$E_{3/2-1/2} = JE^{S=3/2-1/2}(L, S^z)\,, \tag{3.2}$$

3. spin-1/2 on each rung with energy

$$E_{1/2} = -\frac{3}{4}J'L + JE^{S=1/2}(L, S^z)\,. \tag{3.3}$$

Here $E^{\bullet}(L, S^z)$ is the energy of the corresponding spin-chain with coupling constant 1, length L and a given S^z-sector. It should be noted that each spin-1/2 state comes with two chiralities. The eigenvalues of the Hamiltonian of Eq. (1.1) are independent of these chiralities, which is clear from the rewriting of Eq. (1.2). This degeneracy gives rise to an entropy ln(2) for each rung with spin 1/2.

On ladders with $L \leq 8$ (a total of up to 24 sites) we have again checked numerically that the ground states in the presence of a magnetic field can always be found among Eq. (3.1)–(3.3) except for special values of the field where the magnetization jumps. Then we have again used DMRG to compute $E^{S=3/2}(60, S^z)$ and $E^{S=3/2-1/2}(60, S^z)$. Since we are not aware of any previous discussion of the magnetization curve of the $S = 3/2 - 1/2$ ferrimagnetic chain, we present it in Fig. 5. This curve is very similar to the magnetization curve of the $S = 1 - 1/2$ ferrimagnetic chain [30,31], the main difference being the plateau value of $\langle M\rangle$ which is 1/3 in the latter case.

$E^{S=1/2}(\infty, S^z = L\langle M\rangle/2)/L$ was obtained from the Bethe ansatz equations for the thermodynamic limit in the spirit of [32] (the actual program used is a small modification of the one described in [5]). The accuracy of our DMRG results can be assessed by comparison to earlier DMRG studies. We find $E^{S=3/2}(60, 0)/60 \approx -2.82879$ and

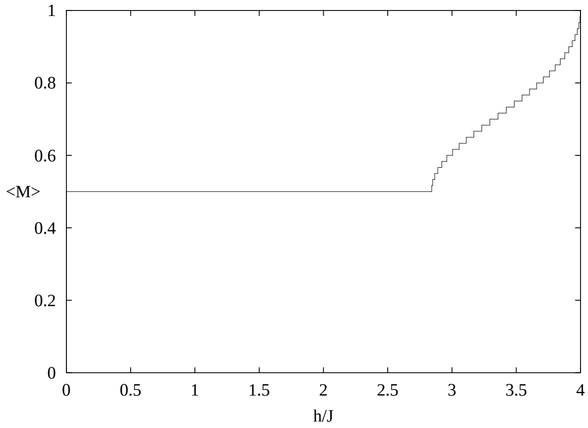

FIG. 5. Magnetization curve of the $S = 3/2 - 1/2$ ferrimagnetic chain for $L = 60$.

$E^{S=3/2-1/2}(60,0)/60 \approx -0.98362$ which should be compared to the extrapolated values $e_\infty^{S=3/2} = -2.82833(1)$ [33] and $e_\infty^{S=3/2-1/2} = -0.98362$ [34], respectively [3].

Proceeding as for the two-leg ladder, the magnetization curves of Eq. (1.1) for $N = 3$ can be constructed from these data for different values of J'/J. The evolution with J'/J is shown in Fig. 6. Figure 7 shows a projection onto the J'/J-h plane. Construction of this ground state phase diagram is somewhat more involved than Fig. 4 and slightly less accurate. We therefore do not quote any number for points in Fig. 7, but all transitions should be accurate to the order of the width of the lines in the figure.

For $J' \lesssim 1.557J$, the magnetization curve of the three-leg ladder is identical to that of the $S = 3/2$ chain. If $J' \geq 2J$, the magnetization process proceeds by polarizing $S = 1/2$ states at $h_{c_1} = 2J$. Then the magnetization jumps from the polarized $S = 1/2$ state ($\langle M \rangle = 1/3$ in the language of the three-leg ladder) to the polarized state of the ferrimagnetic $S = 3/2 - 1/2$ chain ($\langle M \rangle = 2/3$ in the language of the three-leg ladder) at

$$h_{c_2} = J + \frac{3}{2} J' \, . \tag{3.4}$$

Finally, the magnetization jumps again polarizing the complete system at

$$h_{c_3} = 3J + \frac{3}{2} J' \tag{3.5}$$

in this region $J' \geq 2J$.

[3] Our result for the antiferromagnetic gap $\Delta_L = E^{S=3/2-1/2}(L, L/2+1) - E^{S=3/2-1/2}(L, L/2)$ is $\Delta_{60} \approx 2.8420$. This cannot be directly compared to the corresponding result of [34] since that DMRG computation was performed for open boundary conditions and in this case a *bound state* with the boundary is formed. Repetition of our computation with open boundary conditions lead to $\Delta_{60}^{(o)} \approx 1.8558$ which compares well with the extrapolated value $\Delta_\infty^{(o)} = 1.8558(1)$ [34]. Also for open boundary conditions, the next magnetic excitation lies above the antiferromagnetic gap, *i.e.* it can indeed be expected that the magnetization process becomes independent of the boundary conditions in the thermodynamic limit.

