TOPICAL REVIEW

Quantum spin nanotubes—frustration, competing orders and criticalities

Tôru Sakai1,2,3, Masahiro Sato4,8, Kiyomi Okamoto5, Kouichi Okunishi6 and Chigak Itoi7

1 Japan Atomic Energy Agency, Spring-8, 1-1-1 Kouto, Sayo, Hyogo 679-5148, Japan
2 Department of Material Science, University of Hyogo, Kamigori, Hyogo 678-1297, Japan
3 JST TRIP, Japan
4 Condensed Matter Theory Laboratory, RIKEN, Wako, Saitama 351-0198, Japan
5 Department of Physics, Tokyo Institute of Technology, 2-12-1 O-okayama, Meguro-ku, Tokyo 152-8551, Japan
6 Department of Physics, Niigata University, Niigata 950-2181, Japan
7 Department of Physics, Nihon University, Kanda-Surugadai, Chiyoda-ku, Tokyo 101-8308, Japan
8 Department of Physics and Mathematics, Aoyama Gakuin University, 5-10-1 Fuchinobe, Chuo-ku, Sagamihara-shi, Kanagawa 251-5258, Japan

Received 17 June 2010, in final form 20 August 2010
Published 14 September 2010
Online at stacks.iop.org/JPhysCM/22/403201

Abstract
Recent developments of theoretical studies on spin nanotubes are reviewed, especially focusing on the S = 1/2 three-leg spin tube. In contrast to the three-leg spin ladder, the tube has a spin gap in the case of the regular-triangle unit cell when the rung interaction is sufficiently large. The effective theory based on the Hubbard Hamiltonian indicates a quantum phase transition to a gapless spin liquid due to the lattice distortion to an isosceles triangle. This is also supported by the numerical diagonalization and the density matrix renormalization group analyses. Furthermore, combining analytical and numerical approaches, we reveal several novel magnetic-field-induced phenomena: Néel, dimer, chiral and/or inhomogeneous orders, a new mechanism for the magnetization plateau formation, and others. The recently synthesized spin tube materials are also briefly introduced.

(Some figures in this article are in colour only in the electronic version)

Contents
1. Introduction 1
2. Isosceles spin tube 2
3. Effective theory 3
3.1. Global phase diagram derived from the Hubbard model on the tube lattice 4
3.2. Gapless phase for Jr ≪ J′r ≪ J1 4
3.3. Perturbation theory from the strong rung-coupling limit 4
4. Spin gap and ground-state phase diagram—numerical study 5
5. Field-induced phenomena 5

1. Introduction
Geometrically frustrated low-dimensional quantum spin systems have attracted increasing attention in recent years. Among them the spin nanotube is one of the most interesting, because it is expected to lead to a new generation of...
multifunctional devices. Recently, some candidates for spin nanotubes have been synthesized; three-leg tubes [(CuCl2tachH3)2Cl]Cl2 [1, 2] and CsCrF4 [3], a nine-leg tube Na2V3O7 [4], and a four-leg tube Cu3Cl12D3Cl2SO4 [5] and [6]). Several theoretical works have indicated various exotic quantum phenomena of spin tubes [7–21]. Most have concentrated on the $S = 1/2$ three-leg spin tube, because both the frustration and quantum fluctuation are the largest. In this paper, we review the recent theoretical results on the system.

In the $S = 1/2$ three-leg antiferromagnetic spin tube the unit cell consists of three spins. According to the Lieb–Schultz–Mattis theorem [22], the spin gap must be accompanied by at least doubly degenerate ground states. In fact, previous numerical analyses [11, 16, 17] have confirmed such doubly degenerate $S = 0$ ground states due to the spontaneous breaking of the translational symmetry along the leg direction. The ground states have a valence-bond type (dimerized) order [11, 17]. Some numerical works [7, 16, 17] indicated that the spin gap is quite fragile against lattice distortion, changing the unit cell from a regular triangle to an isosceles one. As a result, when one of the three rung-couplings is changed, a quantum phase transition occurs from the spin gap to the gapless phase. Developing an effective theory based on the Hubbard Hamiltonian, using numerical exact diagonalization and the density matrix renormalization group (DMRG) approach, the ground-state phase diagram of the quantum phase transition was presented [7], as reviewed in sections 3 and 4.

This system was also theoretically revealed to exhibit some exotic phenomena in magnetic fields. The numerical diagonalization study [12] suggested that a magnetization plateau appears at $1/3$ of the saturation for sufficiently large rung interactions. Introducing the above lattice distortion, two different plateau-formation mechanisms; the up–up–down (udd) and the dimer–monomer types, are expected to appear, depending on the type of isosceles triangle. Our recent work [23] has indicated a new plateau phase, with a dimer and/or chiral order accompanying the staggered moment. On the other hand, the bosonization for the weak rung-coupling regime [18] has shown that a vector chiral phase is commonly present in the field-induced Tomonaga–Luttinger liquid (TLL) phase. In addition, a spin-wave type approach [19] has predicted that not only the chiral order but also an inhomogeneous magnetization order appears near saturation. These field-induced phenomena will be discussed in detail in section 5.

Valence-bond solid (VBS) ground states were revealed as appearing in various spin tube systems. For example, a quantum Monte Carlo simulation study [24] suggested that several different types of VBS ground state occur in some chiral spin nanotubes without frustration. The recent nonlinear $\sigma$ model and the DMRG approach [25] indicated some three-leg higher spin tubes exhibit several Haldane phases.

One of the most realistic candidates of the $S = 1/2$ three-leg spin tube is [(CuCl2tachH3)2Cl]Cl2 [2]. In this material, each triangle unit cell is oriented upside-down to the adjacent one, differently from the straight spin tube (see section 6). The DMRG calculation of such a twisted spin tube [8, 14, 15] suggested that the material has no spin gap, which is consistent with the magnetization measurement [2].

As a future prospect, we consider the superconductivity in carrier-doped spin nanotubes in section 7. A possible chirality-induced superconductivity will be proposed as a new mechanism.

2. Isosceles spin tube

We consider the $S = 1/2$ isosceles three-leg spin tube [7] shown in figure 1, described by the Hamiltonian

$$\hat{H} = J_1 \sum_{i=1}^{L} S_{i,j} \cdot S_{i,j+1} + J_2 \sum_{i=1}^{L} S_{i,j} \cdot S_{i+1,j} + J' \sum_{j=1}^{L} S_{3,j} \cdot S_{1,j},$$

(1)

where $S_{i,j}$ is the spin-1/2 operator and $L$ is the length of the tube along the leg direction. The exchange interaction constant $J_1$ stands for the neighboring spin pairs along the legs, while $J_2$ and $J'$ are the rung interaction constants. All the exchange interactions are supposed to be antiferromagnetic (namely, positive). The ratio $\alpha = J'/J_1$ expresses the degree of asymmetry of the rung interactions. Throughout this paper, we fix $J_1$ to unity. The effect of the magnetic field $H$ along the $z$ direction is taken into account by adding the Zeeman term $H_Z = -H \sum_{i,j} S_{i,j}^z$ to (1).

3. Effective theory

In this section, we explain low-energy effective theories for the spin tube (1). In section 3.1, we sketch a method to draw a phase diagram in the whole coupling constant space $(\alpha, J_1)$ used in [7]. Next, we investigate two special regimes $J_r \ll J' \ll J_1$ and $J_r \gg J_1$, respectively, in sections 3.2 and 3.3.

