

# Exotic Quantum Phase Transition of the Spin Nanotube

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**Abstract.** The  $S=1/2$  three-leg spin tube is investigated using the numerical diagonalization up to the 42-spin clusters. A precise finite-size scaling analysis, so called the level spectroscopy, is carried out. It indicates a quantum phase transition between the spin-gap and gapless phases, with respect to the ratio of the leg and rung exchange interactions. The present analysis gives a precise estimate for the critical value of the ratio.

## 1. Introduction

The spin nanotube[1] is one of interesting nanomaterials which are expected to be developed towards some functional devices in the near future, like the carbon nanotube. Since the  $S=1/2$  three-leg spin tube  $[(\text{CuCl}_2\text{tach} \cdot \text{H})_3\text{Cl}]\text{Cl}_2$  was synthesized[2], several theoretical works about this systems have been published[3-12]. One of the interesting point of the  $S=1/2$  three-leg spin tube is that it has the spin gap, which is an energy gap between the singlet ground state and the triplet excitation, although the  $S=1/2$  three-leg spin ladder is gapless. The previous density matrix renormalization group (DMRG) calculation[11] revealed that the spin gap is open for sufficiently large exchange interactions in the rung (interchain) direction of the spin tube. On the other hand, the system is gapless in the weak rung coupling limit, because it corresponds to the three independent  $S=1/2$  antiferromagnetic spin chains. Thus a quantum phase transition should occur between the spin-gap and gapless phases, if the ratio of the rung and leg exchange interactions is varied. In our previous level spectroscopy analysis combined with the numerical diagonalization up to 30-spin clusters[8], it was difficult to determine whether a finite critical ratio exists or an infinitesimal rung coupling induces the spin gap, because the finite-size effect is quite large. Recently we performed the numerical diagonalization of the  $S=1/2$  three-leg spin tube with system sizes up to 42 spins. In particular, calculations of the 42-spin cluster was carried out by our program running at the K Computer at RIKEN, Kobe. In the present paper, we report a result from the level spectroscopy analysis applied for the data of the numerical diagonalization up to 42-spin clusters and conclude that the gapless-gapped quantum phase transition occurs at a finite critical ratio.

## 2. Model

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



$$\hat{H} = J_1 \sum_{i=1}^3 \sum_{j=1}^L \bar{S}_{i,j} \cdot \bar{S}_{i,j+1} + J_2 \sum_{i=1}^3 \sum_{j=1}^L \bar{S}_{i,j} \cdot \bar{S}_{i+1,j} \quad (1)$$

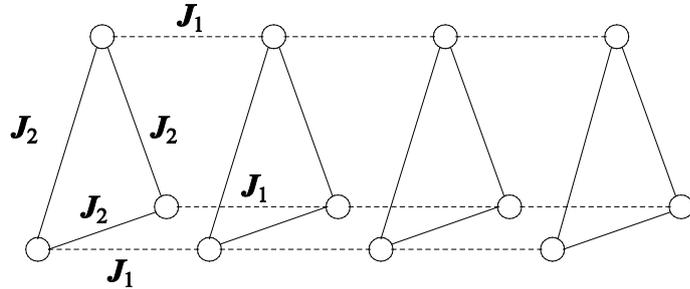


Fig. 1 Structure of the three-leg spin tube (1).

where  $\bar{S}_{i,j}$  is the spin-1/2 operator and  $L$  is the length of the tube in the leg direction. The exchange interaction constant  $J_1$  is for the neighbouring spin pairs along the legs, while  $J_2$  is the rung interaction constant. All the exchange interactions are supposed to be antiferromagnetic (namely, positive).

We performed the numerical diagonalization based on the Lanczos algorithm for finite-size clusters with system sizes up to 42 spins, namely  $L=14$ , under the periodic boundary condition, and obtained the single ground-state and triplet excited-state energies. In addition we calculated the single excitation energy, namely the second eigenvalue in the  $S=0$  sector, for the level spectroscopy analysis. The single-triplet excitation energy and single-singlet one are denoted as  $E_{01}$  and  $E_{00}$ , respectively.

We carried Lanczos diagonalizations using our MPI-parallelized code which was originally developed in the study of the Haldane gaps[13]. The usefulness of our program was confirmed in large-scale parallelized calculations[14,15]. Note also that this program contributed much for the progress of the studies of anomalous magnetization jump in frustrated magnets[16,17,18].

### 3. Quantum Phase Transition

The previous DMRG calculation[11] suggested that the system (1) has a spin gap for sufficiently large  $J_2$ . According to the Lieb-Schultz-Mattis theorem, the spin gap phase of the  $S=1/2$  three-leg spin tube should have two-fold degeneracy in the ground state, due to the translational symmetry break down. A schematic picture of the gapped phase for the symmetric spin tube was proposed as shown in Fig. 2, where the three equivalent singlet dimer covering patterns are resonating at each two unit cell triangles.

