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Novel Quantum Phase Transition in the Frustrated Spin Nanotube

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Abstract

The S=1/2 three-leg quantum spin tube is investigated using the numerical diagonalization. The study indicated a new quantum phase transition between the 1/3 magnetization plateau phase and the plateauless one, with respect to the spin anisotropy. The phase diagram is also presented.

Keywords: Spin tube, frustration, spin gap

1 Introduction

The spin systems of a tube-type structure have attracted a lot of interest in the field of the condensed matter physics[1]. Particularly, the S=1/2 three-leg spin tube is the most important because it has the largest frustration and quantum fluctuation. One of interesting features is that the system has a spin gap[2], while the S=1/2 three-leg spin ladder is gapless. Although no clear evidence of the spin gap has been observed in any candidate materials of the three-leg spin tube so far[3,4], many theoretical works[5-12] have supported the existence of the gap for the strong exchange interaction along the rung. The gap is found to disappear when the rung interaction is decreased. The phase transition between the gapped and gapless phases was clarified[13]; the critical ratio of the rung and leg coupling constants was precisely estimated by level-spectroscopy method based on the numerical-diagonalization data obtained by the MPI-parallelized program[14-16]. Under external fields, on the other hand, a magnetic field induced spin gap was also predicted to appear at the 1/3 of the saturation magnetization of the system by the numerical-diagonalization analysis[12] and the density matrix renormalization group (DMRG) calculation[17]. It should appear as a plateau of the magnetization curve, namely a magnetization plateau.

In this paper, we theoretically investigate the stability of the 1/3 magnetization plateau in the S=1/2 three-leg spin tube against the XXZ anisotropy. The discovery of a quantum phase transition

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from the plateau phase to the gapless one due to the anisotropy would be another evidence of the existence of the magnetization plateau in the isotropic spin tube.

2 Model and Calculation

We consider the S=1/2 three-leg spin tube, shown in Fig. 1, with the XXZ anisotropy described by the Hamiltonian

$$H = J_1 \sum_{i=1}^{3} \sum_{j=1}^{L} (S^x_{i,j} S^x_{i,j+1} + S^y_{i,j} S^y_{i,j-1} + \lambda S^z_{i,j} S^z_{i,j+1})$$
$$+ J_r \sum_{i=1}^{3} \sum_{j=1}^{L} (S^x_{i,j} S^x_{i+1,j} + S^y_{i,j} S^y_{i-1,j} - \lambda S^z_{i,j} S^z_{i+1,j})$$

where S^x, S^y, S^z are the spin-1/2 operators and L is the length of the tube along the leg direction. The exchange interaction constant J_1 stands for the neighboring spin pairs along the legs, while J_r the rung interaction constant. λ is the XXZ anisotropy parameter. All the exchange interactions are supposed to be antiferromagnetic (namely, positive). Throughout this paper, we fix J_r to unity. In this paper, we consider the XY-like anisotropy (λ <1) only.

We performed the numerical diagonalization based on the Lanczos algorithm to calculate the lowest energy eigenvalue in each subspace characterized by $M=\Sigma_j S_j^z$ (M=0, 1, …, 3L/2), which denoted as $E_0(L,M)$.