3.1. Global phase diagram derived from the Hubbard model on the tube lattice

Here, we explain a systematic method to draw global phase diagrams of one-dimensional antiferromagnetic quantum spin systems. It is well known that the $S = 1/2$ Heisenberg model on an arbitrary lattice is obtained from the corresponding half-filled Hubbard model in the limit of strong on-site Coulomb interactions. Especially in one dimension, the spin configurations of the low-energy states in the Heisenberg model agree with those in the half-filled Hubbard model, even with a weak-Coulomb interaction [26–28]. The phases in the
weak-Coulomb regime often smoothly connect to those in the strong-Coulomb regime in one-dimensional electron systems. By these arguments, we obtain a low-energy effective theory for the spin tube (1) from the corresponding Hubbard model. To discuss the wider parameter space, first we diagonalize the kinetic parts of the Hubbard Hamiltonian, including both the leg and rung hopping terms [29–31]. Then, we take account of the on-site Coulomb interaction as the perturbation, with the help of non-Abelian bosonization [32–34] and conformal field theory (CFT).

The Hamiltonian of the Hubbard model on the three-leg tube lattice

\[ H = H_{\text{hop}} + H_{\text{int}} \]

(2)

consists of the hopping part

\[ H_{\text{hop}} = \sum_{n=1}^{L} \sum_{i=1}^{3} \sum_{\sigma = \uparrow, \downarrow} \{ t c_{n+1,i,\sigma}^+ c_{n,i,\sigma} + s_{i+1,j} c_{n+1,i,\sigma} c_{n,i,\sigma} + h.c. \} \]

and the on-site interaction part

\[ H_{\text{int}} = U \sum_{n=1}^{L} \sum_{i=1}^{3} n_{n,i,\uparrow} n_{n,i,\downarrow} \]

(3)

where \( n_{n,i,\sigma} = c_{n,i,\sigma}^+ c_{n,i,\sigma} \) and \( U > 0 \) is the repulsive coupling constant. The electron operators \( c_{n,i,\sigma} \) and \( c_{n,i,\sigma}^\dagger \) satisfy the periodic boundary conditions for both the leg and the rung directions, \( c_{n+1,i,\sigma} = c_{n,i,\sigma} \), \( c_{n+3,i,\sigma} = c_{n,i,\sigma} \), and anticommutation relations. The hopping parameters are given by \( t > 0 \), \( s_{1,2} = s_{2,3} = s > 0 \) and \( s_{3,1} = \beta s > 0 \). The strong-Coulomb regime in one-dimensional electron systems.

By a suitable unitary transformation, the hopping Hamiltonian can be written in the following diagonal form

\[ H_{\text{hop}} = \sum_{k} \sum_{\alpha = \uparrow, \downarrow} \sum_{\sigma = \uparrow, \downarrow} E_{i}(k) d_{k,i,\sigma}^\dagger d_{k,i,\sigma} \]

(4)

where the wavenumber \( k \) is summed over \( \frac{2\pi}{L} \leq k \leq 2\pi \). With an orthogonal matrix \( O_{ij} \), the operators \( d_{k,i,\sigma} \) and \( d_{k,i,\sigma}^\dagger \) are defined by

\[ d_{k,i,\sigma} = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} \sum_{j=1}^{3} \exp(\text{i}kn) O_{ij} c_{n,i,\sigma} \]

(5)

\[ d_{k,i,\sigma}^\dagger = \frac{1}{\sqrt{L}} \sum_{n=1}^{L} \sum_{j=1}^{3} \exp(\text{i}kn) O_{ij} c_{n,i,\sigma}^\dagger \]

(6)

which satisfy the standard anticommutation relations. The energy eigenvalues of the one-electron states are

\[ E_{1}(k) = -\beta s + 2t \cos k, \]

(7)

\[ E_{2}(k) = \frac{1}{2} (\beta s - s \sqrt{\beta^2 + 8 + 4t \cos k}), \]

(8)

\[ E_{3}(k) = \frac{1}{2} (\beta s + s \sqrt{\beta^2 + 8 + 4t \cos k}). \]

(9)

Note that a degeneracy \( E_{1}(k) = E_{2}(k) \) appears at \( \beta = 1 \) due to the permutation symmetry \( (S_{2,j} \leftrightarrow S_{1,j}) \) for \( i = 1, 2, 3 \).

For the half-filled case, \( 3L \) one-electron states should be occupied by electrons with up and down spins. As a result, the ground state of the hopping Hamiltonian has one, two or three pairs of the Fermi points \((k_1, k_2)\) just on the Fermi sea, depending on the parameters \( s/t \) and \( \beta \). Since the low-energy excitations are given by the particle–hole creations around these Fermi points, they can be represented by using the Dirac fermions, the left mover \( \psi_{t,\sigma}(x) \) and the right mover \( \bar{\psi}_{t,\sigma}(x) \), which are defined from the electrons around the \( j \)th pair of Fermi points.

\[ c_{n,i,\sigma} = \sqrt{a} \sum_{j=1}^{3} O_{ij}^{-1} \{ \exp(\text{i}k_j x/a) \psi_{t,\sigma}(x) + \exp(\text{i}k_j x/a) \bar{\psi}_{t,\sigma}(x) \} \]

(10)

where \( a \) is the lattice spacing with dimension of length and \( x = an \) is the continuous position coordinate. We add the on-site Coulomb interaction (3) to this free Dirac fermion system, and use the non-Abelian bosonization techniques. Following the field-theory argument in [28], we expect that if the number of Fermi-point pairs is odd (even), the spin excitations are gapless (gapped) in the half-filled Hubbard tube. In particular, in the cases of one or two Fermi-point pairs, we can explicitly determine whether or not a spin gap exists as follows.

First, we consider the case of one pair of Fermi points \( k_{1} = \frac{2\pi}{L} - \frac{k_{1}}{2} \) and \( k_{1} = \frac{2\pi}{L} + \frac{k_{1}}{2} \). In this case, the interaction (3) is approximated as the sum of an Umklapp interaction and two marginal ones

\[ H_{\text{int}} \sim \int dx \left( g_{1} O_{1}(x) - g_{2} O_{2}(x) - g_{3} O_{3}(x) + \cdots \right) \]

(11)

where \( g_{1,2,3} \) are positive coupling constants proportional to \( U \). The Umklapp term is expressed as

\[ O_{1}(x) = \psi_{t,\uparrow}(x)^{\dagger} \psi_{t,\downarrow}(x) \]

(12)

and the marginal interaction between the \( U(1) \) charge currents is given by

\[ O_{2}(x) = \psi_{t,\uparrow}(x)^{\dagger} \psi_{t,\downarrow}(x)^{\dagger} \psi_{t,\downarrow}(x) \]

(13)

where \( \psi_{t} = (\psi_{t,\uparrow}, \psi_{t,\downarrow}) \). It is known that the bosonized form of \( O_{1,2,3} \) contains only the charge degrees of freedom and they open a charge gap when \( g_{2} \) is positive. Then, the remaining spin degrees of freedom are described by the gapless level-1 SU(2) Wess–Zumino–Witten (WZW) theory [32–34]. This phenomenon, i.e., the charge–spin separation, is well known in the single Hubbard chain model. For this WZW theory, the third interaction

\[ O_{3}(x) = \psi_{t,\uparrow}(x)^{\dagger} \psi_{t,\downarrow}(x)^{\dagger} \psi_{t,\downarrow}(x) \]

(14)

is known to be marginally irrelevant if \( g_{3} > 0 \). Except the above interactions, \( O_{1,2,3}(x) \), there is no relevant operator with invariance under a one-site translation along the leg,

\[ \psi_{t,\sigma}(x) \rightarrow e^{\text{i}k_{1} x/a} \psi_{t,\sigma}(x), \quad \psi_{t,\sigma}(x) \rightarrow e^{\text{i}k_{1} x/a} \psi_{t,\sigma}(x) \]

(15)
as in the case of the Heisenberg chain. The spin excitations remain gapless.

