

**Magnetization plateaux in Bethe ansatz solvable spin- $S$  ladders**M. Maslen,<sup>1</sup> M. T. Batchelor,<sup>2,3,\*</sup> and J. de Gier<sup>4,†</sup><sup>1</sup>*Department of Mathematics, Mathematical Sciences Institute, Australian National University, Canberra ACT 0200, Australia*<sup>2</sup>*Department of Theoretical Physics, Research School of Physical Sciences and Engineering, Australian National University, Canberra ACT 0200, Australia*<sup>3</sup>*Centre for Mathematics and its Applications, Mathematical Sciences Institute, Australian National University, Canberra ACT 0200, Australia*<sup>4</sup>*Department of Mathematics and Statistics, University of Melbourne, Parkville VIC 3010, Australia*

(Received 10 February 2003; published 29 July 2003)

We examine the properties of the Bethe ansatz solvable two- and three-leg spin- $S$  ladders. These models include Heisenberg rung interactions of arbitrary strength and thus capture the physics of the spin- $S$  Heisenberg ladders for strong rung coupling. The discrete values derived for the magnetization plateaux are seen to fit with the general prediction based on the Lieb-Schultz-Mattis theorem. We examine the magnetic phase diagram of the spin-1 ladder in detail and find an extended magnetization plateau at the fractional value  $\langle M \rangle = \frac{1}{2}$  in agreement with the experimental observation for the organic polyradical spin-1 ladder compound BIP-TENO.

DOI: 10.1103/PhysRevB.68.024418

PACS number(s): 75.10.Jm

**I. INTRODUCTION**

After some intensive effort, the properties of the spin- $\frac{1}{2}$  Heisenberg ladder are now well understood.<sup>1,2</sup> The physics of the model is driven by the rung basis states, which dominate in the limit of strong rung coupling  $J$ . The spin gap originating between the singlet and triplet rung states for large  $J$  is known to persist for all finite  $J$ , vanishing only at the decoupling point  $J=0$  where the model reduces to two Heisenberg chains. More generally, the  $n$ -leg spin- $\frac{1}{2}$  Heisenberg ladders possess the rather striking property of being massive for  $n$  even and massless for  $n$  odd. The ladder models also possess interesting magnetic properties, with clear evidence of magnetization plateaux.<sup>3-5</sup> From quite general arguments, the magnetization  $M$  of the spin- $S$   $n$ -leg ladders should satisfy the discrete values

$$nS(1-M) \in \mathbb{Z}. \quad (1)$$

Although the Heisenberg ladders are not solvable in the sense of the spin- $\frac{1}{2}$  Heisenberg chain, a number of solvable ladder models have been found. These include modified models with dimer or matrix product ground states<sup>6-8</sup> and models solved by means of the Bethe ansatz. Here we consider the latter class. These models include a two-leg spin- $\frac{1}{2}$  model,<sup>9</sup> which, compared to the pure Heisenberg ladder, has an additional four-spin interaction. The model is massless in the absence of rung interactions with a transition to a massive phase at a critical (nonzero) value of the rung coupling. In this solvable model the Heisenberg rung interactions appear as chemical potentials which break the underlying  $su(4)$  symmetry. The phase diagram has been established by means of the Bethe ansatz solution.<sup>9,10</sup> In particular, magnetization plateaux are found at the values  $m=0$  and  $m=1$ , in agreement with Eq. (1). However, the Bethe ansatz calculations also reveal an infinitesimally thin magnetization plateaux at  $m=\frac{1}{2}$ , which may open up with the introduction of some anisotropy into the system. This thin plateau may be interpreted as a ‘‘plateau boundary.’’

The solvable two-leg ladder model has been generalized to an arbitrary number  $n$  of legs in which the underlying  $su(2^n)$  symmetry is broken by the Heisenberg rung interactions, which again appear as chemical potentials in the Bethe ansatz solution.<sup>11,12</sup> Solvable ladder models with Hubbard<sup>13</sup> and  $t$ - $J$  (Ref. 14) interactions have also been found. Yet others have been constructed with mixed spin<sup>15</sup> and higher symmetries arising from other known integrable models.<sup>16,17</sup> Other models<sup>18</sup> have been solved via mapping from the Hubbard model with appropriate boundary conditions. The  $su(4)$  ladder model has also been extended to include an additional free parameter.<sup>19</sup> For the solvable three-leg spin- $\frac{1}{2}$  model,<sup>11,12</sup> magnetization plateaux are found at the values  $m=\frac{1}{3}$  and  $m=1$  in agreement with Eq. (1).<sup>10</sup> An additional infinitesimally thin plateau is also seen at  $m=\frac{1}{2}$ .

In this paper we investigate the properties of the Bethe ansatz solvable two- and three-leg ladder models for general spin  $S$ . These models are defined in Sec. II. In Secs. III and IV we look respectively at the magnetization plateaux and their boundaries, and in Sec. V we give a detailed analysis of the two-leg spin-1 ladder. Our work on the solvable spin-1 ladder is motivated by the recent experimental and theoretical work on certain organic materials. For example, the compound BIP-TENO, an organic polyradical of 3,3',5,5'-tetrakis (N-tert-butylaminoxyl), was studied experimentally,<sup>20,21</sup> and found to have magnetization plateaux of 0,  $\frac{1}{2}$ , and 1. The crystal structure of this substance may be modeled effectively by a two-leg spin-1 ladder. Some models have been used to propose mechanisms by which the fractional plateau appears.<sup>22</sup> Relatively little work has been done on the spin-1 Heisenberg ladder. It has been studied in the semiclassical limit via a mapping to the nonlinear sigma model and by quantum Monte Carlo simulation and bosonization techniques.<sup>23,24</sup> Concluding remarks are given in Sec. VI.

