Exotic quantum phase transitions in the spin nanotube

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Abstract. We investigate the S=1/2 three-leg spin tube, which is the simplest spin nanotube, using the density matrix renormalization group (DMRG) and the numerical exact diagonalization (ED), combined with a finite-size scaling analysis. Particularly, we introduce the lattice distortion from the regular triangle unit to the isosceles one. In our previous works, we revealed that the S=1/2 isosceles triangle spin tube exhibits following exotic quantum phenomena: the quantum phase transition between the spin gapped and gapless spin liquid phases, the 1/3 magnetization plateau due to two different mechanisms, and a new phase between the two plateau phases where the translational symmetry is spontaneously broken. We briefly review these results and show our new calculation of the expectation value of the magnetization at each site to specify the spin structure in the new field induced phase.

1. Introduction
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 density matrix renormalization group (DMRG) and the numerical exact diagonalization (ED), combined with a finite-size scaling analysis. Particularly, we introduce the lattice distortion from the regular triangle unit to the isosceles one. In our previous works\cite{1-4}, we revealed that the S=1/2 isosceles triangle spin tube exhibits following exotic quantum phenomena: (1) the quantum phase transition between the spin gapped and gapless spin liquid phases\cite{1,2}; (2) the 1/3 magnetization plateau due to two different mechanisms\cite{1, 4}; (3) the field-induced symmetry breaking between the two plateau phases\cite{1-4}.

In the present paper, we briefly review these results and present the calculated spin excitation values in the new phase between the two 1/3 magnetization plateau phases, to confirm the symmetry breaking and specify the spin structure.
2. Model

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

\[ \hat{H} = J_1 \sum_{j=1}^{3} \sum_{i=1}^{L} \hat{S}_{i,j} \cdot \hat{S}_{i,j+1} + J_r \sum_{j=1}^{L} \sum_{i=1}^{L} \hat{S}_{i,j} \cdot \hat{S}_{i+1,j} + J' \sum_{j=1}^{L} \hat{S}_{3,j} \cdot \hat{S}_{1,j} \]  

(1)

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

where \( \hat{S}_{i,j} \) 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 \( J' \) are the rung interaction constants. All the exchange interactions are supposed to be antiferromagnetic (namely, positive).

The ratio \( \alpha = J'/J_r \) 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 effect of the magnetic fields is incorporated by adding the Zeeman energy

\[ \hat{H}_Z = -H \sum_{i=1}^{3} \sum_{j=1}^{L} \hat{S}_{i,j}^z \]  

(2)

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. The one-site translational symmetry along the leg \( (\hat{S}_{i,j} \to \hat{S}_{i,j+1}) \) was revealed to be spontaneously broken in the symmetric spin tube at least in the strong-rung-coupling regime in the previous works[5,6].

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.

Fig. 2. A schematic picture of the spin gap formation mechanism of the S=1/2 three-leg spin tube. Blue circles and thick red lines are spins and singlet bonds, respectively. The three equivalent patterns at each two unit cells are resonating.
If this picture is valid, a double periodicity in the chain direction should be realized 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

\[
L_1 \Delta_s(\alpha_c, L_1) = L_2 \Delta_s(\alpha_c, L_2),
\]

for two different system sizes \( L_1 \) and \( L_2 \), 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 \( \alpha_c \) for \( L=4, 6 \) and \( 8 \) 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[1,2] is also plotted as a solid line in Fig. 4. Although there is some difference 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 Δ_s plotted versus α 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. [2].

4. 1/3 magnetization plateau

In order to study the 1/3 magnetization plateau, we calculated the spin excitation gap at $m/m_s = 1/3$ ($m$ is the magnetization and $m_s$ is the saturation magnetization), namely

$$
\Delta = E(M+1) + E(M-1) - 2E(M)
$$

(3)

where $E(M)$ is the lowest energy in the subspace $\sum s_j^z = M$ and $M=L/2$, using the numerical exact diagonalization. The scaled gap $L\Delta$ for $\alpha=1$ is plotted versus $J_1$ for $L=4,6$ and 8 in Fig. 5. From the cross point of $L=6,8$ curves, the quantum critical point is estimated as $J_1 \approx 0.5$ between the plateau and gapless (no plateau) phases.

