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The field-induced gap due to four-spin exchange in a spin ladder

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Abstract

The effect of the four-spin cyclic exchange interaction at each plaquette in the $S = 1/2$ two-leg spin ladder is investigated at $T = 0$, focusing especially on the field-induced gap. The strong-rung-coupling approximation suggests that it yields a plateau at half of the saturation moment ($m = 1/2$) in the magnetization curve, which corresponds to a field-induced spin gap with a spontaneous breaking of the translational symmetry. A precise phase diagram at $m = 1/2$ is also presented, based on the level spectroscopy analysis of the numerical data obtained by the Lanczos method. The boundary between the gapless and plateau phases is confirmed to be of the Kosterlitz–Thouless (KT) universality class.

1. Introduction

The multiple-spin exchange interaction has attracted a lot of interest in condensed matter physics. Such many-body exchange interactions are realized in two-dimensional (2D) solid ^{3}He [1, 2] and the 2D Wigner solid of electrons formed in a silicon inversion layer [3], as well as bcc ^{3}He [4]. Recently the four-spin cyclic exchange interaction, called *ring exchange*, has been revealed to be important even in strongly correlated electron systems like the high-temperature cuprate superconductors. Analysis on the low-lying excitation spectrum of the d–p model indicated that the ring exchange should be taken into account in the simplified spin Hamiltonian describing the CuO_2 plane [5]. Study based on the Heisenberg Hamiltonian also revealed evidence of ring exchange in the Raman scattering spectrum [6]. In fact, such a four-spin interaction was derived from the fourth-order perturbation expansion of the square-lattice Hubbard Hamiltonian with respect to t/U near half-filling [7]. A neutron scattering experiment

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also suggested that the effect of the ring exchange appears in the spin-wave excitation spectrum of La_2CuO_4 [8].

Recently, ring exchange has been supposed to be important also in spin-ladder systems. The significant difference between the observed leg and rung bi-linear exchange coupling constants ($J_{\mathrm{leg}} \sim 2J_{\mathrm{rung}}$) of $Sr_{14}Cu_{24}O_{41}$ was explained, assuming the existence of a ring exchange with an amplitude of about 14% of J_{rung} [9]. A four-spin exchange interaction described by a product of two-spin exchanges in a spin ladder was investigated by a field theoretical approach [10], where the possibility of a massive phase of different type to the Haldane phase is indicated [11, 12], in the nonmagnetic ground state. A recent density-matrix renormalization group study suggested that increasing the ring exchange constant J_4 brings about a quantum phase transition at $J_4 \sim 0.3J_{\mathrm{rung}}$ for $J_{\mathrm{leg}} = J_{\mathrm{rung}}$ [13]. However, this feature of the large-J_4 phase is still an open problem. We note that there exist integrable spin-ladder models with four-spin exchange interactions [14, 15]. But these models are somewhat different from our model.

As another interesting phenomenon caused by the ring exchange, a field-induced spin gap [16], which should be observed as a plateau in the magnetization curve, was proposed to occur in an $S = 1/2$ antiferromagnet on the triangular lattice [17]. This was verified by exact diagonalization [18]. In the spin-ladder system, besides the original spin gap [19–21], a magnetization plateau was also revealed to appear in the presence of an additional leg [22], a bond alternation [23, 24] or some frustrated interactions [25–31]. In the previous work [32] by two of the present authors (TS and YH), such a field-induced gap due to the ring exchange in the spin ladder was investigated. In that work, a phenomenological renormalization study [33] suggested that a plateau appeared at half of the saturation magnetization in the spin ladder for a realistic parameter $J_4 > (0.05 \pm 0.04)J_{\mathrm{rung}}$ in the case of $J_{\mathrm{leg}} = J_{\mathrm{rung}}$. However, the critical point J_{4c} estimated from the one-magnon analysis did not agree well with that obtained from the two-magnon one. The critical index at J_{4c} was also different from that of the Kosterlitz–Thouless transition [34] predicted from the behaviour of the energy gap. Thus better studies are necessary to determine the critical point J_{4c} and the universality class for the transition between the plateau and gapless states due to the ring exchange in the spin ladder. In the present paper, a perturbation expansion from the strong-rung-coupling limit is performed to clarify the mechanism of plateau formation and the quantum critical behaviour around the phase boundary. Also, a precise phase diagram is presented, using size scaling analysis based on the conformal field theory [35–37] and the recently developed level spectroscopy method [38–41]. The parameter space is also more generalized than that of the previous work.