**II. MODELS**

We consider the integrable  $n$ -leg spin- $S$  ladders, or spin tubes with periodic boundary conditions. As usual a ‘‘tube’’

is a ladder with an additional interaction between leg  $n$  and leg 1. We restrict our attention to the cases  $n=2$  and  $n=3$  with uniform spins on each leg, and not the more general mixed spin case. The spins along each leg and rung have an isotropic Heisenberg interaction, with the introduction of many-body terms to retain integrability. The  $\text{su}(2)$  spin- $S$  operators  $\mathbf{S}=(S^x, S^y, S^z)$  are defined by

$$S^x = \frac{1}{2}(S^+ + S^-), \quad S^y = -\frac{1}{2}i(S^+ - S^-),$$

$$S^z = \text{diag}\{S, S-1, \dots, -S\}, \quad (2)$$

where, for given  $S$ ,

$$S_{m',m}^+ = \sqrt{S(S+1) - m(m-1)} \delta_{m',m-1}, \quad (3)$$

$$S_{m',m}^- = \sqrt{S(S+1) - m(m+1)} \delta_{m',m+1}. \quad (4)$$

and  $m, m' = -S, -S+1, \dots, S$ . The Hamiltonian of the model is

$$H = \sum_{i=1}^L H_{i,i+1}^{\text{leg}} + \sum_{i=1}^L H_i^{\text{rung}}, \quad (5)$$

where  $L$  is the number of rungs. The leg term is given by

$$H_{i,i+1}^{\text{leg}} = P_{i,i+1}^{(2S+1)} \otimes P_{i,i+1}^{(2S+1)} \otimes \dots \otimes P_{i,i+1}^{(2S+1)} \quad (n \text{ factors}), \quad (6)$$

where

$$P_{i,j}^{(2S+1)} = \sum_{\alpha=0}^{2S} (-1)^{2S-\alpha} \prod_{\beta \neq \alpha} \frac{S_i \cdot S_j - x_\beta}{x_\alpha - x_\beta}, \quad (7)$$

with  $x_\alpha = \frac{1}{2}\alpha(\alpha+1) - S(S+1)$ . Throughout this paper, site  $L+1$  is identified with site 1. For the simplest case of  $S = \frac{1}{2}$ , one recovers the familiar Heisenberg operator. Similarly for  $S=1$  and  $S=\frac{3}{2}$ :

$$P_{i,i+1}^{(3)} = (S_i \cdot S_{i+1})^2 + S_i \cdot S_{i+1} - 1, \quad (8)$$

$$P_{i,i+1}^{(4)} = \frac{2}{9}(S_i \cdot S_{i+1})^3 + \frac{11}{18}(S_i \cdot S_{i+1})^2 - \frac{9}{8}S_i \cdot S_{i+1} - \frac{67}{32}. \quad (9)$$

The rung term has pure Heisenberg interactions, given by

$$H_i^{\text{rung}} = \sum_{l=1}^{n-\epsilon} J_l (\mathbf{S}_i^{(l)} \cdot \mathbf{S}_i^{(l+1)} - 1), \quad (10)$$

where  $\epsilon=0$  for tubes and  $\epsilon=1$  for ladders, and  $\mathbf{S}_i^{(n+1)} = \mathbf{S}_i^{(1)}$ . We take periodic boundary conditions along the ladder, and consider isotropic rung interactions ( $J_l = J$ ). It has been shown that<sup>15</sup>  $[H_{i,j}^{\text{leg}}, H_i^{\text{rung}} + H_j^{\text{rung}}] = 0$ , so  $H$  defined in Eq. (5) is also integrable for sufficiently small  $n$ .

A key ingredient in the models under consideration is that they are built from permutators. Such models can be diagonalized using the (nested) Bethe ansatz.<sup>25</sup> The  $\text{su}(N)$  Bethe ansatz equations are

$$\left( \frac{\lambda_j^{(1)} - \frac{1}{2}i}{\lambda_j^{(1)} + \frac{1}{2}i} \right)^L = \prod_{k \neq j}^{M_1} \frac{\lambda_j^{(1)} - \lambda_k^{(1)} - i}{\lambda_j^{(1)} - \lambda_k^{(1)} + i} \prod_{k=1}^{M_2} \frac{\lambda_j^{(1)} - \lambda_k^{(2)} + \frac{1}{2}i}{\lambda_j^{(1)} - \lambda_k^{(2)} - \frac{1}{2}i},$$

$$\prod_{k \neq j}^{M_r} \frac{\lambda_j^{(r)} - \lambda_k^{(r)} - i}{\lambda_j^{(r)} - \lambda_k^{(r)} + i}$$

$$= \prod_{k=1}^{M_{r-1}} \frac{\lambda_j^{(r)} - \lambda_k^{(r-1)} - \frac{1}{2}i}{\lambda_j^{(r)} - \lambda_k^{(r-1)} + \frac{1}{2}i} \prod_{k=1}^{M_{r+1}} \frac{\lambda_j^{(r)} - \lambda_k^{(r+1)} - \frac{1}{2}i}{\lambda_j^{(r)} - \lambda_k^{(r+1)} + \frac{1}{2}i}, \quad (11)$$

where in this case  $N = (2S+1)^n$ . As usual the eigenenergies of  $\sum_{i=1}^L H_{i,i+1}^{\text{leg}}$  are

$$E = L - \sum_{j=1}^{M_1} \frac{1}{(\lambda_j^{(1)})^2 + \frac{1}{4}}. \quad (12)$$

It is important to note that since permutator (6) is invariant under any ordering of the basis states, this result may be obtained using any choice of reference state (or pseudo-vacuum)  $|\Omega\rangle$  and any assignment of Bethe ansatz pseudoparticles. For each choice, however, one has to reinterpret the numbers  $M_r$  in terms of those corresponding to the ordering chosen. The rung Hamiltonian is dependent on the choice of ordering, but the change is just a rearrangement of its eigenvalues along the diagonal. We use this property to our advantage by doing calculations with that choice of ordering for which the Bethe ansatz reference state is closest to the true ground state of the system.