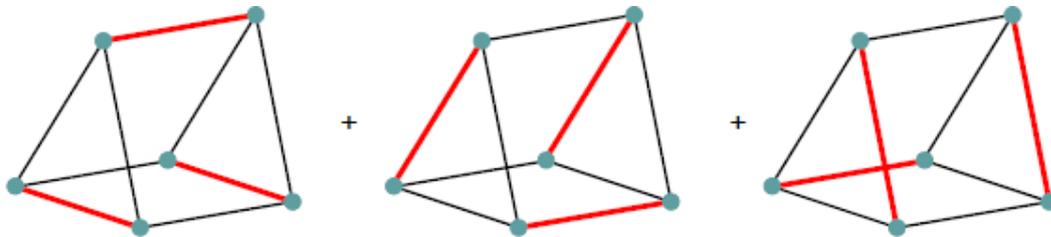


Fig. 2. A schematic picture of the spin gap formation mechanism of the  $S=1/2$  three-leg spin tube. Circles and thick lines are spins and singlet bonds, respectively. The three equivalent patterns at each two unit cells are resonating.

On the other hand, the system is gapless in the weak  $J_2$  limit where it corresponds to three independent spin chains. The purpose of the present work is to determine the critical point of  $J_2/J_1$  where a quantum phase transition occurs between the gapless and gapped phases.

#### 4. Level Spectroscopy

The quantum phase transition in the present case is expected to belong to the universality class of the Berezinkii-Kosteritz-Thouless transition. Around the transition the logarithmic system size correction proportional to  $1/\log L$  sometimes appears and as a result it is difficult to determine a precise critical point in the thermodynamic limit because of quite large finite-size effects. In such a case the level spectroscopy[19] is one of the best method to determine it. According to this method, the critical point is estimated as an intersection between the triplet and singlet excitation energies, where the logarithmic correction vanishes. The result of our previous level spectroscopy analysis up to 30-spin clusters was  $J_2/J_{1c}=0.5 \pm 0.5$ . The error due to the extrapolation to the thermodynamic limit was still too large to determine whether the critical point is finite or zero. Then in the present work, we calculated the triplet and singlet excitation energies up to 42-spin clusters and applied the same method for them. The level cross points for 36- and 42-spin clusters are shown in Figs. 3 and 4, respectively.

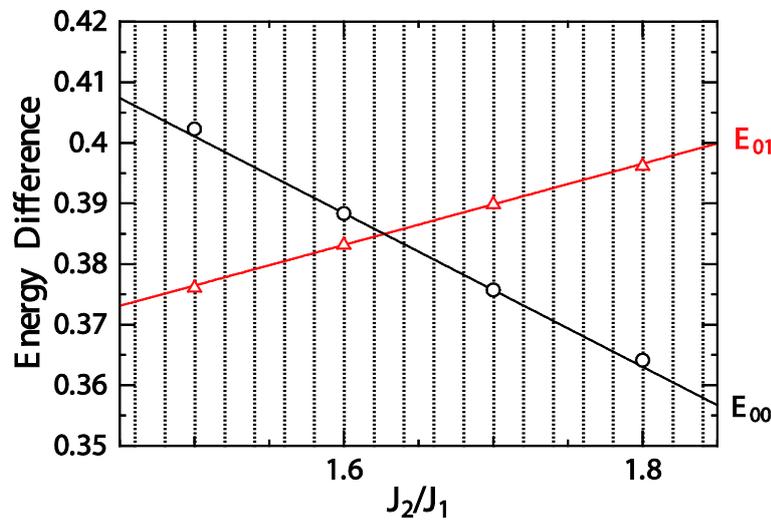


Fig.3. Singlet-triplet excitation energy  $E_{01}$ (triangles) and singlet-singlet one  $E_{00}$ (squares) for  $L=36$  are plotted versus  $J_2/J_1$  to estimate a level cross point.

