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Anomalous magnetization process in frustrated spin ladders

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Abstract
We study, at $T = 0$, the anomalies in the magnetization curve of the $S = 1$ two-leg ladder with frustrated interactions. We focus mainly on the existence of the $M = M_s/2$ plateau, where M_s is the saturation magnetization. We report the results using the degenerate perturbation theory and the density matrix renormalization group, which lead to consistent conclusion with each other. We also touch on the $M = M_s/4$ and $(3/4)M_s$ plateaux and cusps.

1. Introduction

Anomalies in the magnetization process, such as plateau, cusp and jump, in low-dimensional magnets have attracted increasing attention in the past few years. In this paper, we investigate the effect of the frustrated interactions on the plateaux and cusps in the magnetization curve of the $S = 1$ two-leg ladder. Our Hamiltonian, sketched in figure 1, is described by

$$\mathcal{H} = J_0 \sum_{j=1}^{N} \boldsymbol{S}_{j,1} \cdot \boldsymbol{S}_{j,2} + J_1 \sum_{j=1}^{N} (\boldsymbol{S}_{j,1} \cdot \boldsymbol{S}_{j+1,1} + \boldsymbol{S}_{j,2} \cdot \boldsymbol{S}_{j+1,2})$$
$$+ J_2 \sum_{j=1}^{N} (\boldsymbol{S}_{j,1} \cdot \boldsymbol{S}_{j+1,2} + \boldsymbol{S}_{j,2} \cdot \boldsymbol{S}_{j+1,1})$$
$$+ J_3 \sum_{j=1}^{N} (\boldsymbol{S}_{j,1} \cdot \boldsymbol{S}_{j+2,1} + \boldsymbol{S}_{j,2} \cdot \boldsymbol{S}_{j+2,2}) - H \sum_{j=1}^{N} (S^z_{j,1} + S^z_{j,2}) \quad (1)$$

where $\boldsymbol{S}_{j,l}$ is the $S = 1$ operator at the jth site of the lth ladder ($l = 1, 2$), H denotes the magnetic field along the z direction, and all the couplings are supposed to be antiferromagnetic unless otherwise noted.

We focus mainly on the effect of the frustrated interaction J_2 on the $M = M_s/2$ plateau, where M is the magnetization and M_s is the saturation magnetization, although we touch on other topics. In section 2, we investigate the simple two-leg ladder with no frustration. The

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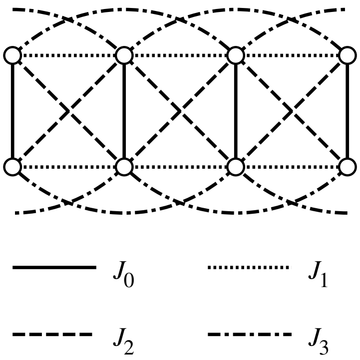

Figure 1. Sketch of the model Hamiltonian (1).

effect of the frustrated interaction J_2 on the $M = M_s/2$ plateau is discussed in section 3. The last section (section 4) is devoted to concluding remarks.

2. $M_s/2$ plateau of a simple $S = 1$ two-leg ladder

In case of the $S = 1/2$ simple ladder, the rung interaction is always relevant. In other words, infinitesimally small rung interactions brings about the spin gap at $M = 0$. The situation is quite different for the $M = M_s/2$ plateau of the present $S = 1$ model. When $J_0 \to \infty$, the $M = M_s/2$ plateau obviously exists, because the problem is reduced to the two-spin problem. On the other hand, there will be no $M = M_s/2$ plateau in the $J_0 \to -\infty$ limit, because the ladder is essentially a single chain of $S = 2$ spins formed by the rung spin pair. Thus there exists the critical value of J_0/J_1. This quantum phase transition is thought to be of the Berezinskii–Kosterlitz–Thouless (BKT) type [1, 2]. We note that this $M_s/2$ plateau state is unique (not degenerate) from the necessary condition for the plateau [3]. It is interesting to note whether the critical point lies on the antiferromagnetic side (i.e. $J_0 > 0$) or the ferromagnetic side ($J_0 < 0$), when $J_1 > 0$ is fixed. Infinitesimally small J_0 yields the $M = M_s/2$ plateau if $J_0^{(cr)} < 0$, while it does not if $J_0^{(cr)} > 0$.