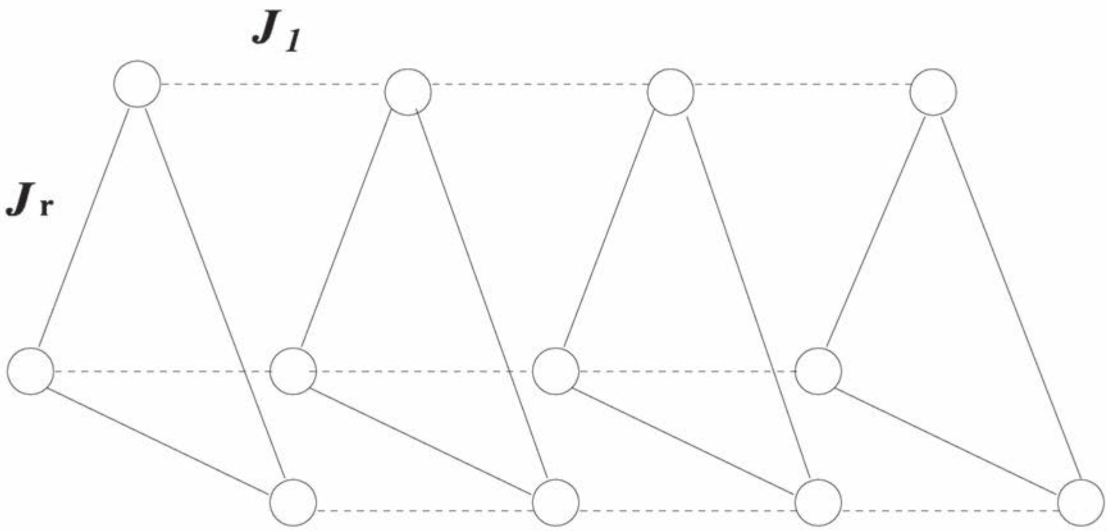

Fig. 1 S=1/2 three-leg spin tube. J_1 and J_r are the exchange coupling constants.

3 Magnetization Process

First, we present the magnetization processes in Fig.2, where the results of the system of L=8 with J_1=0.4 are shown for λ = 0.25, 0.48 and 0.75. Note here that we take the Zeeman term $-h\Sigma_j S_j^z$ into account. In this study, we focus our attention on the behavior at the one-third height of the saturation. One can easily observe the plateau-like behavior at this height for λ = 0.75. On the other hand, the behavior disappears for λ = 0.25. These results suggest that the phase transition occurs between the plateau-plateauless regions with respect to λ. λ=0.48 is the critical point for J_1=0.4 between the plateau and the plateauless phases, estimated by the phenomenological renormalization in the next section. However, it is difficult to determine the critical value of λ from those magnetization curves of the finite-size systems. In the following sections, we carry out a quantitative analysis of this phase transition.