### A. Two-leg ladder

We turn our attention now to the specific case of the two-leg spin- $S$  ladder, for the moment in the absence of a magnetic field. The rung Hamiltonian (10) is given by

$$H^{\text{rung}} = J(\mathbf{S}^{(1)} \cdot \mathbf{S}^{(2)} - 1), \quad (13)$$

which can be rewritten as

$$H^{\text{rung}} = J \left[ \frac{(\mathbf{S}^{(1)} + \mathbf{S}^{(2)})^2 - (\mathbf{S}^{(1)})^2 - (\mathbf{S}^{(2)})^2}{2} - \mathbf{1} \right]. \quad (14)$$

It is convenient to change to the basis where the square and the  $z$ -component of the total spin of a given rung are diagonal. Now, the operators  $(\mathbf{S}^{(1)} + \mathbf{S}^{(2)})^2$ ,  $\mathbf{S}^{(1)2}$ , and  $\mathbf{S}^{(2)2}$  are all diagonal with common eigenstates. As a result we can derive the eigenvalues of  $H^{\text{rung}}$  simply by combining the eigenvalues of these operators as in the above expression. From elementary quantum mechanics, the respective eigenvalues of these operators are  $T(T+1)$ ,  $S(S+1)$ , and  $S(S+1)$ , where the total spin  $T$  can assume the values  $0, \dots, 2S$ . It follows

that, for a two-leg ladder, the  $(2S+1)^2$  rung states fall into  $2S+1$  multiplets of total spin  $T$ , with eigenvalues

$$\lambda_T = \frac{J}{2} [T(T+1) - 2S(S+1) - 2], \quad T=0, \dots, 2S, \quad (15)$$

---


$$H^{\text{rung}} = \text{diag}\{\lambda_0, \lambda_1, \lambda_1, \lambda_1, \dots, \underbrace{\lambda_T, \dots, \lambda_T}_{2T+1}, \dots, \underbrace{\lambda_{2S}, \dots, \lambda_{2S}}_{4S+1}\}. \quad (16)$$


---

In Sec. V we will look at the specific example of a two-leg spin-1 ladder in detail.

### B. Three-leg tube

We follow a similar procedure to the two-leg ladder, rewriting the Hamiltonian and changing the basis appropriately. In the case of the three-tube, the  $(2S+1)^3$  states fall into  $[3S]+1$  types of multiplet ( $[x]$  denotes the integer part of  $x$ ), with total spin  $T$ , whose eigenvalues are given by

$$\lambda_T = \frac{J}{2} [T(T+1) - 3S(S+1) - 6], \quad (17)$$

where

$$T = \frac{2S(\text{mod } 2)}{2}, \frac{2S(\text{mod } 2)}{2} + 1, \dots, 3S. \quad (18)$$

This has clear similarity to Eq. (15). However the situation now is somewhat more complicated. This is because in general there are several multiplets of given spin  $T$ ; for example two distinct doublets having the same energy in the absence of a magnetic field. What follows is an analysis of exactly how the states fall into multiplets in a three-spin system.

Let us consider the addition of three spin- $S$  objects. We first add the spins at sites (1) and (3) to get a combined spin- $S_{13}$  system, and in turn, add the spin at site (2) to this combined system to get a state of total spin  $T$ . Note that the choice of ordering of addition affects only the basis vectors used to represent a state, and not the actual state itself. The order chosen here facilitates computation of ladder eigenvalues in the next subsection. According to quantum mechanical rules for addition of angular momenta, we have

$$0 \leq S_{13} \leq 2S \quad (19)$$

and

$$|S_{13} - S| \leq T \leq S_{13} + S. \quad (20)$$

So the number of spin- $T$  multiplets is given by the number of possible values of  $S_{13}$  which satisfy Eqs. (19) and (20). There are two cases to consider.

and respective multiplicities  $m_T = 2T+1$ .

It is emphasized that Hamiltonian (6) has the same form in this new basis. The rung Hamiltonian (10) now becomes diagonal and is given by

*Case 1:  $T \leq S$ .* In this case the right inequality of Eq. (20) is automatically satisfied. The left inequality is true when  $S_{13}$  assumes values in the range defined by Eq. (19) that satisfy

$$|S_{13} - S| \leq T, \quad (21)$$

namely

$$S_{13} = S - T, S - T + 1, \dots, S + T; \quad (22)$$

and there are  $2T+1$  such values.

*Case 2:  $S \leq T$ .* We note that Eq. (19) implies that  $|S_{13} - S| \leq S$ , so the left inequality of (20) is automatically satisfied. To make the right inequality true,  $S_{13}$  must assume values in the range defined by Eq. (19) that satisfy

$$T \leq S_{13} + S, \quad (23)$$

namely,

$$S_{13} = T - S, T - S + 1, \dots, 2S; \quad (24)$$

and there are  $3S - T + 1$  such values [since  $2S = T - S + (3S - T)$ ].

To summarize these results: In a system of three spin- $S$  objects, the number of spin- $T$  multiplets [that is,  $(2T+1)$ -plets] is given by

$$\Theta(S, T) = \begin{cases} 2T+1 & S \geq T \\ 3S - T + 1 & S < T \leq 3S \end{cases} \quad (25)$$

Multiplets of the same type have the same energy under the tube Hamiltonian, but are distinguishable by their value of  $S_{13}$ , the possible values of which are

$$S_{13} = \begin{cases} S - T, S - T + 1, \dots, S + T, & S \geq T \\ T - S, T - S + 1, \dots, 2S, & S < T \leq 3S. \end{cases} \quad (26)$$

So, to compute the tube eigenvalues we use Eq. (17), and then use Eq. (25) to determine the number of multiplets which will have the given eigenvalues.

### C. Three-leg ladder

The three-leg ladder presents additional difficulty because of the broken symmetry. However, from (10) we see that the ladder and tube rung Hamiltonians are related via

TABLE I. Tabulated results relating tube eigenvalues and ladder eigenvalues.