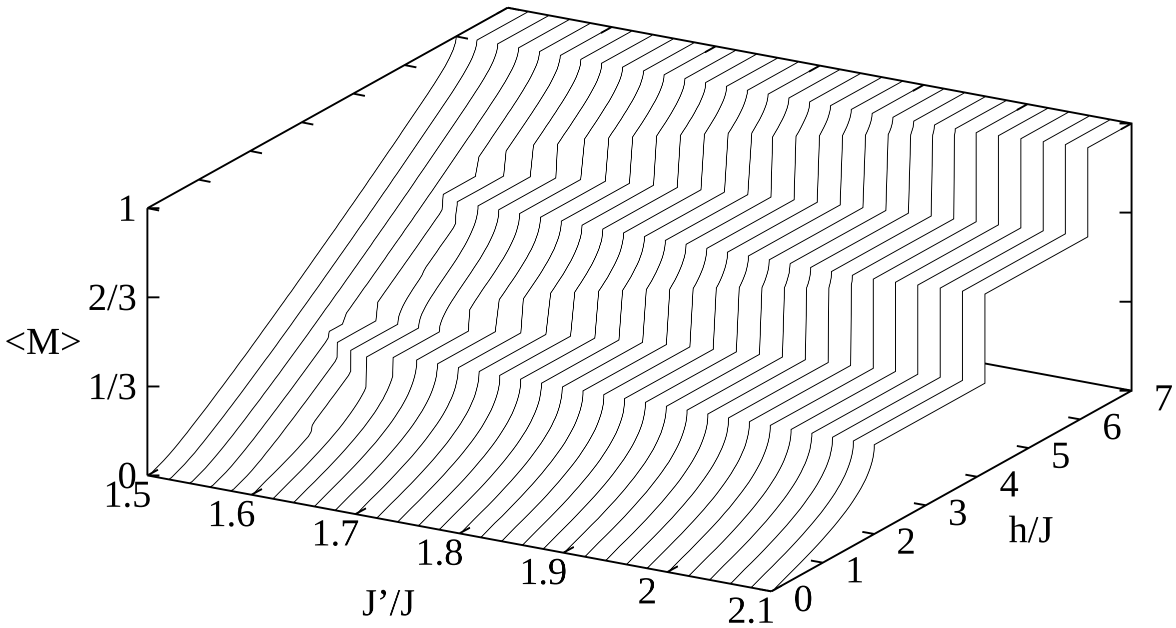

FIG. 6. Magnetization curves of the three-leg ladder (Eq. (1.1)).

For intermediate J' partially polarized states of the ferrimagnetic $S = 3/2 - 1/2$ chain also contribute to the magnetization process, and the plateau state which has $\langle M \rangle = 1/2$ in the language of the $S = 3/2 - 1/2$ chain appears. When translated into the language of the three-leg ladder the latter leads to $\langle M \rangle = 1/3$ and it is this number which we quote in the corresponding region of Fig. 7. At $J' \approx 1.645J$, there is a first order transition between this plateau state and the fully polarized state of the $S = 1/2$ chain. Since the magnetization is the same in both states, there is no jump in the magnetization. Still, the transition occurs via a level crossing and it is therefore first order in the sense that many correlators on the $\langle M \rangle = 1/3$ plateau are discontinuous across this line.

A remarkable property of the Hamiltonian of Eq. (1.1) with $N = 3$ is that it has a plateau at $\langle M \rangle = 2/3$ without giving rise to a gap (or plateau) at $\langle M \rangle = 0$. On general grounds both of them would be permitted for a frustrated $N = 3$-leg ladder when translational invariance is spontaneously broken in the ground state to a period $p = 2$ [4,5,35,36]. The present situation should be contrasted to the case of the regular cylindrical three-leg ladder [4,5] which has a plateau at $\langle M \rangle = 0$ (*i.e.* a gap [37–39]) and presumably no plateau at $\langle M \rangle = 2/3$ [40]. In that case, the plateau at $\langle M \rangle = 0$ is a direct consequence of the coupling of the spin and the chirality of each triangular rung. In the present case, there is no plateau because the chirality is completely decoupled from the spin. We would also like to emphasize that there is a residual entropy both on the $\langle M \rangle = 1/3$ and on the $\langle M \rangle = 2/3$ plateaux of $\ln(2)$ and $\ln(2)/2$, respectively.