2. The spin ladder with ring exchange

We consider the $S = 1/2$ uniform antiferromagnetic spin ladder with the four-spin cyclic exchange at every plaquette, as shown in figure 1. The Hamiltonian of our model is

$$\begin{aligned}
\mathcal{H} &= \mathcal{H}_0 + \mathcal{H}_Z \\
\mathcal{H}_0 &= \sum_{j=1}^{L}(J_1 \boldsymbol{S}_{1,j} \cdot \boldsymbol{S}_{1,j+1} + J_1 \boldsymbol{S}_{2,j} \cdot \boldsymbol{S}_{2,j+1} + J_\perp \boldsymbol{S}_{1,j} \cdot \boldsymbol{S}_{2,j}) + J_4 \sum_{j=1}^{L}(P_{4,j} + P_{4,j}^{-1}) \\
\mathcal{H}_Z &= -H \sum_{j=1}^{L}(S_{1,j}^z + S_{2,j}^z)
\end{aligned} \tag{1}$$

where J_1 and $J_\perp$ are the bi-linear leg and rung exchange constants, respectively. We set $J_\perp = 1$ throughout this paper. $P_{4,j}$ is the cyclic permutation operator which exchanges the four spins

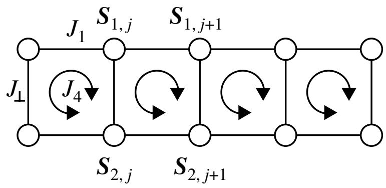

Figure 1. An illustration of a two-leg spin ladder with four-spin exchange interaction at every plaquette.

around the jth plaquette as $S_{1,j} \to S_{1,j+1} \to S_{2,j+1} \to S_{2,j} \to S_{1,j}$; we have

$$P_j \begin{vmatrix} a & b \\ d & c \end{vmatrix}\Big\rangle = \begin{vmatrix} d & a \\ c & b \end{vmatrix}\Big\rangle \qquad P_j^{-1} \begin{vmatrix} a & b \\ d & c \end{vmatrix}\Big\rangle = \begin{vmatrix} b & c \\ a & d \end{vmatrix}\Big\rangle \tag{2}$$

where the (1, 1) component denotes the spin state of $S_{1,j}$ and the (2, 2) component that of $S_{2,j+1}$. The strength of the four-spin ring exchange J_4 is assumed to be positive, as it is in the Cu oxides. The applied magnetic field is denoted by H . The magnetization of the bulk system is defined as $m = M/L$, where $M \equiv \langle \sum_j (S^z_{1,j} + S^z_{2,j}) \rangle$. We focus on a possible plateau at half of the saturation ($m = 1/2$) in the magnetization curve at $T = 0$.

3. The strong-rung-coupling approximation

The condition of quantization of the magnetization [16] predicted that $Q(S - m) =$ integer is necessary for the appearance of the plateau at m, where Q is the period of the ground state and S is the total spin per unit cell. Thus the plateau at $m = 1/2$ should require a spontaneous breakdown of the translational symmetry which results in the period of two unit cells, as in the case of the Néel state.

In order to investigate the possibility and the mechanism of the plateau at $m = 1/2$ in the spin ladder with the ring exchange, we consider the strong-rung-coupling limit ($J_\perp \gg J_1$, J_4) [27, 28] first. The system is separated into isolated rung dimers when $J_1 = J_4 = 0$. In this case, at $m = 1/2$, half of the rung pairs are triplets with $S^z = 1$, and the remaining half are singlets. Since other possible selections have higher energies, we may restrict ourselves to considering these two states for each rung dimer and represent them by states $|\Uparrow\rangle$ and $|\Downarrow\rangle$ of pseudo-spin $\tilde{S}$:

$$\begin{vmatrix} \uparrow \\ \uparrow \end{vmatrix}\Big\rangle \Rightarrow |\Uparrow\rangle \qquad \frac{1}{\sqrt{2}}\left(\begin{vmatrix} \uparrow \\ \downarrow \end{vmatrix}\Big\rangle - \begin{vmatrix} \downarrow \\ \uparrow \end{vmatrix}\Big\rangle \right) \Rightarrow |\Downarrow\rangle. \tag{3}$$