Multiplet type	$T$	Quantity [ $\Theta(S, T)$ ]	$\lambda^{(tube)}$	$S_{13}$ from (26)	$\mu_{S_{13}}$	Shifts	$\lambda^{(ladder)}$
singlet	0	1	-6	1	-1	2	-4
triplet	1	3	-5	0,1,2	-2, -1, 1	3, 2, 0	-2, -3, -5
quintuplet	2	2	-3	1, 2	-1, 1	2, 0	-1, -3
septuplet	3	1	0	2	1	0	0

$$H^{(ladder, rung)} = H^{(tube, rung)} + J(1 - \mathbf{S}^{(1)} \cdot \mathbf{S}^{(3)}). \quad (27)$$

Since  $\mathbf{S}^{(1)} \cdot \mathbf{S}^{(3)}$  commutes with the Hamiltonians (see the Appendix), their eigenvalues are similarly related via

$$\lambda_{T, S_{13}}^{(ladder)} = \lambda_T^{(tube)} + J(1 - \mu_{S_{13}}), \quad (28)$$

where  $\mu_{S_{13}}$  is the eigenvalue of  $\mathbf{S}^{(1)} \cdot \mathbf{S}^{(3)}$  for the state. Up to a shift and scaling, this operator is similar to the two-leg ladder Hamiltonian. By symmetry, the eigenvalues of  $\mathbf{S}^{(1)} \cdot \mathbf{S}^{(3)}$  must be the same as those of  $\mathbf{S}^{(1)} \cdot \mathbf{S}^{(2)}$ , and hence adaptation of Eq. (15) yields

$$\mu_{S_{13}} = \frac{1}{2} S_{13}(S_{13} + 1) - S(S + 1), \quad S_{13} = 0, 1, \dots, 2S. \quad (29)$$

Thus, modifying the Hamiltonian from the tube to the ladder gives rise to an energy shift [ $J(1 - \mu_{S_{13}})$ ] that depends, ultimately, on the value of  $S_{13}$  for the eigenstate (the tube and ladder Hamiltonians have the same eigenstates). So, to calculate the ladder eigenvalues, we proceed as follows: first calculate the tube eigenvalues along with the number of different type of multiplets that will occur using Eq. (25). Then, using Eq. (26), we compute the range of values of  $S_{13}$  that will occur for a given type of multiplet. From these, we use Eq. (29) to calculate  $\mu_{S_{13}}$  and hence the energy shift, and finally, add these to the original tube eigenvalues to obtain the ladder eigenvalues.

The process is perhaps better clarified through an example, and we demonstrate for the case of the three leg spin-1 ladder. We put  $J=1$  for simplicity. From Eq. (17) we determine that the tube eigenvalues are -6, -5, -3, and 0, with respective multiplicities 1 (one singlet), 9 (three triplets), 10 (two quintuplets), and 7 (a septuplet). The eigenvalues  $\mu_{S_{13}}$  in this case are -2, -1, and 1, so the corresponding shifts [ $S(1 - \mu_{S_{13}})$ ] required to give the tube eigenvalues are 3, 2, and 0.

We calculate the possible  $S_{13}$  values (and hence the possible  $\mu_{S_{13}}$  values) that occur for each type of multiplet as given by Eq. (26), and then proceed to compute the energy shifts, and finally the ladder eigenvalues. The results are summarized in Table I.

### III. MAGNETIZATION PLATEAUS

We now analyze the effect of introducing a magnetic field  $h$  along the positive  $z$  direction. This causes the multiplets to

split into individual nondegenerate states according to the  $z$ -component of a state's spin. The relevant physical effect is the existence of magnetization plateaus, which occur when, in some region of phase space (defined by  $J$  and  $h$ ), the groundstate consists of rungs all having the same magnetization. We work with the magnetization per site, which is defined as

$$M = \frac{1}{nLS} \sum_{i=1}^L \sum_{l=1}^n [(S^z)_i^{(l)}]. \quad (30)$$

This definition is constructed in such a way that  $M$  has a saturation value of 1. As we move through phase space, passing through regions where the system is gapless, we find that the magnetization varies continuously. However in regions where there is a nonzero gap, the magnetization remains constant, hence the term "magnetization plateau."

The Lieb-Schultz-Mattis theorem for low-dimensional magnets gives rise to the necessary general condition<sup>3,26</sup>

$$Q(S_c - m_c) \in \mathbb{Z} \quad (31)$$

for the existence of a plateau. Here  $Q$  is the spatial period as measured by the unit cell, and  $S_c$  and  $m_c$  are the total spin and magnetization of the unit cell respectively. Hence for an  $n$ -leg ladder they may be taken as  $nS$  and  $nm$ . In this definition,  $m$  is not designed to have a saturation value of 1, and so we may take  $m = SM$ . For translationally invariant ladders, including those of this paper, we take  $Q=1$ , hence retrieving Eq. (1).

In the case of the two-leg ladder, we note that the introduction of a magnetic field splits the energy levels of the states within a multiplet. Each state is shifted from the value given in Eq. (15) by an amount  $hS^z$ , where  $S^z$  is the  $z$ -component of its spin. Since the multiplet states may be characterized by their value of  $S^z$ , there is a complete loss of degeneracy upon the introduction of a magnetic field. For a rung of total spin  $T$ , the lowest energy state from each one has an eigenvalue

$$\lambda_{T, \min} = \frac{J}{2} [T(T+1) - 2S(S+1) - 6] - hT, \quad T=0, \dots, 2S. \quad (32)$$

We show that it is possible for any of these states to be the groundstate with a nonzero gap, subject to appropriate choice of  $J$  and  $h$ . Consider first the case where the two rung states of lowest energy are from the same multiplet. Since the magnetic energy shifts are given by  $hS^z$ , it is clear that the difference in their energy due to the rung Hamiltonian is  $h$ . The

leg Hamiltonian gives a contribution of 4, so that the energy gap is  $\Delta = h - 4$ . Therefore if  $h > 4$ , all rungs are in the same state, and the system has a gap  $\Delta$ .