On the other hand, when there exist two pairs of the Fermi points, \((k_1, \tilde{k}_1)\) and \((k_2, \tilde{k}_2)\), the spin excitations suffer from relevant interactions. In this case, the spin sector in the hopping part of the Hubbard tube is described by a level-2 SU(2) WZW model derived from two decoupled Dirac fermions. The Coulomb interaction yields several perturbations for this theory. For example, the following term

\[
\psi_{1,\uparrow}(x) \psi_{2,\uparrow}(x) \psi_{1,\downarrow}(x) \psi_{2,\downarrow}(x)
\]

contains a relevant perturbation in the level-2 WZW model which is invariant under the translation

\[
\psi_{j,\sigma}(x) \rightarrow e^{i\delta} \psi_{j,\sigma}(x), \quad \bar{\psi}_{j,\sigma}(x) \rightarrow e^{i\delta} \bar{\psi}_{j,\sigma}(x).
\]

Particularly for \(\beta = 1\), much more relevant operators are allowed by the translational invariance because of the coincident Fermi points \(k_1 = k_2\) and \(\tilde{k}_1 = \tilde{k}_2\). Therefore, we conclude that any gapless spin excitation generally has no chance to survive except in particularly rare cases (e.g., when the coupling constant of (16) is zero). For the case of three Fermi-point pairs, the interactions among three Dirac fermions are generated from (3), and thus it is difficult to analyze them and judge whether or not the spin excitation can survive as gapless. The gapless spin excitation is expected from [28, 35].

From these arguments, we can draw the ground-state phase diagram of the half-filled Hubbard tube shown in figure 2. The phase (I) has three pairs of Fermi points, the phases (II) and (IV) have one pair, and the central phase (III) has two pairs. Therefore, we predict that phases (II) and (IV) have gapless spin excitations, whereas phase (III) possesses a spin gap. By \((t/s)^2 = J'/J_1\) and \(\beta^2 = \alpha^2\) obtained from the strong on-site interaction, figure 2 depicts the phase diagram of the \(S = 1/2\) three-leg spin tube (1). Since we have treated the on-site interaction perturbatively in the effective theory, we should not trust the obtained phase boundaries as accurate ones. Note that the gapful phase (III) is predicted to be extended around the line \(\beta = 1\) for a finite \(s/t\). In the limit \(s/t \rightarrow \infty\), both the left- and right-side phase boundaries of region (III) converge to \(\beta = 1\). This narrowing of phase (III) is consistent with the numerical results [16, 17] in the strong rung-coupling limit \(J_r/J_1 \rightarrow \infty\).

Finally, we argue the universality classes of the phase transitions at two phase boundaries, (II)–(III) and (III)–(IV). For the level-1 SU(2) WZW model in the phases (II) and (IV), the most relevant perturbation is the marginal current–current interaction [32–34], (14), which is the only allowed invariant interaction. Since it can be marginally ‘relevant’ when parameters are finely tuned and then \(g_3\) becomes negative, we speculate that the transition from the phases (II) or (IV) to (III) is caused by this marginal term. Therefore, the transitions are expected to be in the Berezinskii–Kosterlitz–Thouless (BKT) universality class [36, 37].

9 We have neglected the difference between the Fermi velocities of the first and second bands.
The lowest-energy states are \( \psi(0) \).

These wavefunctions do not depend on \( \sigma \) because all of them are completely classified by the eigenvalues \( S_{\text{tot}}, S_{\text{tot}}^\perp \) and \( P \).

The first order perturbation theory with respect to \( J_1 \) retaining the above four states with \( S_{\text{tot}} = 1/2 \) and neglecting the other four states with \( S_{\text{tot}} = 3/2 \) leads to

\[
\mathcal{H}_{\text{eff}} = J_1 \sum_j T_j \cdot T_{j+1} (1 + 8 [\sigma_j^+ \sigma_{j+1}^- + \sigma_j^- \sigma_{j+1}^+])
- (1 - \alpha) \sum_j \sigma_j^z
\]

where \( T_j \) is a spin-1/2 operator acting on \( S_{\text{tot}} \) and \( \sigma \) is also a spin-1/2 operator acting as

\[
\sigma^z \psi_0^{(1)}(S_{\text{tot}}) = \pm \frac{1}{2} \psi_0^{(3)}(S_{\text{tot}}^\perp)
\sigma^+ \psi_0^{(1)}(S_{\text{tot}}) = 0, \quad \sigma^+ \psi_0^{(-)}(S_{\text{tot}}) = \psi_0^{(2)}(S_{\text{tot}}) \quad \sigma^- \psi_0^{(1)}(S_{\text{tot}}) = \psi_0^{(-)}(S_{\text{tot}}), \quad \sigma^- \psi_0^{(-)}(S_{\text{tot}}) = 0
\]

where \( S_{\text{tot}} = 1/2 \) indices were omitted for simplicity. The energy difference between \( \psi_0^{(1)}(S_{\text{tot}}) \) and \( \psi_0^{(-)}(S_{\text{tot}}) \) acts as a ‘magnetic field’ applied on \( \sigma \) spins. This \( \mathcal{H}_{\text{eff}} \) is essentially the same as that obtained by Nishimoto and Arikawa [17].

In the case of sufficiently strong symmetry \( |\alpha - 1| \gg 1 \), the \( \sigma \) spins are completely polarized and only \( T \) spins survive, where \( \mathcal{H}_{\text{eff}} \) is reduced to that of the antiferromagnetic Heisenberg chain having the gapless excitation. Thus phase (III) has a finite width along the line \( J_1/J_1 = \text{const} \gg 1 \). Next, let us focus on the region around the symmetric line \( \alpha \sim 1 \). In the limit \( J_1/J_1 \rightarrow 0 \), the ground state has saturated \( \sigma \) spins at any asymmetric point \( \alpha \neq 1 \). For a finite \( J_1/J_1 \), however, we expect an extended gapful phase around \( \alpha = 1 \) if the energy gap exists at \( \alpha = 1 \) due to the coupling between \( T \) and \( \sigma \) spins. The finite energy gap does not vanish with an infinitesimal external field \( \alpha - 1 \). In other words, the magnetization process of the \( \sigma \) spins should show a zero-magnetization plateau. Therefore, an energy gap would also be present for sufficiently weak asymmetry \( |\alpha - 1| \ll 1 \).