When $J_1 = J_4 = 0$, each pseudo-spin $\tilde{S}$ can be either $|\Uparrow\rangle$ or $|\Downarrow\rangle$ completely freely, which means a high degeneracy of the $m = 1/2$ ground states. The introduction of weak J_1 and J_4 resolves the degeneracy. The effect of a weak inter-dimer coupling can be taken into account by the perturbation expansion with respect to J_1 and J_4, resulting in the following matrix elements by straightforward calculation:

$$\begin{array}{c} \\ \langle \Uparrow_j \Uparrow_{j+1}| \\ \langle \Uparrow_j \Downarrow_{j+1}| \\ \langle \Downarrow_j \Uparrow_{j+1}| \\ \langle \Downarrow_j \Downarrow_{j+1}| \end{array} \begin{array}{c} \quad |\Uparrow_j \Uparrow_{j+1}\rangle \qquad |\Uparrow_j \Downarrow_{j+1}\rangle \qquad |\Downarrow_j \Uparrow_{j+1}\rangle \qquad |\Downarrow_j \Downarrow_{j+1}\rangle \\ \begin{pmatrix} -(1/4)J_1 + 2J_4 & 0 & 0 & 0 \\ 0 & -(1/4)J_1 - J_4 & (1/2)J_1 + J_4 & 0 \\ 0 & (1/2)J_1 + J_4 & -(1/4)J_1 - J_4 & 0 \\ 0 & 0 & 0 & (1/4)J_1 + J_4 \end{pmatrix} \end{array}. \tag{4}$$

By comparing equation (4) with an XXZ-type Hamiltonian including an effective magnetic field $\tilde{H}$:

$$\begin{array}{c} \\ \langle\Uparrow_j\Uparrow_{j+1}| \\ \langle\Uparrow_j\Downarrow_{j+1}| \\ \langle\Downarrow_j\Uparrow_{j+1}| \\ \langle\Downarrow_j\Downarrow_{j+1}| \end{array} \begin{array}{c} \begin{array}{cccc} |\Uparrow_j\Uparrow_{j+1}\rangle & |\Uparrow_j\Downarrow_{j+1}\rangle & |\Downarrow_j\Uparrow_{j+1}\rangle & |\Downarrow_j\Downarrow_{j+1}\rangle \end{array} \\ \begin{pmatrix} (1/4)\tilde{J}^z - \tilde{H} + a & 0 & 0 & 0 \\ 0 & -(1/4)\tilde{J}^z + a & (1/2)\tilde{J}^{xy} & 0 \\ 0 & (1/2)\tilde{J}^{xy} & -(1/4)\tilde{J}^z + a & 0 \\ 0 & 0 & 0 & (1/4)\tilde{J}^z + \tilde{H} + a \end{pmatrix} \end{array} \tag{5}$$

we obtain the effective Hamiltonian for $\tilde{\boldsymbol{S}}$:

$$\tilde{\mathcal{H}} = \sum_j^L \left\{ \tilde{J}^{xy}(\tilde{S}_j^x \tilde{S}_{j+1}^x + \tilde{S}_j^y \tilde{S}_{j+1}^y) + \tilde{J}^z \tilde{S}_j^z \tilde{S}_{j+1}^z \right\} + \tilde{\mathcal{H}}_{\mathrm{Z}} \tag{6}$$

with $\tilde{J}^{xy} = J_1 + 2J_4$ and $\tilde{J}^z = J_1/2 + 5J_4$.

The effective Zeeman term $\tilde{\mathcal{H}}_{\mathrm{Z}}$ and the effective XXZ-anisotropy are given respectively by

$$\tilde{\mathcal{H}}_{\mathrm{Z}} = \tilde{H} \sum_j^L \tilde{S}_j^z \qquad \tilde{H} = \frac{J_1}{4} - \frac{J_4}{2} \tag{7}$$

and

$$\lambda_{\mathrm{eff}} \equiv \frac{\tilde{J}^z}{\tilde{J}^{xy}} = \frac{J_1/2 + 5J_4}{J_1 + 2J_4}. \tag{8}$$