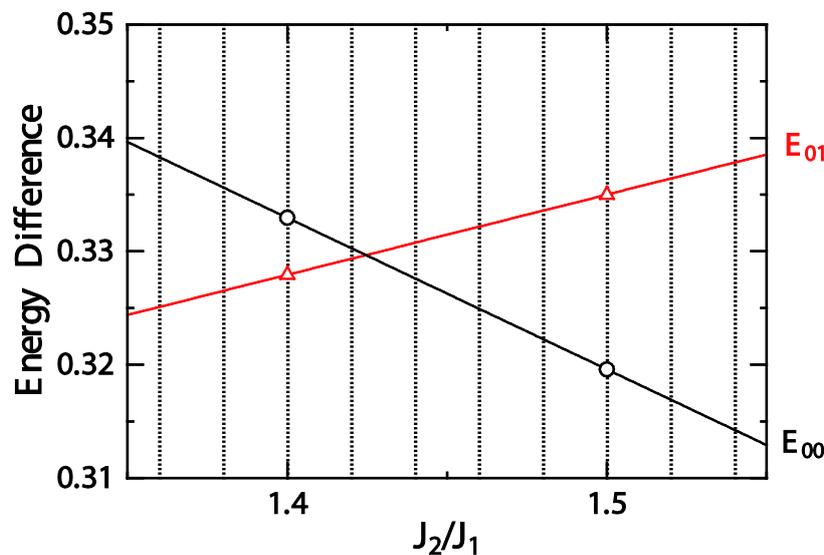


Fig.4. Singlet-triplet excitation energy  $E_{01}$ (triangles) and singlet-singlet one  $E_{00}$ (squares) for  $L=42$  are plotted versus  $J_2/J_1$  to estimate a level cross point.

Since the size correction of the level cross points is expected to be proportional to  $1/L^2$ , we estimated a quantum critical point in the thermodynamic limit by plotting them versus  $1/L^2$  shown in Fig. 5. It includes the present results for  $L=12$  (36 spins) and 14 (42 spins), as well as previous ones up to  $L=10$ . The present extrapolation indicates  $J_2/J_{1c}=0.71\pm 0.21$ . If we estimate it only from the largest two system sizes ( $L=12$  and 14), the result is  $J_2/J_{1c}=0.864$ . This is a strong evidence to confirm that the quantum phase transition occurs at a finite critical point of  $J_2/J_1$ . Thus the  $S=1/2$  three-leg spin tube is gapless for weak rung exchange interactions. The present result suggests that the spin gap is not open, until the rung coupling is comparable with the leg one.

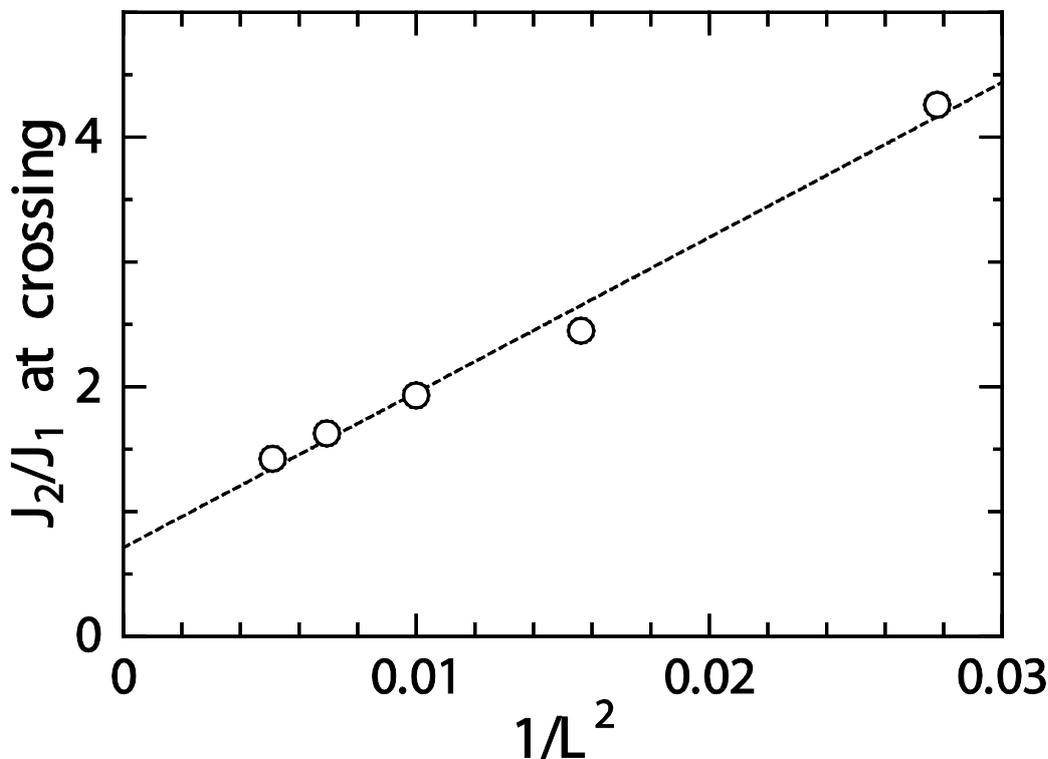


Fig.5. Extrapolation of the level cross point to the thermodynamic limit, assuming that the size correction is proportional to  $1/L^2$ . The estimated critical point is  $J_2/J_1=0.71\pm 0.21$ .

## 5. Summary

The  $S=1/2$  three-leg spin tube is investigated by the level spectroscopy combined with the numerical diagonalization up to the 42-spin cluster. It leads to the conclusion that a quantum phase transition between the gapless and spin-gap phases occurs at a finite critical ratio of the rung and leg coupling constants. The critical value is estimated as  $J_2/J_1=0.71\pm 0.21$ .

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