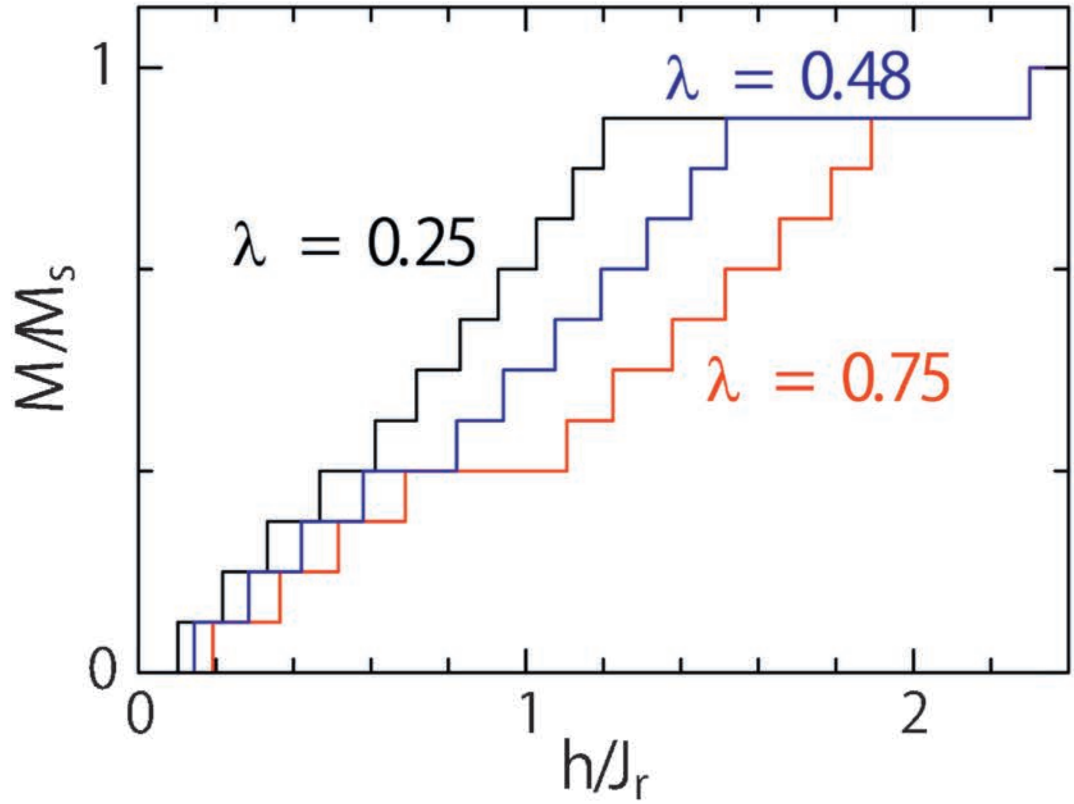

Fig. 2 Magnetization processes of the S=1/2 three-leg spin tube of L=8 and J_1=0.4 for λ = 0.25, 0.48 and 0.75. The saturated magnetization is denoted by M_s. λ=0.48 is the phase boundary between the plateau and the plateauless phases, estimated by the phenomenological renormalization in the next section.

4 Phenomenological Renormalization

Some previous theoretical works suggested that the XY-like anisotropy gives rise to the quantum phase transition between a magnetization plateau phase and a gapless one[18]. Thus we examine whether the same transition occurs or not in the present model. The phenomenological renormalization is one of good methods to detect a critical point where the magnetization plateau which is the field induced spin gap vanishes. The width of the 1/3 magnetization plateau which is calculated as $E_0(L, M+1)+E_0(L, M-1)-2E_0(L,M)$, where M=L/2 is 1/3 of the saturation magnetization(3L/2), is denoted as Δ. Using the numerical diagonalization, we calculate Δ for L=4, 6 and 8. According to the phenomenological renormalization, the equation of the scaled gap (plateau) $L\Delta$

$$L\Delta(L, \lambda) = (L-2)\Delta(L+2, \lambda).$$

gives the size-dependent fixed point λ_c (L+1). In Fig. 3 the scaled gap for J_1=0.2 is plotted versus λ, where dashed, dotted, and solid lines are for L=4, 6, and 8, respectively. The cross point of the scaled gaps for L and L+2 gives the fixed point $\lambda_c(L+1)$. Although the scaled gaps for L=4 and 6 do not cross to each other due to the finite-size effect, the ones for L=6 and 8 cross and we can obtain $\lambda_c(7)$. Thus we use $\lambda_c(7)$ as the estimated phase boundary between the plateau and plateauless phases at 1/3 of the saturation magnetization.