Thus the problem of magnetized states with $m = 1/2$ of the *original* system is mapped onto that of nonmagnetic states of the Hamiltonian (6). It is well known for the $\tilde{S} = 1/2$ XXZ-chain that the ground state has Néel order for $\lambda_{\mathrm{eff}} > 1$ and magnetic/nonmagnetic excitations are gapped. The ordered phase is separated from the gapless one by a critical point $\lambda_{\mathrm{eff}} = 1$; the transition at the critical point is of the Kosterlitz–Thouless type with $\eta = \eta^z = 1$, where η and η^z are critical indices defined by

$$\langle S_0^x S_r^x \rangle \sim (-1)^r r^{-\eta} \qquad \text{and} \qquad \langle S_0^z S_r^z \rangle \sim (-1)^r r^{-\eta^z} \qquad (r \to \infty) \tag{9}$$

respectively. Turning back to the original system, this implies that the original ladder (1) has a magnetization plateau at $m = 1/2$ under the condition

$$J_4 > \frac{1}{6} J_1. \tag{10}$$

The plateau state is Néel ordered in the language of the pseudo-spin $\tilde{\boldsymbol{S}}$, as shown in figure 2.

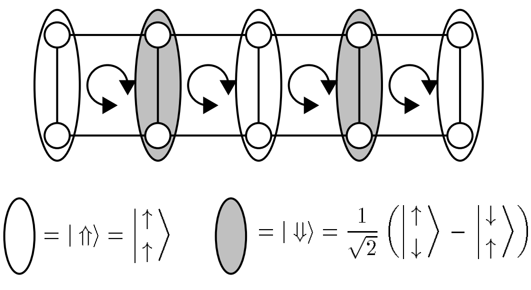

Figure 2. A physical picture of the $m = 1/2$ plateau state. Open ellipses represent $|\Uparrow\rangle$ and shadowed ellipses $|\Downarrow\rangle$ in the language of the pseudo-spin $\tilde{\boldsymbol{S}}$.

4. Numerical approach

The phase boundary $J_4 = (1/6)J_1$ obtained in the previous section is valid for $J_1, J_4 \ll 1$. To obtain a phase diagram for a wider range of the parameters, we have performed the numerical diagonalization of the original Hamiltonian (1) by the Lanczos method.

The most powerful method at the present stage for determining the KT phase boundary is level spectroscopy (LS), which was developed by one of the present authors (KO) and Nomura [38–41]. In the LS analysis the critical point is determined from the level cross between the two relevant low-lying excitation gaps with a common scaling dimension—that is, the same dominant size correction including the logarithmic one. In the present case, we use the following three gaps:

$$\Delta_1 = \frac{1}{2}[E_\pi(L, M+1) + E_\pi(L, M-1) - 2E_0(L, M)] \tag{11}$$

$$\Delta_\pi = E_\pi(L, M) - E_0(L, M) \tag{12}$$

$$\Delta_\pi^{(2)} = E_\pi^{(2)}(L, M) - E_0(L, M) \tag{13}$$

where $E_k(L, M)$ and $E_k^{(2)}(L, M)$ respectively denote the lowest and the second-lowest eigenvalues of the Hamiltonian $\mathcal{H}_0$ with the system size L, and $\langle \sum_j (S_{1,j}^z + S_{2,j}^z) \rangle = M$. These gaps Δ_1, Δ_π and $\Delta_\pi^{(2)}$ govern the long-distance behaviours of the $S^x - S^x$, $S^z - S^z$ and dimer correlations, respectively, in the language of the pseudo-spin $\tilde{S}$. The critical indices η, η^z and η^{d} can be connected with Δ_1 and Δ_π by

$$\eta = \frac{L\Delta_1}{\pi v_{\mathrm{s}}} \qquad \eta^z = \frac{L\Delta_\pi}{\pi v_{\mathrm{s}}} \qquad \eta^{\mathrm{d}} = \frac{L\Delta_\pi^{(2)}}{\pi v_{\mathrm{s}}} \qquad (L \to \infty) \tag{14}$$

respectively, where v_{s} is the spin-wave velocity estimated by

$$v_{\mathrm{s}} = \frac{L}{2\pi}\big(E_{k_1}(L, M) - E_0(L, M)\big) \qquad (L \to \infty) \tag{15}$$

with $k_1 \equiv 2\pi/L$.