For the rest of this subsection we suppose \( \alpha = 1 \) (i.e. regular-triangle case), where the translational invariance by one site along the rung direction holds and the lowest-energy states are four-fold degenerate. In this case another set of useful expressions for the lowest-energy states is

\[
\begin{align*}
|\uparrow L\rangle &= \frac{1}{\sqrt{3}}(|\uparrow \uparrow \downarrow \rangle + \omega |\uparrow \downarrow \downarrow \rangle + \omega^{-1} |\downarrow \downarrow \downarrow \rangle) \quad (21a) \\
|\uparrow R\rangle &= \frac{1}{\sqrt{3}}(|\uparrow \downarrow \uparrow \rangle + \omega^{-1} |\downarrow \uparrow \uparrow \rangle + \omega |\downarrow \downarrow \uparrow \rangle) \quad (21b) \\
|\downarrow L\rangle &= \frac{1}{\sqrt{3}}(|\downarrow \downarrow \uparrow \rangle + \omega |\downarrow \uparrow \uparrow \rangle + \omega^{-1} |\uparrow \downarrow \uparrow \rangle) \quad (21c) \\
|\downarrow R\rangle &= \frac{1}{\sqrt{3}}(|\downarrow \uparrow \downarrow \rangle + \omega^{-1} |\uparrow \downarrow \downarrow \rangle + \omega |\downarrow \uparrow \downarrow \rangle) \quad (21d)
\end{align*}
\]

where \( \omega = \exp(2\pi i/3) \) and indices \( L \) and \( R \) denote the wavenumber \( k = 2\pi/3 \) and \( k = -2\pi/3 \) along the rung direction, respectively. The first order perturbation theory with respect to \( J_1 \), retaining the above four states with \( S_{\text{tot}} = 1/2 \), and neglecting the other four states with \( S_{\text{tot}} = 3/2 \) leads to \[10, 11\]

\[
\mathcal{H}_{\text{eff}} = J_1 \sum_{j} T_j \cdot T_{j+1} [1 + 4 (\tau_j^+ \tau_{j+1}^- + \tau_j^- \tau_{j+1}^+)]
\]

where \( T \) is a spin-1/2 operator acting on the first indices of the above states and \( \tau^\pm \) are the spin-1/2 matrices acting on the second indices as

\[
\tau^+ |L\rangle = 0, \quad \tau^+ |R\rangle = |L\rangle, \quad \tau^- |L\rangle = |L\rangle, \quad \tau^- |R\rangle = 0.
\]

Of course this \( \mathcal{H}_{\text{eff}} \) can be obtained from (19) through the unitary transformation and letting \( \alpha = 1 \).

Schulz [10] analyzed \( \mathcal{H}_{\text{eff}} \) using the Jordan–Wigner transformation and concluded that the system is gapped. Kawano and Takahashi [11] performed the DMRG calculation for \( \mathcal{H}_{\text{eff}} \) to find that Hamiltonian \( \mathcal{H}_{\text{eff}} \) has a spin gap of 0.277\( J_1 \). When the next-nearest-coupling term having a
Phases (I), (II), (III) and (IV) in the thermodynamic limit vanish just at $\alpha$. Here, we should recall that the logarithmic correction normally corresponds to the phase boundary (II)–(III) and that between (III)–(IV), respectively. At least these boundaries for the strong coupling regime $J_1 \ll J_2$ are precise enough to justify that a finite gapful phase (III) exists. However, it is difficult to obtain $\alpha_c$ for $J_1 > 2$, because the DMRG calculation does not converge well there. In order to determine the phase boundaries for the weak rung-coupling regime $J_1 > 2$, we use the minimum points of $L_1 \Delta L_1 - L_2 \Delta L_2$, calculated by the numerical diagonalization up to $L = 10$ under the periodic boundary condition. Using the estimated phase boundaries for $(L_1, L_2) = (6, 8)$ and $(8, 10)$, and assuming the size correction is proportional to $1/L^2$ in both directions of $J_1$ and $\alpha$, the phase boundaries among the phases (I), (II), (III) and (IV) in the thermodynamic limit were estimated. The phase boundaries are also shown as solid curves in figure 3. At least the phase boundaries (II)–(III) and (III)–(IV) are consistent with the DMRG results for $J_1 \ll 1$. The boundary (III)–(IV), however, significantly deviates from the DMRG estimation for $J_1 \sim 1$. This discrepancy is supposed to be due to the error of extrapolation. This analysis also justifies the existence of the phase (I). However, the error of extrapolation becomes larger as we approach the line $1/J_1 = 0$ in the case of $\alpha < 1$. Thus it is difficult to conclude that the phase (I) really exists for $\alpha < 1$, within the present numerical demonstration. It is also difficult to confirm the boundary (I)–(II), and the phase (I) might combine with the phase (II) in a certain regime with $\alpha < 1$.

The phase boundaries between the phases (I) and (III), as well as (II) and (III) and (II) and (IV), for smaller $J_1$ ($0 < J_1 < 0.5$), were reproduced well by the level-spectroscopy method [39, 42–44], which is one of precise techniques to estimate the critical point for the BKT transition. But the level-spectroscopy method does not work well for larger $J_1$, because of too large finite-size corrections.

In our previous work [7], applying the conformal field-theory analysis [45–50], the central charge and the critical exponents of the spin correlation functions were estimated. The results suggested that all the phase boundaries in figure 3 belong to the BKT universality class.

### 5. Field-induced phenomena

In this section, we consider the effects of an applied magnetic field in three-leg spin tubes. Particularly, we focus on field-induced phases (vector chiral order and magnetization plateau) and quantum phase transitions.
5.1. Vector chiral phase in the weak rung-coupling regime

Here, we consider the weak rung-coupling regime in a magnetic field [18], namely, the Hamiltonian,

$$\mathcal{H}_H = \mathcal{H} + \mathcal{H}_Z$$  \hspace{1cm} (24)

with $J_1 \gg |J_i|, |J'_i|$. If a sufficiently strong magnetic field is applied and a finite magnetization occurs, the spin-rotational SU(2) symmetry is reduced to the U(1) type, in which the Abelian bosonization [33, 34, 51] becomes reliable at least for the weak rung-coupling regime. At the zero rung-coupling limit, the low-energy properties of the $i$th spin chain in the tube can be described by a free boson theory whose Hamiltonian is given by

$$\mathcal{H}'_{\text{eff}} = \int dx \frac{v}{2} [K^{-1}(\partial_x \phi)^2 + K (\partial_x \theta)^2].$$  \hspace{1cm} (25)

Here, $\phi(x)$ and $\theta(x)$ are a pair of dual scalar fields ($x = j/a_0$), and $K$ and $v$ respectively denote the TCL parameter and the exciton velocity. The spin operator is also bosonized as

$$S_{i,j}^z \approx \frac{a_0}{\sqrt{\pi}} \partial_x \phi(x) + (-1)^j A_0 \cos(\sqrt{4 \pi \phi} + 2 \pi M j) + \cdots$$

$$S_{i,j}^z \approx \exp(i \sqrt{\theta} \pi)((-1)^j B_0 + B_1 \cos(\sqrt{4 \pi \phi} + 2 \pi M j) + \cdots),$$  \hspace{1cm} (26)

with $A_0$ and $B_0$ being nonuniversal constants. Here, $M = \langle S_{i,j}^z \rangle$ is the magnetization per site. In the present notation, $K$ runs from $1/2$ to 1 when the magnetization $M$ is increased from 0 to the saturated value $1/2$. Using the formula (26), we can obtain the bosonized form of the perturbative rung-coupling, and the resultant effective Hamiltonian for the spin tube is expressed as

$$\mathcal{H}'_{\text{eff}} = \int dx \sum_{q=0}^{\infty} \frac{v}{2} [K^{-1}(\partial_x \phi)^2 + K (\partial_x \theta)^2]$$

$$+ 2 \sqrt{\frac{3}{\pi}} M J_1 \partial_x \Phi_0 + \frac{M}{\sqrt{3 \pi}} (J_1 - J'_1) (2 \partial_x \Phi_0 + \sqrt{2} \partial_x \Phi_2)$$

$$+ \frac{a_0}{\sqrt{\pi}} (2 J_1 - J'_1) (\partial_x \Phi_0)^2 - \frac{a_0}{\sqrt{\pi}} (2 J_1 - J'_1) (\partial_x \Phi_2)^2$$

$$+ \frac{a_0}{\sqrt{\pi}} (2 J_1 - J'_1) (\partial_x \Phi_2 a_0^{-1} \cos(\sqrt{2 \pi \Theta_1}))$$

$$\times \exp(\sqrt{2 \pi \Phi_1}) + \cdots.$$  \hspace{1cm} (27)