In the case where the two lowest energy states are from different multiplets (say,  $\lambda_p$  and  $\lambda_q$ , where  $\lambda_p > \lambda_q$ ), the gap is given by

$$\Delta = \lambda_p - \lambda_q - 4 = \frac{J}{2} [p(p+1) - q(q+1)] - h(p-q) - 4. \quad (33)$$

This can be guaranteed to be greater than zero for any  $p$  and  $q$  simply by taking

$$J > 2 \left[ \frac{h(p-q) + 4}{p(p+1) - q(q+1)} \right] \quad (34)$$

in the antiferromagnetic case (with a similar result in the ferromagnetic case). Hence, the lowest energy state from each multiplet has some corresponding region of phase space where it is the sole rung state occurring in the ground state, and the ladder is gapped. The different multiplets take on all possible values of  $S_z$  allowed under the restriction that the system consists of intrinsic spins  $S$ . Consequently, it is apparent that a plateau of every allowable magnetization is realized somewhere in phase space. This analysis can also be applied to the three-leg case without significant modification.

It is simple to check that the magnetization plateaus we have found here satisfy the requirements of Eq. (31). We note that, if the gaps discussed above are nonzero, then all rungs are in the same ground state. Hence  $Q=1$ , and we require that  $S-m=k$ , where  $S$  and  $m$  are the spin and magnetization of a rung, and  $k$  is an integer. However, since  $m$  can take values ranging from  $-S$  to  $S$  in integer steps, it is clear that this relation will be satisfied.

#### IV. PLATEAU BOUNDARIES

It is of some interest to explore what happens on the boundary between two magnetization plateaux. We examine the two-leg case. The boundary may be defined by the line on which the groundstate of each plateau is degenerate.<sup>10</sup> In general, we see that the states that can have minimum energy in the quadrant  $J, h > 0$  are the states from each multiplet with the largest  $z$  component of the spin, namely,

$$\lambda_{T,\min} = \frac{J}{2} [T(T+1) - 2S(S+1)] - hT. \quad (35)$$

It is also clear that as we steadily increase the ratio  $h/J$  that  $T$  will progress in order through its possible values  $0, \dots, 2S$ . That is, the plateau boundaries will occur between successively ordered states as in Eq. (35). Thus the equations of the plateau boundaries are given by  $\lambda_{T,\min} - \lambda_{T+1,\min} = 0$  or, more explicitly,

$$h = \frac{J}{2} (T+1), \quad T=0, 1, \dots, 2S-1. \quad (36)$$

Now it is a simple matter to determine what the magnetization will be on these lines. As usual we normalize so that

$\langle M \rangle = 1$  if  $S_z = S$  on each site. We calculate the magnetization on these boundary lines by averaging the two states that meet there. Now the state corresponding to  $\lambda_{T,\min}$  must have  $S_z$  as large as possible, that is,  $S_z = T$ . On boundary line  $T$ , then, we simply average  $T$  and  $T+1$ , which is spread over two sites and normalized for spin. That is,

$$\langle M \rangle_T = \left( \frac{T+T+1}{2} \right) / 2S = \frac{2T+1}{4S}, \quad T=0, 1, \dots, 2S-1. \quad (37)$$

Although we would not, strictly speaking, consider this a magnetization plateau, it still satisfies Eq. (31) in some sense. We can think of the ground state now as being a mixture of two types of rung. Hence for the two-leg ladder, we take  $Q=2$  to be a unit cell. The magnetization of the unit cell is then  $2T+1$ , with the total spin being some integer between 0 and  $4S$ . Hence  $2(S-m)$ , as defined in Eq. (31), is clearly an integer.

#### V. EXAMPLE—THE TWO-LEG, SPIN-1 LADDER

We look at the specific case of the two-leg, spin-1 ladder in the presence of a magnetic field. In this example the leg Hamiltonian is

$$H_{i,j}^{\text{leg}} = [\mathbf{S}_i^{(1)} \cdot \mathbf{S}_j^{(1)} + (\mathbf{S}_i^{(1)} \cdot \mathbf{S}_j^{(1)})^2 - 1] \\ \times [\mathbf{S}_i^{(2)} \cdot \mathbf{S}_j^{(2)} + (\mathbf{S}_i^{(2)} \cdot \mathbf{S}_j^{(2)})^2 - 1], \quad (38)$$

while the rung Hamiltonian is given by

$$H_i^{\text{rung}} = J(\mathbf{S}_i^{(1)} \cdot \mathbf{S}_i^{(2)} - 1) - h[(S^z)_i^{(1)} + (S^z)_i^{(2)}], \quad (39)$$

where

$$S^x = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}, \quad S^y = \frac{1}{\sqrt{2}} \begin{pmatrix} 0 & -i & 0 \\ i & 0 & -i \\ 0 & i & 0 \end{pmatrix}, \\ S^z = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}, \quad (40)$$

are the spin-1 operators. We will work in the basis where the square and the  $z$ -component of the total spin of a given rung,  $S = \mathbf{S}^{(1)} + \mathbf{S}^{(2)}$ , are diagonal. It follows that the nine states on a given rung fall into a spin-2 quintuplet, a spin-1 triplet, and a spin-0 singlet. Let  $S = |\mathbf{S}|$  and let  $S^z$  be the  $z$  component of the total spin. We denote the rung basis by  $|S, S^z\rangle$  and it is given in terms of the  $(S^z)^{(l)}$  eigenstates by

$$\begin{aligned}
|0\rangle &= |0;0\rangle = \frac{1}{\sqrt{3}}(|+\rangle|-\rangle - |0\rangle|0\rangle + |-\rangle|+\rangle), \\
|1\rangle &= |1;1\rangle = \frac{1}{\sqrt{2}}(-|+\rangle|0\rangle + |0\rangle|+\rangle), \\
|2\rangle &= |1;0\rangle = \frac{1}{\sqrt{2}}(-|+\rangle|-\rangle + |-\rangle|+\rangle), \\
|3\rangle &= |1;-1\rangle = \frac{1}{\sqrt{2}}(-|0\rangle|-\rangle + |-\rangle|0\rangle), \\
|4\rangle &= |2;2\rangle = |+\rangle|+\rangle, \\
|5\rangle &= |2;1\rangle = \frac{1}{\sqrt{2}}(|+\rangle|0\rangle + |0\rangle|+\rangle), \\
|6\rangle &= |2;0\rangle = \frac{1}{\sqrt{6}}(|+\rangle|-\rangle + 2|0\rangle|0\rangle + |-\rangle|+\rangle), \\
|7\rangle &= |2;-1\rangle = \frac{1}{\sqrt{2}}(|0\rangle|-\rangle + |-\rangle|0\rangle), \\
|8\rangle &= |2;-2\rangle = |-\rangle|-\rangle.
\end{aligned} \tag{41}$$