To estimate the above-mentioned critical point analytically, we employ the degenerate perturbation theory (DPT) [4]. Hereafter we set $J_0 = 1$ (energy unit) for convenience and due to the fact that the critical point lies on the antiferromagnetic side, as will be seen later. Let us begin with the strong rung coupling limit $J_1 \ll J_0$. In this limit, around $M = M_s/4$, we can take only two states for the rung states, neglecting the other seven states: the lowest state with $S_{\rm rung}^{z({\rm tot})} = 0$ and that with $S_{\rm rung}^{z({\rm tot})} = 1$. We can express these states by the $T^z = 1/2$ and $-1/2$ states, respectively, of the psuedo spin $\boldsymbol{T}$. The lowest order perturbation with respect to J_1 leads to the effective Hamiltonian

$$\mathcal{H}_{\rm eff} = \sum_j \{J_{\rm eff}^{xy}(T_j^x T_{j+1}^x + T_j^y T_{j+1}^y) + J_{\rm eff}^z T_j^z T_{j+1}^z - H_{\rm eff} T_j^z\} \tag{2}$$

$$J_{\rm eff}^{xy} = \frac{8J_1}{3}, \qquad J_{\rm eff}^z = \frac{J_1}{2}, \qquad H_{\rm eff} = H - 1 - \frac{J_1}{2}. \tag{3}$$

The $M = 0$, $M_s/4$ and $M_s/2$ states of the original $\boldsymbol{S}$ system correspond to the $M^{(T)} = -M_s^{(T)}$, 0 and $M_s^{(T)}$ states, respectively, where $M^{(T)}$ ($M_s^{(T)}$) denotes the magnetization (saturation magnetization) of the $\boldsymbol{T}$ system. It is easy to obtain the field corresponding to $M^{(T)} = M_s^{(T)}$

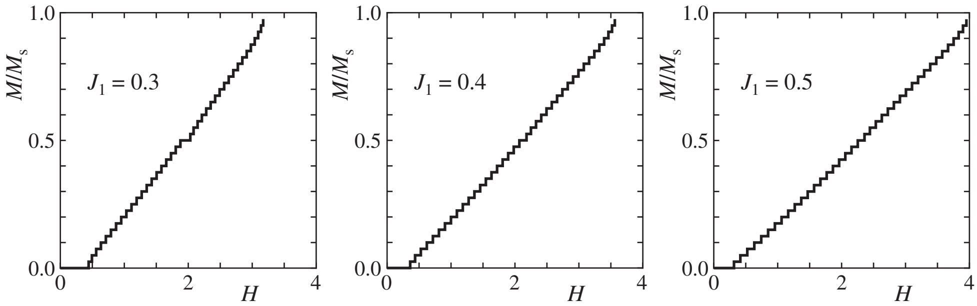

Figure 2. Magnetization curves of the simple ladder ($J_2 = J_3 = 0$) when $J_1 = 0.3$, 0.4 and 0.5 for 40 spins obtained by the DMRG. The $M_s/2$ plateau clearly exists for $J_1 = 0.3$, while it does not for $J_1 = 0.5$. It is difficult to judge for the $J_1 = 0.4$ case.

by considering the one-spin-down spectrum of $\mathcal{H}_{\rm eff}$ as

$$H^{(1)}_{M_s/2} = 1 + \frac{11J_1}{3}. \tag{4}$$

This $H^{(1)}_{M_s/2}$ gives the lower edge of the $M = M_s/2$ plateau.

A similar DPT can be developed around $M = (3/4)M_s$, resulting in

$$H^{(2)}_{M_s/2} = 2 - J_1, \tag{5}$$

where $H^{(2)}_{M_s/2}$ gives the upper edge of the $M = M_s/2$ plateau. Thus, the critical value $J_1^{(\rm cr)}$, where the $M = M_s/2$ plateau vanishes, can be estimated from $H^{(1)}_{M_s/2} = H^{(2)}_{M_s/2}$, resulting in

$$J_1^{(\rm cr)} = \tfrac{3}{14} = 0.214. \tag{6}$$

We remark that there is no $M = M_s/2$ plateau for the so-called isotropic case $J_1 = 1$.

We have calculated the magnetization curves (figure 2) by use of the density matrix renormalization group (DMRG) method. The DMRG result is consistent with the level spectroscopy (LS) result $J_1^{(\rm cr)} = 0.491$, if we consider the pathological nature of the BKT transition. We can clearly see the $M_s/2$ plateau for $J_1 = 0.3$, while we cannot for $J_1 = 0.5$. It is difficult to judge for the $J_1 = 0.4$ case. This situation is qualitatively consistent with the DPT results, although the critical value is slightly larger than the DPT prediction (6). This is reasonable because the plateau region will narrowly extend, like a beak of a bird, onto the J_1–H plane, as was seen in the diamond-type spin chain case [5].

