Exotic Quantum Phase Transitions in Spin Nanotubes

Tōru Sakai\textsuperscript{A,B}, Masahiro Sato\textsuperscript{C}, Kouichi Okunishi\textsuperscript{D}, Kiyomi Okamoto\textsuperscript{E} and Chigak Itoi\textsuperscript{F}

\textsuperscript{A}Japan Atomic Energy Agency, SPring-8, Sayo, Hyogo 679-5148, Japan
\textsuperscript{B}Graduate School of Material Science, University of Hyogo, Kamigori, Hyogo 678-1297, Japan
\textsuperscript{C}Department of Physics and Mathematics, Aoyama Gakuin University, Kanagawa 229-8558, Japan
\textsuperscript{D}Department of Physics, Niigata University, Niigata 950-2181, Japan
\textsuperscript{E}Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan
\textsuperscript{F}Department of Physics, Nihon University, Tokyo 101-8308, Japan
E-mail: sakai@spring8.or.jp

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 and the finite-size scaling analysis. In our previous works the quantum phase transition between the spin-gap and gapless phases was revealed to occur due to the asymmetric lattice distortion. In addition the transition between the magnetization plateau and gapless phases at 1/3 of the saturation magnetization induced by the same distortion. Recently we found that the Tomonaga-Luttinger liquid is realized in the 1/3 magnetization plateau phase for the symmetric three-leg spin tube.

The quantum spin nanotube [1] is one of interesting objects in the low-temperature physics. 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 [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 [(\text{CuCl$_2$tachH})$_3$Cl|Cl$_2$ ]\textsuperscript{3}, several theoretical works on the $S=1/2$ three-leg spin tube have been published [4–10], as well as another experimental work for CsCrF$_4$ [11]. In our previous study [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 asymmetric lattice distortion was investigated. The phenomenological renormalization combined with the numerical diagonalization of finite-size clusters derived the phase diagram.

The numerical diagonalization study [12] also indicated that the system exhibits a plateau of the ground-state magnetization curve at 1/3 of the saturation magnetization for sufficiently large rung interaction. Our previous work [1, 13] suggested that a new plateau phase appears between the two different mechanisms of the plateau formation depending on the asymmetric lattice distortion.
In the present paper, we briefly review the above properties of the $S = 1/2$ three-leg spin tube and present some new results at 1/3 of the saturation magnetization for the regular triangle unit cell.

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

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

(1)

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 neighboring spin pairs along the legs, while $J_\tau$ and $J'_\tau$ are the rung interaction constants. All the exchange interactions are supposed to be antiferromagnetic (namely, positive). The ratio $\alpha = J'_\tau/J_\tau$ 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 $J_\tau$ 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 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 $J_\tau$ 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. The complete phase diagram including the I, II, III and IV phases was obtained by the phenomenological renormalization with the numerical diagonalization up to $L = 10$ in our previous work [9]. According to the standard phenomenological renormalization, the size-dependent fixed point $J_{1c,L}$ with fixed $\alpha$ is given by the equation

$$L_1 \Delta L_1(J_{1c,L}) = L_2 \Delta L_2(J_{1c,L}),$$

(2)

where $\Delta L$ is the calculated spin gap for $L$ and $L$ is the average of $L_1$ and $L_2$, namely $L = (L_1 + L_2)/2$. Since no solutions of (2) were found due to the logarithmic size correction, we took the minimum of the difference between both sides of (2) as the fixed point [9]. The obtained phase diagram is shown in Figure 2.

Next, we consider the 1/3 magnetization plateau of the system (1). Our previous phenomenological renormalization study derived the phase diagram at $m = 1/3$ shown in Figure 3, including three plateau and a plateauless phases [1, 14]. The plateau I and II phases correspond to the up-up-down and the dimer-monomer mechanisms, respectively. In the plateau III phase, the translational symmetry is broken and the Néel order along the two bottom legs appears, as shown in Figure 4. Even in the phase, the regular triangle ($\alpha = 1$) is a special case, where
Figure 2. The phase diagram in the $J_1$-$\alpha$ plane. The phase boundaries are obtained by the phenomenological renormalization with the numerical diagonalization up to $L = 10$.