The leg Hamiltonian (6) has the same form in this new basis. The rung Hamiltonian (39) now becomes diagonal and is given by  $H^{\text{rung}} = \text{diag}\{-3J, -2J-h, -2J, -2J+h, -2h, -h, 0, h, 2h\}$ .

We now consider the possible orderings of the states according to their energy in the presence of the magnetic field  $h$ . The energy considerations in this case are quite simple, as there is no degeneracy. The number of possible orderings is now quite large because the field can cause varying amounts of energy level splitting within a given multiplet, leading to overlaps between them. In fact there are 12 physically possible orderings for  $h > 0$ . From now on we will restrict our attention to the first quadrant ( $J > 0$ ) which contains six orderings. We will list these below, computing energy gaps, and hence deriving the phase diagram.

In computing energy gaps for each ordering, we will use a procedure similar to that used in work on the  $\text{su}(8)$  tube.<sup>12</sup> Since the rung Hamiltonian is diagonal, it is a simple matter to compute its contribution to this gap. However, calculating the contribution of the leg Hamiltonian is more complicated. This requires taking the thermodynamic limit of the Bethe ansatz equations, taking Fourier transforms, and then solving. The final step comes down to the evaluation of an integral, which gave us our final result.

This integral, and hence the energy gap, ultimately depends on the type of mode we need to create in order to compute the energy gap. This follows directly from the degeneracy of the ground state. It is therefore possible to give a general form of this integral, which depends only on the type of mode we are creating. This allows us to easily and quickly

compute the gap contribution of a Hamiltonian that is to be solved by the Bethe ansatz method.

If we denote by  $\alpha_k$  the integral corresponding to creating a  $\lambda^{(k)}$  excitation, the general result is

$$\alpha_k = \frac{-2}{k} \left[ \gamma + \log 4 + \psi \left( \frac{1}{2} + \frac{1}{k} \right) \right], \tag{42}$$

where  $\gamma$  is the Euler gamma constant and  $\psi(x)$  is the digamma function. This can be simplified for a specified  $k$ . Here, we will only need the values  $\alpha_1 = 4$  and  $\alpha_2 = 2 \log 2 = 1.38629 \dots$ . We now proceed to analyze each ordering in turn.

(1)  $h < \frac{2}{3}J$ . In this case the ordering is  $\{|0\rangle, |1\rangle, |2\rangle, |3\rangle, |4\rangle, |5\rangle, |6\rangle, |7\rangle, |8\rangle\}$ . The energy is given by  $E = E_{\text{leg}} + M_1(J-h) + (M_2 + M_3)h + M_4(2J-3h) + (M_5 + M_6 + M_7 + M_8)h$ , where  $M_k = \sum_{r=k}^9 N_{Pr}$ , where  $N$  is the number of states  $|j\rangle$  occurring in an excited state, and  $P$  takes the numbers 0, 1, 2, 3, 4, 5, 6, 7, and 8 to the ordering we present. (In this case,  $P$  is the identity permutation, in the cases below, it will be some other permutation.) Hence the first energy gap is  $\Delta = (-2J-h) - (-3J) - 4 = J-h-4$ , leading to a critical line  $h_c = J-4$ . There is another crossover curve on which the second excitations ( $|2\rangle$  states) also become massless. Although we cannot calculate this exactly, we can see that it intersects the above critical line at the point  $(J, h) = (4, 0)$ . This curve moves as  $M_1$  changes, eventually traversing regions (1) and (2) to the point  $(J, h) = (2 \log 2, 2 \log 2)$  on the boundary of region (3)  $h = J$ . Below the line  $h_c = J-4$ , all rungs are in state  $|0\rangle$ , so the total magnetization of the system is  $\langle M \rangle = 0$ , as would be expected. Above this line a finite number of rungs exist in the lowest-energy triplet state, and the magnetization varies continuously.

(2)  $\frac{2}{3}J < h < J$ . Now the ordering is  $\{|0\rangle, |1\rangle, |2\rangle, |4\rangle, |3\rangle, |5\rangle, |6\rangle, |7\rangle, |8\rangle\}$ . This gives the same calculation as for case 1, so the critical line is the same. Regions (1) and (2) become distinguishable only when considering the third or higher excitations.

(3)  $J < h < \frac{3}{2}J$ . Now the ordering is  $\{|1\rangle, |0\rangle, |4\rangle, |2\rangle, |5\rangle, |3\rangle, |6\rangle, |7\rangle, |8\rangle\}$ . The first energy gap is  $E = -J+h-4$ , giving rise to a critical line of  $h_c = J+4$ . The second excitations become massless on this line at  $(J, h) = (8, 12)$ , and move to the point  $(J, h) = (2 \log 2, 2 \log 2)$ . That is, the same point as that calculated for region (1). Now above this line, the ground state consists entirely of rungs in state  $|1\rangle$ . As a result there is a magnetization plateau of  $\langle M \rangle = \frac{1}{2}$  here.

