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Energy gap of spin nanotube

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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 a first step of theoretical study on the spin nanotube, we investigate the $S=\frac{1}{2}$ three-leg spin tube, which is the simplest one, using numerical analyses of finite clusters and a finite-size scaling technique. The spin gap, which is one of the most interesting quantities reflecting the macroscopic quantum effect, was revealed to be open for any finite rung exchange couplings, in contrast to the three-leg spin ladder system which is gapless. We also found a quantum phase transition caused by an asymmetric rung interaction. When one of the three rung coupling constants is changed, the spin gap vanishes very rapidly.

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Keywords: Spin nanotube; Spin gap; Quantum phase transition

1. Introduction

The spin nanotube is one of the interesting new materials in the nanoscience and technology, like the carbon nanotube. It would be possibly a new type of low-dimensional magnet towards a fruitful application in the near future. Recently, some candidates of the spin nanotube have been synthesized; the dioxygen molecules absorbed in a microporous copper coordination polymer [1], $[(CuCl_2tachH)_3Cl]Cl_2$ [2] and $Na_2V_3O_7$ [3]. Although these materials exhibited some characteristic features of the low-dimensional magnet, only a few theoretical works on spin nanotubes have been done [4–7]. As a first step, we theoretically investigate the simplest spin nanotube, the $S=\frac{1}{2}$ three-leg spin tube, using the numerical exact diagonalization and the density

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matrix renormalization group (DMRG) approach. In this paper, we focus our attention on the quantum phase transition related to the spin gap Δ, which reflects the quantum effects.

2. Model

The $S = \frac{1}{2}$ three-leg spin tube, shown in Fig. 1, is described by the Hamiltonian

$$H = J_1 \sum_{i=1}^{3} \sum_{j=1}^{L} \vec{S}_{i,j} \cdot \vec{S}_{i,j+1} + J_r \sum_{i=1}^{2} \sum_{j=1}^{L} \vec{S}_{i,j} \cdot \vec{S}_{i+1,j} + J'_r \sum_{j=1}^{L} \vec{S}_{3,j} \cdot \vec{S}_{1,j}, \qquad (1)$$

where $\vec{S}$ is the quantum spin-$\frac{1}{2}$ operator and L is the length of the tube in the leg direction. The exchange coupling constants J_l and J_r are the neighboring spin pairs along each leg and rung, respectively. All the exchange interactions are antiferromagnetic here. One of the three rung couplings is denoted by J'_r and the ratio $\alpha = J'_r/J_r$ will be varied to investigate the quantum phase transition in the next section.

3. Spin gap

Model (1) corresponds to the three-leg ladder for $\alpha = 0$, which was revealed to be gapless. On the other hand, the symmetric three-leg tube ($\alpha = 1$) was predicted to have the spin gap between the singlet ground state and triplet excited one, using the Luttinger liquid analysis [8] and an effective Hamiltonian approach [9]. According to the Lieb–Schultz–Mattis theorem [10], if system (1) has a gap, the ground state should be at least doubly degenerated. The scaled gaps $L\Delta$ of the singlet ($S = 0$) and triplet ($S = 1$) excitations for $J_l = 0.2$ and $\alpha = 1$ calculated by numerical diagonalization of finite clusters are shown in Fig. 2. The increasing $L\Delta$ with increasing L implies that the gap is open, while the decreasing one indicates that the excited state degenerates with the ground state in the thermodynamic limit. Fig. 2 suggests that the spin gap exists and the singlet ground state is doubly degenerated for $J_r > 0$, and the gap is close at $J_r \sim 0$. The results are consistent with the previous predictions [8,9].

As already stated, system (1) is gapless when $\alpha = 0$. Further, it should be also gapless for large α, because it is decomposed into a single chain and a two-leg ladder in the limit $\alpha \to \infty$. We note that the central charge of the conformal field theory [11] is $c = 1$ in both limits, $\alpha = 0$ and ∞. Thus, we will see two quantum phase transitions between the gapped and gapless phases, if the ratio α varies from 0 to ∞. We have numerically calculated the scaled gaps $L\Delta$ of the triplet excitations by DMRG for $J_r = 1$ and $J_l = 0.2$ with varying α from 0 to 2 to investigate the above-mentioned quantum

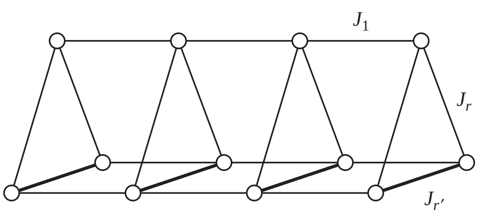

Fig. 1. Schematic figure of the three-leg spin tube.

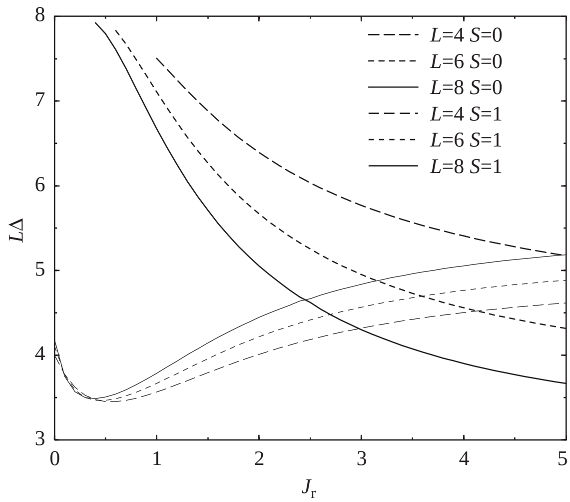

Fig. 2. Scaled gaps of singlet and triplet excitations calculated by numerical diagonalization, versus the rung coupling J_r with $J_l = 0.2$ and $\alpha = 1$.