Figure 3. Phase diagram at $m = 1/3$ obtained by the phenomenological renormalization with the numerical diagonalization up to $L = 8$ [1]. The plateau I and II phases correspond to the up-up-down and the dimer-monomer mechanisms, respectively. In the plateau III phase the Néel order exists at the two equivalent legs. Solid and dashed lines correspond to the Berezinskii-Kosterlitz-Thouless (BKT) and the 2nd-order quantum phase boundaries, respectively [1].

The translational symmetry is still kept. In order to clarify features on the line $\alpha = 1$, the phenomenological renormalization is applied for the excitation gaps with $k = 0$ and $k = \pi$, respectively, keeping the magnetization $m = 1/3$. The scaled gaps $L\Delta$ with $k = 0$ and $k = \pi$ are plotted versus $J_1$ in Figures 5(a) and (b), respectively, calculated for $L = 4$ and 8. Both figures indicate the critical point $J_{1c}$ about 0.45 and the two excitations are gapless (gapped) for $J_1 < J_{1c}$ ($J_1 > J_{1c}$). It suggests that the Tomonaga-Luttinger liquid is realized on the $\alpha = 1$ line, while the Néel order exists along the two legs for $\alpha \neq 1$ in the plateau III phase.

In summary, the phase diagrams of the $S = 1/2$ asymmetric three-leg spin tube at $m = 0$ and $m = 1/3$ obtained by our previous works were reviewed. Our present phenomenological renormalization study revealed that the Tomonaga-Luttinger liquid is realized in the symmetric regular triangle unit case in the plateau III phase in Figure 3.

This work was partly supported by Grants-in-Aid for Scientific Research and Priority Areas “Novel States of Matter Induced by Frustration” from the Ministry of Education, Culture,
Figure 4. Calculated $S_j^z$ at the apical (stars), left (pluses), and right (crosses) bottom sites of the triangular unit for $J_1=0.1$ by DMRG ($L=48$).

Figure 5. Scaled gaps with $k=0$ (a) and $k=\pi$ (b) are plotted versus $J_1$ for $L=4$ and 8.

Sports, Science and Technology of Japan. A part of the computations was performed using facilities of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo.

[1] See, for example, Sakai T, Sato M, Okunishi K, Okamoto K and Itoi C 2010 J. Phys.: Condens. Matter 22 403201
[2] Kawano K and Takahashi M 1997 J. Phys. Soc. Jpn. 66 4001
[3] Schnack J, Nojiri H, Kögerler P, Cooper G J T and Cronin L 2004 Phys. Rev. B 70 174420
[4] Sakai T, Matsumoto M, Okunishi K, Okamoto K and Sato M 2005 Physica E 29 633
[5] Fouet J-B, Läuchli A, Pilgram S, Noack R M and Mila F 2006 Phys. Rev. B 73 014409
[6] Okunishi K, Yoshikawa S, Sakai T and Miyashita S 2005 Prog. Theor. Phys. Suppl. 159 297
[7] Sato M and Sakai T 2007 Phys. Rev. B 75 014411
[8] Nishimoto S and Arikawa M 2008 Phys. Rev. B 78 054421
[9] Sakai T, Sato M, Okunishi K, Otsuka Y, Okamoto K and Itoi C 2008 Phys. Rev. B 78 184415
[10] Sakai T, Okunishi K, Okamoto K, Itoi C and Sato M 2010 J. Low. Temp. Phys. 159 55
[11] H. Manaka, Y. Hirai, Y. Hachigo, M. Mitsunaga, M. Ito and N. Terada 2009 J. Phys. Soc. Jpn. 78 093701
[12] D. C. Cabra, A. Honecker and P. Pujol 1998 Phys. Rev. B 58 6241
[13] K. Okamoto, M. Sato, K. Okunishi, T. Sakai and C. Itoi 2011 Physica E 43 769
[14] Okamoto K, Sato M, Okunishi K, Sakai T and Itoi C 2011 Physica E 43 769