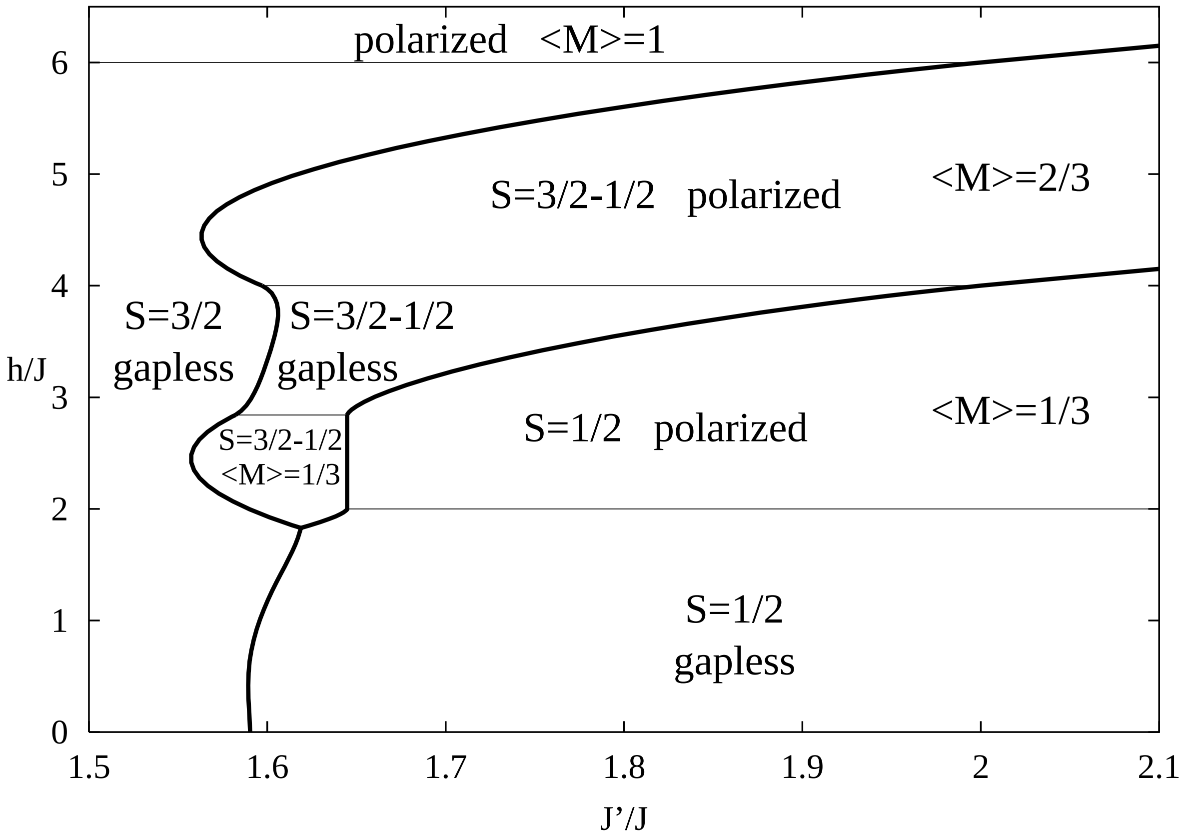

FIG. 7. Ground state phase diagram for the three-leg ladder. The heavy lines denote first order transitions, the thin ones second order transitions.

IV. CONCLUSION

We have proposed and studied a class of frustrated ladders for which the magnetization curve can be calculated by elementary methods once the magnetization of a few, much simpler systems is known. There are many further models in this class beyond the one studied in the present paper. For example, the models studied in [41] and [42] come to mind as natural generalizations of the two- and three-leg ladders which we have studied. A modified version of the model of [41] has in fact been proposed to describe the $S = 1/2$ trimer system $Cu_3Cl_6(H_2O)_2{\cdot}2H_8C_4SO_2$ [43,44]. Since the synthesis and investigation of many quasi-one dimensional magnets is under way, also the models discussed here should soon become relevant to experimental systems.

A remark is in order regarding a small detuning of the coupling constants from the case where the reasoning of the present paper applies. After such a detuning, the spins on each rung are no longer conserved and therefore one will find avoided crossings rather than real crossings. Since the plateau-state is gapped, magnetization plateaux are stable against small perturbations but a softening of the transitions between them is to be expected. This can indeed be seen easily in the strong-coupling region $J' \gg J, J_\times$ where magnetization plateaux can be shown to exist using perturbative arguments and transitions between them can be described by first-order effective Hamiltonians (see e.g. [3–6,9,35,40,45]). With the choice

$J = J_\times$ one eliminates the kinetic energy part of the first-order effective Hamiltonian and therefore we find steps in the magnetization curves even at finite $J = J_\times < 2J'$ whereas for $J \neq J_\times$ one would find a smooth transition. However, the fact that we found jumps in these special models is still interesting since it points towards the possibility of steep increases of the magnetization in frustrated models in general, a possibility not emphasized so far in that context.

The main advantage of the models Eq. (1.1) is that the features of the magnetization curve - plateaux and jumps - can be traced back to level crossings. The underlying physical picture is thus clear and simple, and at the same time a very precise determination of the critical fields is possible. The price to pay is not horrendous - the Hamiltonian can still be written down compactly, and its visualization is straightforward. So, in the spirit of the Affleck-Kennedy-Lieb-Tasaki model of a spin-1 chain with a gap [46], we hope that these models will be a useful reference to understand the physics of the magnetization of low-dimensional magnets.

Note added

After completion of this work, we became aware of [47] which uses similar ideas to compute the magnetization curve of a two-dimensional model.

ACKNOWLEDGMENTS

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