(4)  $\frac{3}{2}J < h < 2J$ . The ordering is  $\{|1\rangle, |4\rangle, |0\rangle, |2\rangle, |5\rangle, |3\rangle, |6\rangle, |7\rangle, |8\rangle\}$ . The gap now is  $\Delta = 2J-h-4$  and the critical curve is  $h_c = 2J-4$ . This intersects the critical curve of region (3) on the boundary between them. Again the second excitations become massless at  $(J, h) = (8, 12)$ , and move to the point  $(J, h) = (2 \log 2, 4 \log 2)$  on the line  $h = 2J$ . Below the line  $h_c = 2J-4$  the ground state consists entirely of rungs in the  $|1\rangle$  state, yielding a magnetization of  $\langle M \rangle = \frac{1}{2}$ , being part of the same plateau as found in region (3).

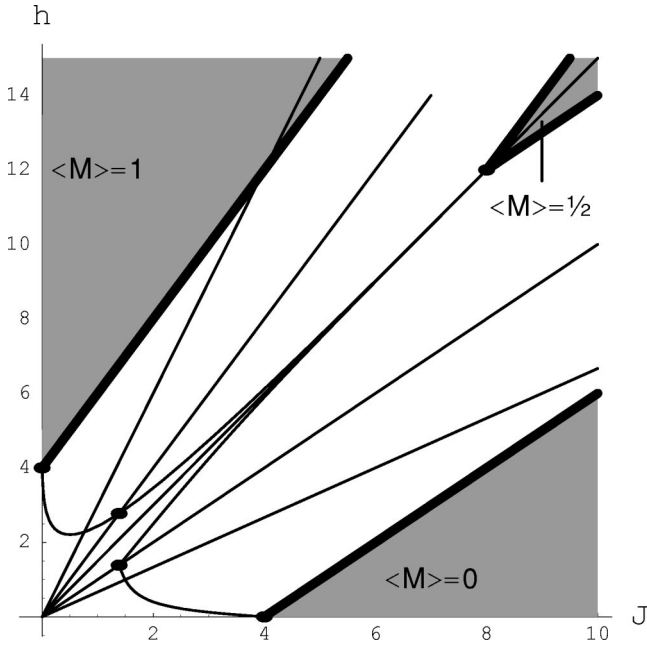


FIG. 1. The magnetic phase diagram of the two-leg spin-1 ladder. The thin lines are  $h = \frac{2}{3}J$ ,  $h = J$ ,  $h = \frac{3}{2}J$ ,  $h = 2J$ , and  $h = 3J$ , which together with the y axis divide the quadrant into regions 1–6. The thick lines are the exactly derived phase boundaries, and the curved lines are sketches of higher phase boundaries.

(5)  $2J < h < 3J$ . We now have an ordering of  $\{|4\rangle, |1\rangle, |0\rangle, |5\rangle, |2\rangle, |6\rangle, |3\rangle, |7\rangle, |8\rangle\}$ . The critical line here is  $h_c = 2J + 4$ . The second excitations do not become massless on this curve. They do, however, become massless at the point  $(J, h) = (2 \log 2, 4 \log 2)$ .

(6)  $h > 3J$ . The ordering is  $\{|4\rangle, |1\rangle, |5\rangle, |0\rangle, |2\rangle, |6\rangle, |3\rangle, |7\rangle, |8\rangle\}$ , yielding an extension of the critical line found in case (5). The second excitations become massless on this line at  $(J, h) = (0, 4)$ . Above the line  $h_c = 2J + 4$  in regions (4) and (5) the ground state consists entirely of rungs in state  $|4\rangle$ , and the system reaches a magnetization plateau of  $\langle M \rangle = 1$ . Outside the three plateaux found here the magnetization varies continuously.

The results of this analysis are encapsulated in the phase diagram (Fig. 1). We show its first quadrant. The shape of the curved line is interesting, showing a sharp spike with its cusp on the line  $h = \frac{3}{2}J$ . Although we have calculated some exact points, its overall shape cannot be determined analytically. We can predict some features using perturbation theory, and it is possible that the shape of the curve could be accurately determined using numerical series methods. Note also that there is more structure inside this curve, corresponding to the points at which higher excitations become massless.

## VI. CONCLUDING REMARKS

We have investigated the behavior of some Bethe ansatz solvable two- and three-leg ladder models with general spin  $S$ . These models include multispin interactions in order to be exactly solvable. Most importantly, the solvable ladder models include Heisenberg rung interactions of arbitrary strength which drive the physics for strong rung coupling. The values

of the magnetization on each of the magnetization plateaux are seen to fit with the general prediction based on application of the Lieb-Schultz-Mattis theorem. Additionally, the plateau boundaries, which may be thought of as infinitesimally thin plateaux, also satisfy this criterion. We calculated the phase diagram (Fig. 1) of the spin-1 ladder in detail. Distinct plateaux occur at the values  $\langle M \rangle = 0, \frac{1}{2}, 1$  in agreement with the experimentally observed<sup>20,21</sup> values for the spin-1 ladder compound BIP-TENO. It will be most interesting to derive the thermodynamic properties of this model.

## ACKNOWLEDGMENTS

This work was supported by the Australian Research Council through Grant Nos. A6990558, F69700124, and DP0208925. M.M. was supported by an Australian Postgraduate Research Award.

## APPENDIX: COMMUTATION OF $S^{(1)}, S^{(3)}$ WITH THE HAMILTONIANS

We first show that  $S^{(1)} \cdot S^{(3)}$  commutes with the rung Hamiltonian. For the three-leg case we have

$$H^{\text{rung}} = -J(2 - S^{(1)} \cdot S^{(2)} - S^{(2)} \cdot S^{(3)}), \quad (\text{A1})$$

so

$$\begin{aligned} [S^{(1)} \cdot S^{(3)}, H^{\text{rung}}] &= -J(2[S^{(1)} \cdot S^{(3)}, \mathbf{I}] - [S^{(1)} \cdot S^{(3)}, S^{(1)} \cdot S^{(2)}] \\ &\quad - [S^{(1)} \cdot S^{(3)}, S^{(2)} \cdot S^{(3)}]) \\ &= J([S^{(1)} \cdot S^{(3)}, S^{(1)} \cdot S^{(2)}] \\ &\quad + [S^{(1)} \cdot S^{(3)}, S^{(2)} \cdot S^{(3)}]) \\ &= J([S^{(1)} \cdot S^{(3)}, S^{(1)} \cdot S^{(2)} + S^{(2)} \cdot S^{(3)}]). \end{aligned} \quad (\text{A2})$$