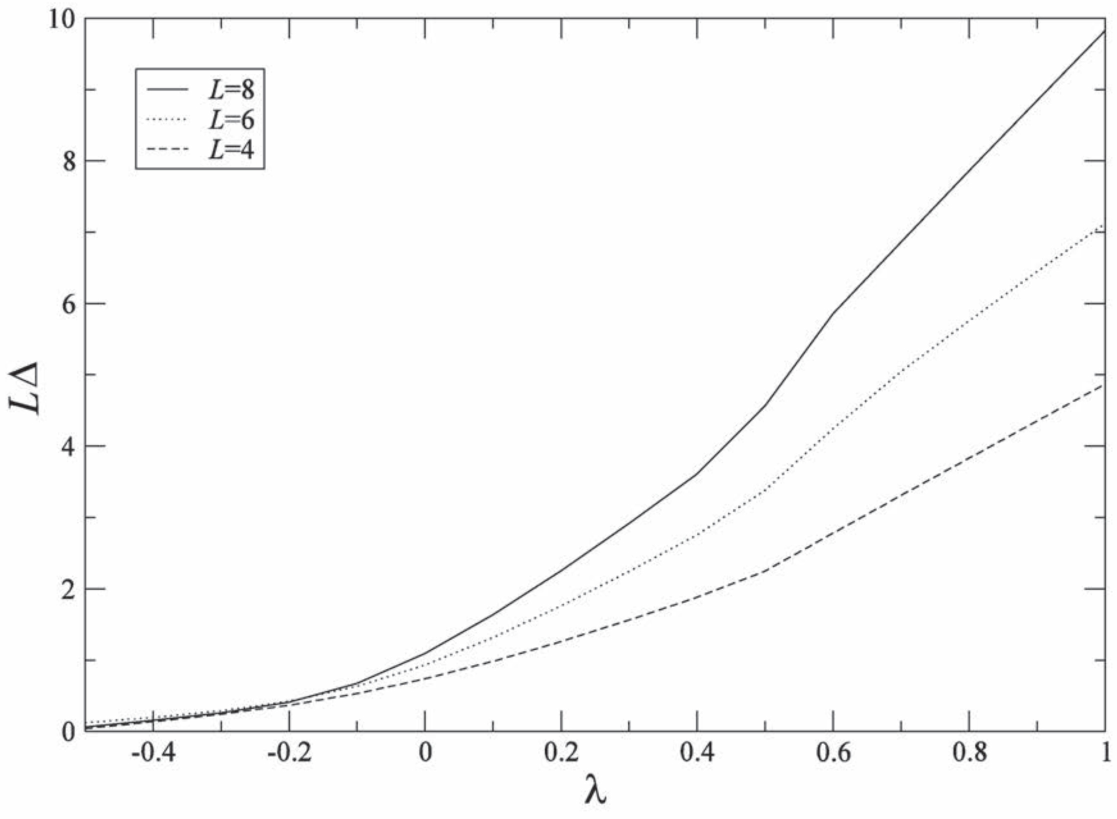

Fig. 3 Scaled gap (plateau width) $L\Delta$ is plotted versus λ for L=4, 6, and 8 for J_1=0.2.

5 Phase Diagram

The boundary between the 1/3 plateau (gapped) and plateauless(gapless) phases is shown in Fig. 4. Since the phase boundary was obtained only for one system size(L=7), it is difficult to estimate precise boundary in the thermodynamic limit. The calculation for larger systems would be desirable. However, even within the present analysis, we can expect that the region of the plateauless phase should be larger in the thermodynamic limit. Because the finite-size effect overestimates the plateau phase, as shown in Fig. 3 where the behavior of the scaled gaps for L=4 and 6 (the absence of the fixed point) indicates the existence of the plateau in the whole region. Thus the present estimation of the phase boundary would give a lower bound of the correct one in the phase diagram in Fig. 4. If we assume the existence of the 1/3 magnetization plateau in the isotropic case (λ=1), the present result is a strong evidence of the quantum phase transition to the plateauless phase.

