Exotic Quantum Critical Phenomena of the Spin Nanotubes

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Abstract. Recently some quantum spin systems on tube lattices, so called spin nanotubes, have been synthesized. They are expected to be interesting low-dimensional systems like the carbon nanotubes. As the first step of theoretical study on the spin nanotube, we investigate the S=1/2 three-leg spin tube, which is the simplest one, using the numerical exact diagonalization (ED), combined with the recently developed level spectroscopy analysis. Particularly, we introduce the lattice distortion from the regular triangle unit to the isosceles one. We revealed that the S=1/2 isosceles triangle spin tube exhibits the quantum phase transition between the spin gapped and gapless spin liquid phases.

1. Introduction

The quantum spin nanotube \cite{1} are one of interesting objects in the nanoscience and the nanotechnology. Among them the three-leg spin tubes have been extensively studied both theoretically and experimentally in recent years, because they have a strong spin frustration at each unit cell. The density matrix renormalization group (DMRG) analysis \cite{2} indicated a large spin gap in the strong rung coupling limit, in contrast to the three-leg spin ladder which is gapless. After the synthesisization of the S=1/2 three-leg spin tube [(CuCl\textsubscript{2}tachH)\textsubscript{3}Cl]Cl\textsubscript{2} \cite{3}, several theoretical works on the S=1/2 three-leg spin tube have been published \cite{4–10}. In our previous study \cite{4,9,10}, the asymmetric rung interaction was introduced and the quantum phase transition from the gapped to the gapless phases with respect to the lattice distortion was investigated. Although the phase boundary was clearly determined by the DMRG method for strong rung coupling region, it is still ambiguous for small one because the DMRG calculation is not converged well. In this paper, using the level spectroscopy analysis which is one of the most precise method to the phase boundary of the Berezinskii-Kosterlitz-Thouless (BKT) transition, we present a phase diagram including the week rung coupling region.
2. Model
We consider the $S = \frac{1}{2}$ asymmetric three-leg spin tube, shown in Fig. 1, described by the Hamiltonian

$$
\hat{H} = J_1 \sum_{i=1}^{3} \sum_{j=1}^{L} \vec{S}_{i,j} \cdot \vec{S}_{i,j+1} + J_t \sum_{i=1}^{2} \sum_{j=1}^{L} \vec{S}_{i,j} \cdot \vec{S}_{i+1,j} + J_r' \sum_{j=1}^{L} \vec{S}_{3,j} \cdot \vec{S}_{1,j},
$$

(1)

where $\vec{S}_{i,j}$ is the spin-$\frac{1}{2}$ operator and $L$ is the length of the tube in the leg direction. The exchange interaction constant $J_1$ is for the neighboring spin pairs along the legs, while $J_t$ and $J_r'$ are the rung interaction constants. All the exchange interactions are supposed to be antiferromagnetic (namely, positive). The ratio $\alpha = J_r'/J_r$ stands for the degree of the asymmetry of the rung interactions. We will vary $\alpha$ and $J_1$ to investigate the quantum phase transitions. Throughout this paper, we fix $J_r$ to one.

![Figure 1. $S = 1/2$ three-leg quantum spin tube.](image)

The present model includes three typical models as limiting cases; (a) $\alpha = 0$: the three-leg spin ladder, (b) $\alpha = 1$: the symmetric spin tube, and (c) $\alpha \to \infty$: the single chain plus rung dimers. Since the system is gapless in the cases (a) and (c), while gapful in the case (b), at least two quantum phase transitions should occur with increasing $\alpha$ from 0 to infinity. As we already mentioned, the one-site translational symmetry along the leg ($\vec{S}_{i,j} \to \vec{S}_{i,j+1}$) is spontaneously broken in the symmetric spin tube at least in the strong-rung-coupling regime. [2,8] On the other hand, the weak $J_t$ limit is also gapless, because the system consists of three independent chains. This gapless phase is denoted as the phase I. We also denote the gapless phase around (a), the gapful one around (b) and the gapless one around (c) as the phases II, III, and IV, respectively.

3. Level spectroscopy
The level-spectroscopy method [11–14] is a very powerful tool to determine the critical point of the BKT transition in one-dimensional quantum systems. For the SU(2)-symmetric cases including the present spin tube, its strategy becomes easier [11]. According to this method, the critical point can be determined as an intersection between the singlet and the triplet excitation gaps, where their logarithmic finite-size corrections vanish.

The phase boundaries II-III and III-IV estimated by this method are shown in Fig. 2. Here we have applied the results of the numerical diagonalization up to $L = 10$ for $J_1 = 0.1$. The numerical data are well converged to those of the thermodynamic limit by use of the $1/L^2$ extrapolation. The $1/L^2$ extrapolation is justified by considering the most important finite-size correction to the excitation gaps $\Delta$ next to the logarithmic term [11].

On the other hand, when we consider the transition between two phases III and I, we search for the level cross value of $1/J_1$ with fixed $\alpha$. In Fig. 3, the size-dependent level cross points are plotted versus $1/L^2$ for $\alpha =0.98$ and 1.02.
Figure 2. Level cross values of $\alpha$ for $L = 6, 8$ and 10 with fixed $J_1$ to 0.1.

Figure 3. Level cross values of $1/J_1$ for $L = 6, 8$ and 10 with fixed $\alpha$ to 0.98 and 1.02. They correspond to the boundary between the I and III phases.

Figure 4. Phase diagram on the $J_1$-$\alpha$ plane by the level spectroscopy method.

4. Phase diagram
All the estimated phase boundaries in the thermodynamic limit are plotted in Fig. 4. The phase diagram justifies that the gapless phase (I) lies in a finite region.

The phase I in the present study is larger than the phenomenological renormalization up to $L = 10$. It is consistent with the fact that the phenomenological renormalization always underestimates gapless phases for the boundaries among the phases II, III and IV, as shown in our previous work [9]. The present level spectroscopy study qualitatively justifies the phase diagram obtained by the effective Hubbard Hamiltonian approach in the work [9].

The present system also exhibits the 1/3 magnetization plateau for sufficiently small $J_1$. This plateau was discussed in detail in [1] and the $J_1$-$\alpha$ phase diagram determined by numerical methods was presented in our recent paper [15].
5. Summary
The $S = 1/2$ three-leg spin tube with the asymmetric interaction is investigated using the level spectroscopy method combined with the numerical diagonalization of finite-size clusters up to $L = 10$. The present result indicates that the gapless phase I lies in a finite area continued to the infinite $J_1$ limit. It is consistent with our previous phenomenological renormalization study and effective theory [9].

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