Topological aspects of the quantum spin nanotube

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Abstract. The spin nanotube has attracted a lot of interest as an intersection between the strongly correlated electronics and the nanoscience. Among spin nanotubes we focus on the $S=1/2$ three-leg spin tube, because it has the largest quantum fluctuation and the strongest frustration. Using the numerical exact diagonalization of the finite-cluster Heisenberg model, we reveal that two singlet ground states are degenerated in the spin gap phase of the spin tube. It is also found that the spin gap is characterized by the quantized Berry phase.

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 $[\text{CuCl}_2\text{ach} \cdot \text{H}, \text{H})_3\text{Cl}]_2$ was synthesized[2], several theoretical works about this systems have been published[3-11]. In the previous theoretical work by the numerical exact diagonalization and the density matrix renormalization group (DMRG) calculation [8], the spin gap was revealed to be very fragile against the lattice distortion from the regular triangle to the isosceles one, and the Berezinskii-Kosterlitz-Thouless (BKT) quantum phase transition was predicted from the gapped to the gapless phases with respect to such an asymmetry of the rung exchange interactions. A purpose of the present study is to propose a physical picture of the spin gap formation mechanism for the spin tube. Using the numerical exact diagonalization of the $S=1/2$ three-leg spin tube, we calculate the singlet excitation gap and the quantized Berry phase, which proposed by Hatsugai[12], to investigate topological aspects of the spin gap phase and the quantum phase transition between the gapped and the gapless Tomonaga-Luttinger liquid phases.

2. Model

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

$$\hat{H} = J_1 \sum_{i} \sum_{j \neq i} \hat{S}_{i,j} \cdot \hat{S}_{i+1,j} + J_2 \sum_{i} \sum_{j \neq i} \hat{S}_{i,j} \cdot \hat{S}_{i+1,j} + J'_r \sum_{j} \hat{S}_{r,j} \cdot \hat{S}_{r,j} \quad (1)$$

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where $\vec{s}_{i,j}$ 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 $J_r$ 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.

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 gap-full 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.

### 3. Spin gap

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.

If this picture is valid, a double periodicity in the chain direction should be realised in the ground state. In order to confirm it, we calculate the singlet excitation energy with the momentum $k = \pi$ and test the degeneracy of it with the ground state in the thermodynamic limit. The phenomenological renormalization is a good method to determine the parameter region where the two states are
degenerated in the infinite length limit. For each value of $J_1$, the critical point $\alpha_c$ is determined by the fixed point equation
\[
\Delta_s(\alpha_c, N_1) = \Delta_s(\alpha_c, N_2),
\]
for two different system sizes $N_1$ and $N_2$, where $\Delta_s$ is the energy difference between the singlet excitation and ground states. The calculated $\Delta_s$ is plotted versus $\alpha$ for $L=4$, 6 and 8 with fixed $J_1=0.5$ in Fig. 3. Extrapolating the size-dependent fixed point $\alpha_c(4,6)$ and $\alpha_c(6,8)$ with respect to the system size $L$ (we assume the size correction is proportional to $1/L^2$), we determine $\alpha_c$ in the thermodynamic limit. The result is shown as solid circles in the $\alpha$-$J_1$ plane in Fig. 4. The phase boundary between the spin gap and gapless phases determined by the phenomenological renormalization applied for the singlet-triplet gap in the previous work[8] is also plotted as a solid line in Fig. 4. Although some discrepancy between the two boundaries due to finite size effects at larger $J_1$, Fig. 4 suggests that the two singlet states are degenerated in the thermodynamic limit in the spin gap phase. It is consistent with that the translational symmetry is broken and double periodicity is realized in the gapped phase.

![Fig. 3 Scaled singlet-singlet excitation gap $L \Delta_s$ plotted versus $\alpha$ with fixed $J_1=0.5$.](image-url)
Fig. 4  Phase boundaries between the spin gap and gapless phases. Solid circles are determined by the phenomenological renormalization of the singlet-singlet excitation gap, a solid line is determined by the singlet-triplet excitation gap from Ref. [8].

4. Quantized Berry phase

The quantized Berry phase, which was proposed by Hatsugai, is a useful quantity to characterize a topological order like the string order in the Haldane gap system. It can be used to detect some hidden topological order characterized by a local gauge connection. Now we make a local SU(2) twist $\theta$ only at one link as,

$$J_{ij} \tilde{S}_j \cdot \tilde{S}_j \rightarrow J_{ij}/2(e^{-i\theta}S_i^+S_j^- + e^{i\theta}S_i^-S_j^+ + 2S_i^zS_j^z)$$

and sum up the Berry connection

$$\gamma = \text{Arg} \prod_C \{\psi_{\theta_j}^U|\psi_{\theta_{j+1}}^U\}, \quad |\psi_{\theta_j}^U\rangle = |\psi_{\theta_j}\rangle\langle\psi_{\theta_j}|\phi\rangle$$

where $|\phi\rangle$ is a reference state to fix the gauge. If the singlet dimer covering in Fig. 2 is realised, the Berry connection is expected to quantized to be one for $\theta = \pi$ at each bond, like the string order parameter in the Haldane gap phase of the $S=1$ antiferromagnetic chain. The calculated $\gamma$ by the numerical exact diagonalization for $L=4$ is plotted in the $\alpha$-$J_1$ plane in Fig. 5. It indicates that the
Berry connection is quantized and it corresponds to one in the spin gap phase, while zero in the gapless phase. It suggests that the spin gap phase of the S=1/2 three-leg spin tube is characterized by the quantized Berry phase and it can be formulated as some topological order parameters.

Fig. 5 Quantized Berry connection calculated by the numerical exact diagonalization for L=4.

5. Summary
The S=1/2 three-leg spin tube is investigated by the numerical exact diagonalization. It is found that the ground state has a two-fold degeneracy in the S=0 space, which is consistent with the translational symmetry break down. The spin gap phase is revealed to be characterized by the quantized Berry phase, which is related to some topological orders.

Acknowledgments
This work has been partly supported by Grants-in-Aid for Scientific Research (B) (No.17340100, No.20340096) and Priority Areas "Invention of Anomalous Quantum Materials --- New Physics through Innovation Materials ---" (No.19014019), "Physics of New Quantum Phases in Super-clean Materials" (No.17071011, No.18043023, No.20029020), "High Field Spin Science in 100T" (No.20030008, No.20030003) and "Novel states of matter induced by frustration" (No. 22014012) from the Ministry of Education, Culture, Sports, Science and Technology of Japan. We further thank the Supercomputer Center, Institute for Solid State Physics, University of Tokyo, the Cyberscience Center, Tohoku University, and the Computer Room, Yukawa Institute for Theoretical Physics, Kyoto University for computational facilities. This workshop was supported in part by the Grant-in-Aid for the Global COE Program "The Next Generation of Physics, Spun from Universality and Emergence" from the Ministry of Education, Culture, Sports, Science and Technology (MEXT) of Japan. The authors also thank the Yukawa Institute for Theoretical Physics at Kyoto University, where this work was initiated completed during the YITP-W-10-12 on "International and Interdisciplinary Workshop on Novel Phenomena in Integrated Complex Sciences: from Non-living to Living Systems".
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