The LS method [6–8] is very powerful in finding the quantum critical point of the BKT and Gaussian types. We have also performed the LS method, the details of which will be published elsewhere. Our conclusion is

$$J_1^{(\rm cr)} = 0.491 \tag{7}$$

which is consistent with the DMRG result. We have also performed the non-Abelian bosonization approach, finding a qualitatively consistent conclusion with those by the above methods. Details of the LS method and the non-Abelian bosonization approach will be published elsewhere.

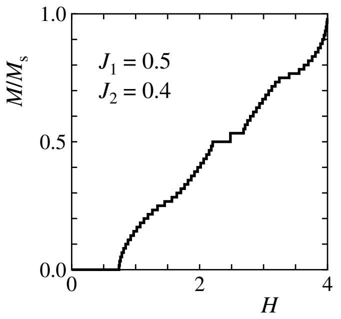

Figure 3. Magnetization curve for 60 spins when $J_1 = 0.5$ and $J_2 = 0.4$.

3. Effect of frustrated interactions

Let us consider the effect of J_2 interactions on the $M_s/2$ plateau problem. The DPT in the previous section can be easily extended to the case with J_2. We obtain

$$H^{(1)}_{M_s/2} = 1 + \frac{11J_1}{3} - \frac{5J_2}{3}, \qquad H^{(2)}_{M_s/2} = 2 - J_1 + 3J_2, \tag{8}$$

yielding the critical line

$$J_2 = J_1 - \tfrac{3}{14}. \tag{9}$$

The magnetization curve for the $J_1 = 0.5$, $J_2 = 0.4$ cases calculated by the DMRG method is shown in figure 3. There exists the $M_s/2$ plateau which is not seen in the $J_1 = 0.5$, $J_2 = 0$ cases (no frustration cases), as shown in figure 2. Furthermore we can see the $M_s/4$ and $(3/4)M_s$ plateaux, which are attributed to the Néel ordering of the $\boldsymbol{T}$ system, which was first pointed out by our group [9]. The Néel ordering condition is known from $\mathcal{H}_{\mathrm{eff}}$ as $J^{xy}_{\mathrm{eff}} < J^{z}_{\mathrm{eff}}$, from which we obtain

$$J_2 > \tfrac{13}{19}J_1 = 0.684J_1 \tag{10}$$

for the $M_s/4$ plateau. This condition is satisfied for the parameter set of figure 3. The Néel ordering condition for the $(3/4)M_s$ plateau is $J_2 > 0.6J_1$, which explains the fact that the width of the $M = (3/4)M_s$ plateau is wider than that of the $M_s/4$ plateau. Both the $M_s/4$ and $(3/4)M_s$ plateaux require the spontaneous breaking of the translation symmetry as is known from the necessary condition for the plateau [3]. We have also employed the LS method for this case, finding consistent results with that of the DMRG.

4. Concluding remarks

Here we briefly touch on the effect of J_3. In the framework of the DPT, the J_3 interaction brings about the frustrated next-nearest-neighbour interaction between $\boldsymbol{T}_j$ and $\boldsymbol{T}_{j+2}$, while the J_2 interaction does not. Thus, for sufficiently large J_3, the magnetization curve has cusps as found in figure 4. These cusps are due to the mechanism proposed by Okunishi *et al* [10].

The condition for the existence of the $M_s/4$ plateau is $J_3 > 0.31J_1$ from the DPT [9]. The width of the plateau may be too narrow to be observed clearly in figure 4.

We have discussed the plateaux and cusps in the magnetization curve of the $S = 1$ frustrated two-leg ladder by use of the DPT as well as the DMRG. We have also used the non-Abelian bosonization approach and the LS method, although we did not go into detail. The results obtained by these methods are consistent with each other. We remark that the $M_s/4$

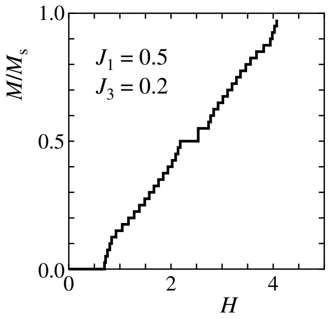

Figure 4. Magnetization curve for 40 spins when $J_1 = 0.5$, $J_2 = 0$ and $J_3 = 0.2$. We can see cusps near $M = 0.15M_s$ and $0.85M_s$.

plateau of the present mechanism is possibly related to that observed in organic $S = 1$ spin ladder 3,3′,5,5′-tetrakis(*N-tert*-butylaminxyl)biphenyl (abbreviated as BIP-TENO) [11].

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