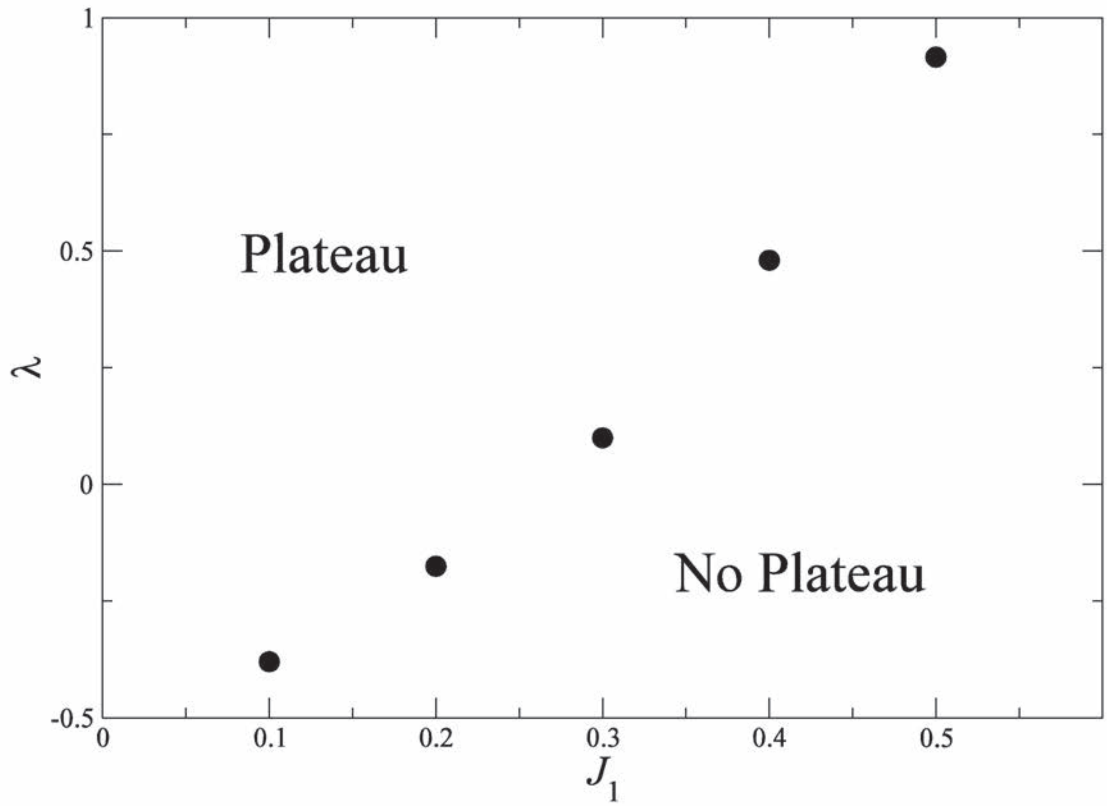

Fig. 4 Phase diagram in the λ-J_1 plane.

6 Summary

The S=1/2 three-leg spin tube with the XY-like anisotropy is investigated using the phenomenological renormalization applied to finite-size numerical-diagonalization data. We have successfully observed cases of the existence and the absence of the magnetization plateau at one-third height of the saturation magnetization when the anisotropy is tuned. The phenomenological-renormalization analysis has clarified a quantum phase transition between the magnetization plateau and plateauless phases at this height. The phase diagram in the λ-J_1 plane is presented. The precision of the phase boundary should be examined in future studies because there may be finite-size effects due to the small clusters that we treated. Calculations of larger-size systems would be necessary to determine the precise phase diagram.

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References

[1] For a review, T. Sakai, M. Sato, K. Okunishi, K. Okamoto and C. Itoi, J. Phys.: Condens. Matter 22 (2010) 403201.
[2] K. Kawano and M. Takahashi, J. Phys. Soc. Jpn. 66 (1997) 4001.
[3] J. Schnack, H. Nojiri, P. Kögerler, G. J. T. Cooper and L. Cronin, Phys. Rev. B 70 (2004) 174420.
[4] H. Manaka, Y. Hirai, Y. Hachigo, M. Mitsunaga, M. Ito and N. Terada, J. Phys. Soc. Jpn. 78 (2009) 093701.
[5] T. Sakai, M. Matsumoto, K. Okunishi, K. Okamoto and M. Sato, Physica E 29 (2005) 633.
[6] J. -B. Fouet, A. Läuchli, S. Pilgram, R. M. Noack and F. Mila, Phys. Rev. B 73 (2006) 014409.
[7] K. Okunishi, S. Yoshikawa, T. Sakai and S. Miyashita, Prog. Theor. Phys. Suppl. 159 (2005) 297.
[8] M. Sato and T. Sakai Phys. Rev. B 75 (2007) 014411
[9] S. Nishimoto and M. Arikawa, Phys. Rev. B 78 (2008) 054421.
[10] T. Sakai, M. Sato, K. Okunishi, Y. Otsuka, K. Okamoto and C. Itoi, Phys. Rev. B 78 (2008) 184415.
[11] T. Sakai, K. Okunishi, K. Okamoto, C. Itoi and M. Sato, J. Low. Temp. Phys. 159 (2010) 55.
[12] D. C. Cabra, A. Honecker and P. Pujol, Phys. Rev. B 58 (1998) 6241.
[13] T. Sakai, H. Nakano and K. Okunishi, J. Phys. Conf. Series 568 (2014) 042024.

[14] H. Nakano and A. Terai, J. Phys. Soc. Jpn.78 (2009) 014003.
[15] H. Nakano and T. Sakai, J. Phys. Soc. Jpn. 80 (2011) 053704.
[16] H. Nakano and T. Sakai, J. Phys. Soc. Jpn. 83 (2014) 104710.
[17] K. Okunishi, M. Sato, T. Sakai, K. Okamoto and C. Itoi, Phys. Rev. B 85 (2012) 054416.
[18] T. Sakai and M. Takahashi, Phys. Rev. B 57 (1998) R3201.