Here we have neglected all the terms with oscillating factors $\exp(i \gamma M \pi j)$ or $(-1)^j$, and have introduced new pairs of boson fields: $(\Phi_0, \Theta_0) = (\sum_{i=1}^{3} \Psi_i, \sum_{i=1}^{3} \Theta_i)/\sqrt{3}$, $(\Phi_1, \Theta_1) = (\phi_1 - \phi_2 - \phi_3)/\sqrt{2}$, and $(\Phi_2, \Theta_2) = (\phi_1 + \phi_2 - \phi_3)/\sqrt{2}$. The first line in (27) is equivalent to three copies of TLs in decoupled chains. The second line is linear terms which induce just a small correction to the magnetization $M$. In the isosceles case $J_i \neq J'_i$, $(S_{i,j}^z) = (S_{i,j}^z) \neq (S_{i,j}^z)$ would be realized. The third and fourth lines are quadratic terms changing the values of $K$ and $v$. In the regular-triangle case, the quadratic part is diagonalized in the basis of $(\Phi_0, \Theta_0)$, and resultant TLL parameters and velocities for $(\Phi_1, \Theta_1)$ sector, $V_0, v_1, v_2, v_3$, are calculated as

$$K_0 = K(1 + \frac{2 K_0}{a_0})^{-1/2},$$

$$K_1 = K(1 - \frac{K_0}{a_0})^{-1/2},$$

$$v_0 = v(1 + \frac{2 K_0}{a_0})^{1/2}$$

and $v_1 = v_2 = v(1 - \frac{K_0}{a_0})^{1/2} = v_3$. The fifth and sixth lines correspond to the vertex type perturbations, and the function $V(\epsilon_1, \epsilon_2)$ is defined by

$$V(\epsilon_1, \epsilon_2) = 2 \cos(\sqrt{2 \pi \epsilon_1}) \cos(\sqrt{3 \pi \epsilon_2}) + \cos(\sqrt{2 \pi \epsilon_1}).$$  \hspace{1cm} (28)

In our notation, the scaling dimensions of the vertex operators are given as $[\exp(in \sqrt{2 \pi \epsilon_1})] = n^2 K$ and $[\exp(in \sqrt{2 \pi \epsilon_1})] = n^3/(4K)$ in the decoupled case. We should emphasize that (27) does not include any relevant terms with $\Phi_0$ and $\Theta_0$ except for commensurate cases with $M = q/p$ ($q$ and $p$: integer). This property is protected by $U(1)$ spin-rotational and translational symmetries of the spin tube. Therefore, the $(\Phi_0, \Theta_0)$ sector is described by a TLL. On the other hand, the remaining sectors are subject to the vertex terms.

We first focus on the regular-triangle case $J_i = J'_i$, analyzing the above effective Hamiltonian (27). In this case, two vertex perturbations $\cos(\sqrt{2 \pi \Phi_1})$ and $\cos(\sqrt{2 \pi \Phi_1})$ in (27) vanish, and the scaling dimensions of $V(\Theta_1, \Theta_2)$ and $V(2\Phi_1, 2\Phi_2)$ are readily evaluated: $[V(\Theta_1, \Theta_2)] = 1/(2K)$ and $[V(2\Phi_1, 2\Phi_2)] = 2K$. In the weak rung-coupling regime, $K_0$ is very close to $K$ and $K > 1/2$ holds in the magnetization process. Therefore, $V(\Theta_1, \Theta_2)$ is more relevant, and $(\Phi_1, \Theta_1)$ sectors have gapped spectra. The form of the potential $V(\Theta_1, \Theta_2)$ is shown in figure 4(a), in which the diamond region is meaningful in the full $\Theta_1 - \Theta_2$ plane and here it is called the physically relevant zone. Remarkably there are two minimum points in the diamond zone: $(\Theta_1, \Theta_2) = (\pm \sqrt{2 \pi}/3, \pm \sqrt{4 \pi}) \equiv \pm X$. One minimum is mapped to the other via a sign change $\Theta_1 \rightarrow -\Theta_1$ that can be realized by the exchange of two chains $S_{i,j} \leftrightarrow S_{i+1,j}$ and $\theta_1 \leftrightarrow \theta_2$. This suggests a spontaneous breakdown of rung-parity symmetry. Vector chiralities in rung bond $\kappa_i^{z,j} = (S_{i,j}^z \times S_{i+1,j}^z)^z$ are natural candidates for the order parameter, and the bosonized forms of their $z$ components are given as

$$\kappa_i^{z,j} \approx -B_0^2 \sin(\sqrt{\pi/2} \Theta_1 + \sqrt{3 \pi/2} \Theta_2) + \cdots$$

$$\kappa_i^{z,j} \approx -B_0^2 \sin(\sqrt{\pi/2} \Theta_1 - \sqrt{3 \pi/2} \Theta_2) + \cdots$$

$$\kappa_i^{z,j} \approx B_0^2 \sin(\sqrt{2 \pi \Phi_1}) + \cdots.$$  \hspace{1cm} (29)

At the point $X_+ (X_-)$, $\kappa_i^{z,j}$ becomes positive (negative). From the translational symmetry along the rung, we can predict $(\kappa_i^{z,j}) = (\kappa_{i+1}^{z,j} = (\kappa_0^{z,j})$. We thus conclude that in the weak rung-coupling regime with $J_i = J'_i$ and a finite $M$, the low-energy physics is governed by the TLL in the $(\Phi_0, \Theta_0)$ sector and the remaining gapped sectors generate a vector chiral long-range order with spontaneous breaking of the rung-parity symmetry. In the commensurate case of $M = 1/3$, the magnetization plateau appears, at least in a strong rung-coupling regime (see section 5.2). It has been predicted in [12] that the plateau survives up to a fairly weak rung-coupling regime ($J_i \sim 0.1 J_1$) in the regular-triangle case $J_i = J'_i$. 


uniform magnetization mentioned, the boson linear terms just slightly change the kinds of rung-coupling terms in (27) are modified. As already several values of $\alpha$ magnetization process. To observe both gapless and gapped vector chiral phases in the has a gapped spectrum and the vector chirality is long-range ordered. In other words, the spin tube offers a unique chance to observe both gapless and gapped vector chiral phases in the magnetization process.