Fig. 5 Scaled gaps for $L=4,6$ and 8 plotted versus $J_1$ with fixed $J'/J_c = 1$.

In comparison with the spin gap at $H=0$, the 1/3 plateau is expected to be stable against the asymmetry ($\alpha \neq 1$), because it was also predicted to exist even for the three-leg ladder ($\alpha = 0$).

At the 1/3 plateau phase close to $\alpha = 0$, the state $|\uparrow \downarrow \uparrow\rangle$ is expected to be stabilized at each triangle unit, while $|\text{singlet}, \uparrow\rangle$ for the other limit $\alpha \to \infty$. We call the two mechanisms of the plateau
formation as the udu mechanism and dimer-monomer mechanism, respectively. Thus the three phases; the udu plateau, the dimer-monomer plateau and gapless phases are expected to occur at \( m/m_s = 1/3 \).

Next we consider the boundary between the two different plateau phases. It is expected to appear around \( \alpha = 1 \) and \( J_1 < 0.5 \). The \( \alpha \) dependences of the plateau width estimated by the DMRG calculation for \( L=128 \) for \( J_1 = 0.1, 0.3, \) and 0.5 are shown in Fig. 6. Figure 6 indicates clear anomalous increases of the plateau width for \( J_1 = 0.1 \) and 0.3. The anomalous increase region is supposed to be a new phase between the two plateau phases. According to the perturbation study in the strong \( J_r \) region in our previous work [1], the translational symmetry in the leg direction is broken and two different low-lying states at each triangle unit alternate like the Neel order in the new phase. The lowest excitation gap within the \( M=M_s/3 \) space, \( \Delta_0 \), with \( k=\pi \) and the odd parity for the inversion with respect to the center line of the isosceles triangle, is a useful order parameter to distinguish the new phase with the other two plateau phases. The gap closes in the new phase, while it is open in the other ones. Thus the phase boundary of the new plateau phase can be determined by the same phenomenological renormalization as the one used to obtain the ground state phase diagram in Fig. 4, applied for \( \Delta_0 \). We just show the phase diagram at \( m/m_s = 1/3 \) obtained by the method in Fig. 7, where the plateau 1, 2, and 3 phases are the udu, dimer-monomer, and new plateau phases, respectively. The boundaries between different plateau phases belong to the Ising universality class, while the one between the plateau and gapless phases the Berezinskii-Kosterlitz-Thouless (BKT) universality class [1].

Fig. 6 \( \alpha \) dependence of the plateau width normalized by the saturation magnetic field \( H_s \) calculated by DMRG for \( J_1 = 0.1, 0.3 \) and 0.5.

Fig. 7 Phase diagram at \( m=1/3 \).
5. Spin structure of the new phase
Finally we show the calculated spin structure in the new phase by the DMRG. The expectation value of $S^z$ at each site calculated by DMRG is plotted versus $\alpha$ in Fig. 8, where blue stars, green pluses and red crosses correspond to the apical, the left, and right bottom sites of the triangle unit, respectively for $J_1=0.3$. The spins have different values between the two bottom sites in the new phase ($0.84<\alpha<1.24$) and they are switched at the adjacent triangle. It implies that the long-range Neel order is realized at the two bottom sites along the leg. Thus the present calculation justifies the existence of the new phase characterized by the staggered long-range order at the two bottom sites.

![Fig. 8](image_url)

### 6. Summary
The S=1/2 isosceles triangle spin tube was investigated by the DMRG and numerical diagonalization. The present study indicated that two singlet states are degenerated in the $m=0$ ground state, which is consistent with the translational symmetry breaking. In addition in the new phase between the two different 1/3 magnetization plateau phases, the staggered long-range order was revealed to realized.

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### References
[1] T. Sakai et al., *J. Phys.: Condens. Matter* **22**, 403201 (2010).
[2] T. Sakai et al., *Phys. Rev. B*, **78**, 184415 (2008).
[3] M. Sato and T. Sakai, *Phys. Rev. B*, **75**, 014411 (2007).
[4] K. Okamoto et al., *Physica E*, **43**, 769 (2011).
[5] K. Kawano and M. Takahashi, *J. Phys. Soc. Jpn.*, **66**, 4001 (1997).
[6] S. Nishimoto and M. Arikawa, *Phys. Rev. B*, **78**, 054421 (2008).