This commutator may be expressed as a linear combination of commutators of the form

$$[(S^a)^{(k)}(S^a)^{(l)}, (S^b)^{(k)}(S^b)^{(m)} + (S^c)^{(l)}(S^c)^{(m)}], \quad (\text{A3})$$

where  $a, b$  and  $c$  represent the coordinate variables  $x, y$ , and  $z$ , and  $k, l$ , and  $m$  represent the site numbers. Using standard properties of commutators, this can be expanded to give

$$[(S^a)^{(k)}, (S^b)^{(k)}](S^a)^{(l)}(S^b)^{(m)} + [(S^a)^{(l)}, (S^c)^{(l)}](S^a)^{(k)}(S^c)^{(m)}, \quad (\text{A4})$$

and, using the quantum mechanical relation  $[S_j, S_k] = i\epsilon_{jkl}S_l$ , this becomes

$$\begin{aligned} i\epsilon_{abc}(S^c)^{(k)}(S^a)^{(l)}(S^b)^{(m)} + i\epsilon_{acb}(S^b)^{(l)}(S^a)^{(k)}(S^c)^{(m)} \\ = i(\epsilon_{abc} + \epsilon_{cba})(S^c)^{(k)}(S^a)^{(l)}(S^b)^{(m)} = 0, \end{aligned} \quad (\text{A5})$$

where a summation is implied over repeated indices, and we have used the fact that spins from different sites commute.

That  $S^{(1)} \cdot S^{(3)}$  commutes with the leg Hamiltonian follows directly from Eq. (17) of a previous paper.<sup>15</sup> As was

noted after that equation, arbitrary  $XYZ$  interactions introduced on the rungs will commute with leg Hamiltonians of the type we are working with here. Of course, the same statement is true for removing such interactions, which is how the

tube Hamiltonian is transformed into the ladder Hamiltonian. Since the Hamiltonians and the operator  $S^{(1)} \cdot S^{(3)}$  are mutually commutative, the eigenvalues may be related directly as in Eq. (28).

\*Electronic address: Murray.Batchelor@anu.edu.au

†Electronic address: jdegier@unimelb.edu.au

<sup>1</sup>E. Dagotto and T.M. Rice, *Science* **271**, 618 (1996).

<sup>2</sup>E. Dagotto, *Rep. Prog. Phys.* **62**, 1525 (1999).

<sup>3</sup>M. Oshikawa, M. Yamanaka, and I. Affleck, *Phys. Rev. Lett.* **78**, 1984 (1997).

<sup>4</sup>D.C. Cabra, A. Honecker, and P. Pujol, *Phys. Rev. B* **58**, 6241 (1998).

<sup>5</sup>See, e.g., D.C. Cabra, M.D. Grynberg, A. Honecker, and P. Pujol, in *Condensed Matter Theories*, Vol. 16, edited by S. Hernandez and J. W. Clark (Nova, New York, 2001), p. 17.

<sup>6</sup>A.K. Kolezhuk and H.-J. Mikeska, *Int. J. Mod. Phys. B* **12**, 2325 (1998).

<sup>7</sup>A. Honecker, F. Mila, and M. Troyer, *Eur. Phys. J. B* **15**, 227 (2000).

<sup>8</sup>E. Chattopadhyay and I. Bose, *Physica A* **318**, 14 (2003).

<sup>9</sup>Y. Wang, *Phys. Rev. B* **60**, 9236 (1999).

<sup>10</sup>J. de Gier and M.T. Batchelor, *Phys. Rev. B* **62**, R3584 (2000).

<sup>11</sup>M.T. Batchelor and M. Maslen, *J. Phys. A* **32**, L377 (1999).

<sup>12</sup>J. de Gier, M.T. Batchelor, and M. Maslen, *Phys. Rev. B* **61**, 15 196 (2000).

<sup>13</sup>H. Fan, *J. Phys. A* **32**, L509 (1999).

<sup>14</sup>H. Frahm and A. Kundu, *J. Phys.: Condens. Matter* **11**, L557 (1999).

<sup>15</sup>M.T. Batchelor, J. de Gier, and M. Maslen, *J. Stat. Phys.* **102**, 559 (2001).

<sup>16</sup>M.T. Batchelor, J. de Gier, J. Links, and M. Maslen, *J. Phys. A* **33**, L97 (2000).

<sup>17</sup>A. Foerster, K.E. Hibberd, J.R. Links, and I. Roditi, *J. Phys. A* **34**, L25 (2001).

<sup>18</sup>J. Links and A. Foerster, *Phys. Rev. B* **62**, 65 (2000).

<sup>19</sup>A.P. Tonel, A. Foerster, J. Links, and A.L. Malvezzi, *Phys. Rev. B* **64**, 054420 (2001).

<sup>20</sup>K. Katoh, Y. Hosokoshi, K. Inoue, and T. Goto, *J. Phys. Soc. Jpn.* **69**, 1008 (2000).

<sup>21</sup>T. Goto *et al.*, *Physica B* **294&295**, 43 (2001).

<sup>22</sup>K. Okamoto, N. Okazaki, and T. Sakai, in *Orbital2001 (International Conference on Strongly Correlated Electrons with Orbital Degrees of Freedom)* (Sendai, 2001).

<sup>23</sup>D. Sénéchal, *Phys. Rev. B* **52**, 15 319 (1995).

<sup>24</sup>D. Allen and D. Sénéchal, *Phys. Rev. B* **61**, 12 134 (2000).

<sup>25</sup>B. Sutherland, *Phys. Rev. B* **12**, 3795 (1975).

<sup>26</sup>E. Lieb, T.D. Schultz, and D.C. Mattis, *Ann. Phys. (N.Y.)* **16**, 407 (1961).