Next, we consider the effects of the rung deformation, $J_1 \neq J'_1$. Even in this isosceles case, the chirality between the first and third chains $(\kappa_3, j)$ is still useful as a order parameter because the tube is invariant under rung-parity operation between these two chains. Due to the rung deformation, all kinds of rung-coupling terms in (27) are modified. As already mentioned, the boson linear terms just slightly change the uniform magnetization $M$. The quadratic term $\partial_x \Phi_0 \partial_x \Phi_2$ cannot be diagonalized in the present basis, but its effects would be quite small and the qualitative nature of the vector chiral phase is expected not to be changed. The most important point of the rung deformation is the change of the vertex potential due to an additional term $\cos(\sqrt{2\pi} \Theta_1)$ in the fifth line of (27). The modified potential is expressed as follows:

$$V_a(\Theta_1, \Theta_2) = V(\Theta_1, \Theta_2) - \frac{J_0 - J'_0}{J'_0} \cos(\sqrt{2\pi} \Theta_1)$$

$$= 2 \cos(\sqrt{2\pi} \Theta_2) \cos(3\pi/\sqrt{2\Theta_2}) + \alpha \cos(\sqrt{2\pi} \Theta_1).$$

(30)

Figure 4(b) presents this potential as a function of $\Theta_1$, fixing $\Theta_2 = \sqrt{2\pi}/3$. It clearly shows that the potential form is changed from a double-well type to a single-well type for $\alpha < 1$, while the form is always a double-well type for $\alpha > 1$. This classical argument predicts the critical point $\alpha_c = 0.5$, and the chiral order is expected to disappear in $\alpha < \alpha_c$. To gain a deeper understanding of this expectation, we consider the effective theory for the $(\Phi_1, \Theta_1)$ sector. If we naively replace $\cos(\sqrt{2\pi}/2 \Theta_2)$ with its mean value $C_2 = \langle \cos(\sqrt{2\pi}/2 \Theta_2) \rangle$ in the potential $V_a(\Theta_1, \Theta_2)$, the effective Hamiltonian for the $(\Phi_1, \Theta_1)$ sector is obtained as

$$H_{\text{eff}}^{(\Phi_1, \Theta_1)} = \int dx \left[ \frac{V_1}{2} \left( \partial_x \Phi_1 \right)^2 + K_1 \left( \partial_x \Theta_1 \right)^2 \right]$$

$$+ B_0 J_0 \partial_x \Phi_0 \cos(\sqrt{2\pi} \partial_x \Theta_1) + \alpha \cos(\sqrt{2\pi} \Theta_1) \right] + \cdots.$$

(31)

This is nothing but a double-frequency sine-Gordon model. Under the condition $K_1 > 1/4$, this model is believed to exhibit an Ising type quantum phase transition by tuning the ratio of two coupling constants $\alpha/(2C_2)$ [52, 53]. We can hence predict the phase diagram of the isosceles spin tube with a weak rung-coupling and a finite magnetization $M \neq 1/3$, as shown in figure 5. The chiral ordering occurs in the region $0 < \alpha < 1$. The true critical value $\alpha_c$ must deviate from its classical one 0.5. The order parameter $(\kappa_3, j)$ behaves as $\sim(\alpha - \alpha_c)^{1/8}$ near the transition point. From this figure, one also finds that once a coupling between a two-leg ladder and a single chain is introduced, a vector chiral order immediately emerges.

Similar scenarios of a vector chiral order and an Ising transition are also expected in other tubes consisting of spin

---

**Figure 4.** (a) Contour lines of potential $V(\Theta_1, \Theta_2)$ in the regular-triangle case, and (b) potential $V_a(\Theta_1, \sqrt{2\pi}/3)$ in the isosceles case with several values of $\alpha$.

**Figure 5.** Ground-state phase diagram of the isosceles spin tube in a magnetic field in the weak rung-coupling regime $J_1 \gg |J_1|, |J'_1|$.
chains with a TLL parameter $K > 1/2$. For instance, even in the zero-field case, spin tubes with easy-plane XXZ anisotropy must yield a chiral order in the weak rung-coupling regime. It is known that the field-induced TLL phase satisfies $K > 1$ in a spin-1 antiferromagnetic Heisenberg chain [54] and the leading term of the bosonized spin operator $S^+_i$ has the same form as that of (26) [55, 56]. Therefore, three-leg spin-1 tubes have a vector chiral order at least in the high-field and weak rung-coupling regime. In the vicinity of the saturation field, three-leg spin-S tubes can be analyzed by a spin-wave type approach [19]. It also predicts the emergence of the vector chiral order in a certain weak rung-coupling regime. These results obviously suggest that a vector chiral order is generally induced by an applied magnetic field in three-leg spin-S antiferromagnetic tubes with a weak rung-coupling.

The spin-wave approach also indicates the possibility of an inhomogeneous magnetization phase with $(S_{1,j}^z) \neq (S_{2,j}^z)$ in the regular-triangle case.

5.2. 1/3 plateau

The magnetization plateau at $M = M_{1/3}$ surely exists for $J_1/J_t \to 0$, since the triangle unit cell is composed of three $S = 1/2$ spins, while it does not exist for $J_1/J_t \to \infty$ because the system is reduced to three independent $S = 1/2$ spin chains in this limit. Thus the $M_{1/3}$ plateau phase diagram on the $J_1 - \alpha$ plane is of immense interest.

As discussed in section 3.1, we study magnetization plateaux in the effective Hubbard model under external field. The Zeeman term for electrons is given by

$$
\mathcal{H}_Z = -H/2 \sum_{n=1}^{L} \sum_{i=1}^{3} (c_{n,i,\uparrow}^\dagger c_{n,i,\uparrow} - c_{n,i,\downarrow}^\dagger c_{n,i,\downarrow}),
$$

(32)

which should be added to the Hubbard Hamiltonian. An elaborated analysis of the effective theory for this Hubbard model gives the conditions for the existence of the spin excitation gap. Then, we show the existence of the 1/3 magnetization plateau and nonexistence of any other nonzero-magnetization plateaux. Details will be published elsewhere [57]. The phase diagram of the 1/3 magnetization plateau is depicted in figure 6. This agrees with the numerical calculation qualitatively, as shown later.

Let us discuss the 1/3 plateau problem by making use of the effective Hamiltonian (19) proposing $J_t \gg J_1$. In the 1/3 plateau case we can fix $T^x = +1/2$ and retain the degree of freedom with respect to $\sigma$, resulting in

$$
\mathcal{H}^{(1/3)}_{\text{eff}} = \frac{2J_t}{3} \sum_{j} (\sigma^+_j \sigma^+_j + \sigma^-_j \sigma^-_j) - (1 - \alpha) \sum_j \sigma^-_j.
$$

(33)

In other words, we take only two states $\psi^\pm(1/2, +1/2)$ in (18) into consideration. We note that $\mathcal{H}^{(1/3)}_{\text{eff}}$ describes $M = M_{1/3}$ states only, because both of $\psi^{(i)}(1/2, +1/2)$ have $S_{\text{tot}} = +1/2$ corresponding to $M = M_{1/3}$.

$\mathcal{H}^{(1/3)}_{\text{eff}}$ is nothing but the $S = 1/2XY$ chain in a transverse magnetic field, which is a special case of the $S = 1/2XXZ$ chain in a transverse magnetic field, of which ground state was investigated by Dmitriev et al [58–60], and Capraro and Gros [61]. Their results read as follows in our cases. Both of $(\sigma^+_j \sigma^-_j)$ and $(-1)^{\alpha-j} (\sigma^+_j \sigma^-_j)$ have long-range order for the weak ‘magnetic field’ case (i.e. $0 < |1 - \alpha| \ll J_1$), while only $(\sigma^+_j \sigma^-_j)$ has long-range order for the strong ‘magnetic field’ case (i.e. $|1 - \alpha| \gg J_1$). The boundary between the above two cases will be approximately given by $|1 - \alpha| \approx J_1$. In the latter case the state of the unit triangle is essentially either $\psi_0^{(+)}(1/2, +1/2)$ or $\psi_0^{(-)}(1/2, +1/2)$ according as $\alpha < 1$ or $\alpha > 1$. In the former case, on the other hand, there exists long-range Néel order of $\sigma$ spins along the $x$ direction associated with the spontaneous breaking of the translational symmetry (SBTS) and the two-fold degeneracy of the ground state. In this case the ground-state energy (the energy of the $M_{1/3}$ state in the original spin language) will be considerably lowered by the interaction effects, which leads to the remarkable increase of the width of $M_{1/3}$ plateau. Further the SBTS of the $\sigma$ system results in the SBTS and the spontaneous breaking of the inversion symmetry of $(S_i^z)$ in the original spin representation. If we suppose the complete Néel order of $\sigma$ along the $x$ direction $(\sigma^x_{j}) = +1/2$, $(\sigma^x_{j+1}) = -1/2$ for simplicity (this situation will be a good approximation of the ground state in the case of an extremely weak ‘magnetic field’ $0 < |1 - \alpha| \ll J_1$), the expectation values of $S^z$ are

$$
\langle \sigma^z_{1,j} \rangle = \langle S^z_{3,j+1} \rangle = 0.455
$$

$$
\langle \sigma^z_{2,j} \rangle = \langle S^z_{4,j+1} \rangle = 0.167
$$

(34)

$$
\langle \sigma^z_{2,j} \rangle = \langle S^z_{4,j+1} \rangle = -0.122
$$

which shows the spontaneous breaking of the translational symmetry $(j \Rightarrow j+1)$ and inversion symmetry $(S_{1,j} \Leftrightarrow S_{2,j})$.

Figure 7(a) shows the $\alpha$ dependence of the $M_{1/3}$ magnetization plateau width $\Delta$, from which we can see the anomalous increase of the $\Delta$ near $\alpha = 1$, at least for the
$J_1 = 0.1$ and $0.3$ cases, as predicted by the above theoretical consideration. In usual cases the plateau width (or the spin gap) remarkably decreases near the mechanism-changing point and often becomes zero at that point, as shown in figure 7(b). Thus, we find a new and exotic behavior of the plateau width, which is completely opposite to that of the usual cases [62]. In the $J_1 = 0.1$ case, for instance, the plateau is realized by the $\psi_0^{(+)}/\Delta_1 (1/2, +1/2)$ and $\psi_0^{(-)} (1/2, +1/2)$ mechanisms for $\alpha < 0.9$ and $1.1 < \alpha$, respectively, while by the cooperative effects of both mechanisms for $0.9 < \alpha < 1.1$. We note that the excitation gap (i.e., magnetization plateau width) $\Delta$ from the $M = M_s/3$ state to the $M = M_s/3 \pm 1$ states is always finite when $\alpha$ is varied. When $J_1 = 0.1$ and $\alpha = 0.95$, the expectation values $\langle S^i \rangle$ obtained by DMRG are

\[
\begin{align*}
\langle S^i_{1,2j} \rangle &= \langle S^i_{1,2j+1} \rangle = 0.46 \\
\langle S^i_{2,2j} \rangle &= \langle S^i_{2,2j+1} \rangle = 0.08 \\
\langle S^i_{1,2j} \rangle &= \langle S^i_{2,2j+1} \rangle = -0.04
\end{align*}
\]

which agree well with the theoretically predicted values in (34). Details will be published elsewhere [57].

Let us explain why the new and exotic behavior of the plateau width is realized in our model, by comparing our model with the $S = 1/2$ bond-alternating Heisenberg chain described by

\[ \mathcal{H}_{b-a} = J \sum_j [1 + (-1)^j/2] \mathbf{S}_j \cdot \mathbf{S}_{j+1} \]  (36)

where $\delta$ is the bond alternation parameter. Any small amount of $\delta$ produces the dimer spin gap as $\Delta \propto |\delta|^{1/2}$ [63–65] (with leading logarithmic correction [66]). Thus the spin gap $\Delta$ of (36) behaves as the sketch in figure 7(b) near $\delta = 0$. When $\delta > 0$ ($\delta < 0$), the spins $\mathbf{S}_{2n}$ and $\mathbf{S}_{2n+1}$ ($\mathbf{S}_{2n-1}$ and $\mathbf{S}_{2n}$) effectively form a singlet dimer pair, which brings about the dimer spin gap. These two mechanisms, the $\delta > 0$ and the $\delta < 0$ mechanism, are completely competing and the reconstruction of the unit cell occurs at the mechanism-changing point $\delta = 0$. At $\delta = 0$, the system is of the Tomonaga–Luttinger state, which is characterized by the gapless excitation. In our case, on the other hand, the unit cell is always the isosceles triangle for both the $\alpha < 1$ and $\alpha > 1$ cases. Then the reconstruction of the unit cell never occurs in our case, which enables the cooperation of two plateau-formation mechanisms, the $\psi^{(+)}/\Delta_1 (1/2, +1/2)$ and the $\psi^{(-)} (1/2, +1/2)$ mechanism.

The phase boundary between the traditional plateau phases and the new plateau phase where the plateau width remarkably increases can be determined by the phenomenological renormalization equation for the scaled gap $L \Delta_0$ obtained by the numerically exact diagonalization method

\[ (L + 2) \Delta_0 L = L \Delta_0 L \] (37)

where $\Delta_0$ is the excitation gap within the $M_s/3$ space and $\alpha_{c,L}$ is the size-dependent fixed point of $\alpha$. The plateau–plateauless phase boundary can be estimated also by the phenomenological renormalization equation where $\Delta_0$ is replaced by $\Delta$ (plateau width), as in case of the spin gap at $M = 0$. Figure 8 shows our preliminary results on the phase diagram at $M_s/3$. This phase diagram qualitatively agrees with figure 6. However more detailed analyses will be necessary to draw a precise phase diagram.

### 6. Twisted tube

Although we have discussed theoretical aspects of the $S = 1/2$ isosceles quantum spin tube, a compound corresponding to our model has not been found yet. In this section, we review the twisted spin tube, which is of particular importance for actual experiments; recently, the interesting compound [(CuCl$_2$-tachH)$_3$Cl]Cl was actually synthesized as an assembly of triangular clusters conformed by Cu$^{2+}$ ions and magnetization measurements were performed [2]. As is
in the magnetization curve \[67\]. investigated in the context of the triangular lattice spin system, the quantum spin tube with the easy-plane anisotropy was as twisted quantum spin tube. we will review the quantum phase transition peculiar to the theoretical results. This suggests that a kind of dual structure region (\(T < 0.5\) K) [68], which is consistent with the theoretical results. This suggests that a kind of dual structure associated with the quantum phase transition of the first order may be captured by the experimental measurements. Below, we will review the quantum phase transition peculiar to the twisted quantum spin tube.

The model Hamiltonian of the twisted spin tube is written as

\[ \mathcal{H} = J_1 \sum_{i=1}^{3} \sum_{j=1}^{3} \left[ S_{i,j} \cdot S_{i,j+1} + S_{i,j} \cdot S_{i+1,j+1} \right] + J_3 \sum_{i=1}^{3} \sum_{j=1}^{3} S_{i,j} \cdot S_{i+1,j} \]  

(38)

Figure 8. Phase diagram of the \(M_1/3\) magnetization plateau. The plateau 1, 2 and 3 correspond to the \(\psi^{(\pm)}(1/2, +1/2)\), the \(\psi^{-}(1/2, +1/2)\), and the new plateau phases, respectively. Dashed lines are the second order lines, while solid curves are expected to be of the Berezinskii–Kosterlitz–Thouless (BKT) transition.

Figure 9. Twisted quantum spin tube. \(J_i\) indicates the exchange coupling in the unit triangle and \(J_r\) indicates inter-triangle coupling. The expansion of the twisted spin tube has a triangular lattice structure.

\[ J_1 \gg J_3 \] indicates inter-triangle coupling.

\[ \psi(-\pi/3) \]

\[ \psi(\pi/3) \]

the rhombus lattice has no frustration. Thus we can expect a quantum phase transition between decoupled triangles and rhombus lattice phases.

In the decoupled triangle limit \((J_r \gg J_1)\), the degenerate perturbation with respect to \(J_1\) leads us to the effective spin-chirality model,

\[ \mathcal{H}_{\text{eff}} = \frac{2J_1}{3} \sum_j T_j \cdot T_{j+1} \left[ 1 + 2\exp(i\pi/3) \tau_j^+ \tau_{j+1}^- + \exp(-i\pi/3) \tau_j^+ \tau_{j+1}^- \right] \]  

(39)

where \(T\) represents the spin-1/2 operator and \(\tau\) indicates an effective spin matrix representing the chirality degrees of freedom as in (22). This effective Hamiltonian is very similar to (22); the phase factor \(\exp(i\pi/3)\) originates from the \(\pi/3\) rotation of the lattice along the tube direction and it can be removed by the gauge transformation. On the same line of the argument as (22), the effective Hamiltonian (39) has a spin gap [10, 11, 13]. Indeed, a detailed DMRG computation of the full Hamiltonian (38) actually confirms that the spin gap exists for \(J_1/J_r < 1.21\) [14, 15]. For \(J_1/J_r > 1.21\), on the other hand, the finite-size scaling analysis of the spin gap basically indicates the gapless ground state [15]. Although the usual singlet–triplet spin gap for the open boundary condition captures a boundary excitation in 1.21 < \(J_1/J_r < 1.5\), such an anomalous behavior due to the boundary can be settled down by using the single-spin termination of the tube [8].

In order to resolve the nature of the quantum phase transition of the twisted tube, an important quantity is the total-\(S\) on the unit triangle [14]. For the decoupled triangle, the ground state is in doubly degenerating doublets of the unit triangle, while for \(J_r = 0\), the ground state basically belongs to the \(S = 3/2\) sector. Here, we define the projection operator of the total-\(S\) of the unit triangle to the doublet sector as \(P_{1/2}(= \frac{1}{2} - \frac{1}{2}(S_1 \cdot S_2 + S_2 \cdot S_3 + S_3 \cdot S_1))\) for each unit triangle. As discussed in [14], then, this projection operator \(P_{1/2}\) is a good order parameter of the twisted tube; the detailed computation of the expectation value \(\langle P_{1/2} \rangle\) shows a discontinuity at the critical value \((J_1/J_r) \simeq 1.22\), not at \(J_1/J_r \simeq 1.47\), which is consistent with the spin gap result. In addition to this, we should remark that an extended spin tube with the diagonal interaction shows the exact first order phase transition, for which total-\(S\) on the unit triangles is independently conserved [69]. We have thus investigated how to connect the twisted tube to the diagonal interaction model.
a certain density of states originating from the ground state itself is gapless, this implies that, although the ground state itself is gapless, the overview of the first order quantum phase transition is clarified.

We add to the Hamiltonian (38), and then vary $-1 \leq \gamma \leq 1$. Note that $\gamma = 0$ corresponds to the original twisted tube and $\gamma = 1$ corresponds to the diagonal spin tube, which shows the first order transition at $J_1/J_t \simeq 0.63$ [69].

In figure 10, we show $\langle P_{1/2} \rangle$ at the center of the extended tube calculated by DMRG for $L = 36$ with $J_t = 1$. In the figure, $\langle P_{1/2} \rangle$ jumps exactly from zero to unity at $J_1/J_t \simeq 0.63$ along the line of $\gamma = 1$, where the total-$S$ of the unit triangle is the exact symmetry. Then, we can see that the ‘gap’ of the $\langle P_{1/2} \rangle$ is adiabatically continued to $\gamma = 0$. This implies that the transition at $(J_1/J_t)_{c} \simeq 1.21$ on the line of $\gamma = 0$ corresponding to the twisted tube (38) is of first order. As $J_1$ increases in $\gamma < 0$, this gap reduces, but we cannot confirm whether the end point of the first order transition exists or not within the present calculations for $L = 36$. However, we think that the overview of the first order quantum phase transition is clarified.

In connection with the experiments, an interesting point is that the parameter $J_1/J_t \simeq 2.16$ for [(CuCl$_3$-tachH)$_2$Cl]Cl$_2$ is located in the gapless $S = 3/2$ sector, but it is surrounded by the ‘gap’ of the first order transition, as in figure 10. This implies that, although the ground state itself is gapless, a certain density of states originating from the $S = 1/2$ sector can be expected above the ground state. Thus we can expect that such a dual structure of $S = 1/2$ and $3/2$ sectors affects the experimentally observed quantities of the twisted tube at a finite temperature. Indeed, a recent specific heat result illustrates that the linear temperature dependence at very low temperature ($T < 0.5$ K), which can be described as an effective $S = 3/2$ chain, crosses over to spin-gap-like behavior around $T \sim 2$ K [68]. Also for the low-field magnetization curve of $J_1/J_t > 1.21$, we can see that, after a linear increase of the magnetization in the very low-field region, the slope of the magnetization curve rapidly increases, as if it had a spin gap [15].

7. Future prospects

As a future prospect, it would be interesting to consider carrier-doped spin nanotubes like the high-$T_c$ cuprates, where the system is effectively described by the Hubbard model near the half-filling case. A mechanism for the superconductivity based on the spin gap had been proposed for the carrier-doped two-leg spin ladder [70] and actually a pressure-induced superconductivity was observed on the spin ladder cuprate [71]. Motivated by this discovery, spin gap mediated superconductivity was theoretically proposed even for the three-leg spin ladder, using the quantum Monte Carlo simulation [72, 73]. If the carrier-doped three-leg spin tube is realized, it would be a better candidate for the superconductor, rather than the three-leg ladder, because it has a spin gap. In addition the three-leg spin tube was also revealed to have an energy gap in the chirality degrees of freedom [13]. It suggests that a chirality-induced superconductivity could possibly be realized as a new mechanism of superconductivity in the near future.

Acknowledgments

We thank Dr Yuichi Ohtsuka for co-working in the initial stage of this work. We also thank Professors I Affleck, A Läuchli, C Lhuillier, H Manaka, F Mila, H Nojiri, D Poilblanc, P Pujol, J Schnack, P Sindzingre, and Drs D Charrier and G Nénert for fruitful discussions. This work has been partly supported by Grants-in-Aid for Scientific Research (B) (Nos 17340100, 20340096), Scientific Research (C) (No. 18540340), for Young Scientists (B) (No. 21740295), and on Priority Areas ‘Invention of Anomalous Quantum Materials—New Physics through Innovation Materials’—(No.19014019), ‘Physics of New Quantum Phases in Superclean Materials’ (Nos 17071011, 18043023, 20029020), ‘High Field Spin Science in 100T’ (Nos 20030008, 20030030) and ‘Novel States of Matter Induced by Frustration’ (Nos 22014016, 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.

References

[1] Seeger G, Kögerler P, Kariuki B M and Cronin L 2004 Chem. Commun. 1580
[2] Schnack J, Nojiri H, Kögerler P, Cooper G J T and Cronin L 2004 Phys. Rev. B 70 174420
[3] Manaka H, Hirai Y, Hachigo Y, Mitsunaga M, Ito M and Terada N 2009 J. Phys. Soc. Japan 78 093701
[4] Millet P, Henry J Y, Mila F and Galy J 1999 J. Solid State Chem. 147 676
[5] Garlea V O, Zheludev A, Regnault L-P, Chung J-H, Qiu Y, Boehm M, Habicht K and Meissner M 2008 Phys. Rev. Lett. 100 037206