The behaviours of η and η^z near the KT critical point for large L are

$$\eta = 1 - \frac{1}{2}y_0 \qquad \eta^z = 1 - \frac{1}{2}y_0(1+2t) \tag{16}$$

respectively, where t denotes the distance from the KT critical point, and y_0 represents the lowest-order finite-size correction, which leads to a logarithmic size correction of the order of $1/\log L$ at the KT critical point. Thus the KT critical point can be obtained from $\eta = \eta^z$ within the lowest order of the finite-size corrections. As shown in equation (16), the logarithmic corrections to η and η^z are serious for finite systems. Then the relation $\eta = 1$ (or $\eta^z = 1$) is not a good indicator for the KT critical point.

Figure 3 shows the behaviours of η and η^z as functions of J_4 for two cases: (a) $J_1 = 0.5$ and (b) $J_1 = 1.0$, for the length of the ladder $L = 16$. From the crossing points between η and η^z, we see that the critical point $J_{4\mathrm{c}} = 0.10$ for $J_1 = 0.5$, and $J_{4\mathrm{c}} = 0.22$ for $J_1 = 1.0$. The quantity $1 - \eta = 1 - \eta^z$ at $J_{4\mathrm{c}}$ represents the magnitude of the logarithmic size correction $y_0/2$ around $L = 8$–16. If we determine the KT critical points from the condition $\eta = 1$, we obtain $J_{4\mathrm{c}} = 0.18$ for $J_1 = 0.5$, and $J_{4\mathrm{c}} = 0.36$ for $J_1 = 1.0$, which are fairly large compared to those obtained by use of the LS.

To check the KT universality class, we also calculated the central charge c by use of

$$\frac{E_0(L, M)}{L} = \epsilon_{\mathrm{g}} - \frac{\pi c v}{6L^2}\left\{1 + \mathrm{O}\left(\frac{1}{(\log L)^3}\right)\right\} \tag{17}$$

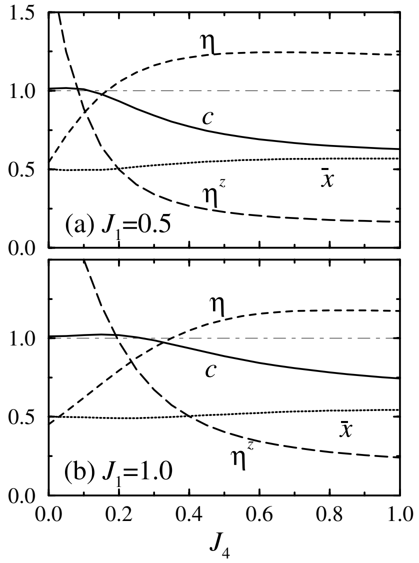

Figure 3. Critical exponents η and η^z as functions of J_4 for the (a) $J_1 = 0.5$ and (b) $J_1 = 1.0$ cases. The central charge c (see equation (17)) and the quantity $\overline{x}$ (see equation (18)) are also shown.

where ϵ_g is the ground-state energy per rung at $m = 1/2$ for an infinite system. As can be seen from figure 3, the central charge is $c = 1$ near the KT critical point and rapidly decreases in the gapped region, as is expected from [42, 43]. This fact supports the KT nature of this transition.

We also checked the KT nature by calculating

$$\overline{x} = \frac{(\eta^z + \eta^d)\eta}{2} \tag{18}$$

which should be $1/2$ in the lowest order of the renormalization equation in the gapless region, as was shown by Kitazawa and Nomura [44]. We can clearly read from figure 3 that the quantity $\overline{x}$ is very close to $1/2$ in the gapless region, also verifying the KT nature.

In figure 4 we show the KT critical points estimated from LS (i.e. $\eta = \eta^z$), as well as those obtained by assuming $\eta = 1$ (conventional method), for the system sizes $L = 8, 12, 16$. We see that the LS result is consistent with that obtained by the strong-coupling approach in section 2, while the result obtained by using the relation $\eta = 1$ is not.

5. Discussion

In the previous section, we have obtained the phase diagram from the numerical diagonalization data through LS analysis, and shown the KT nature of the transition between the plateau and gapless states. Our numerical results are quite consistent with those of the strong-coupling approach in section 3.

In our previous work [32], where we restricted our consideration to the case of $J_1 = 1$, the KT transition was also suggested by the Roomany–Wyld approximation for the Callen–Symanzik β-function [45]. However, the critical exponent η calculated numerically on the basis of the conformal field theory indicated a different value, $\eta \sim 0.5$, around $J_{4c} \simeq 0.05$ estimated by means of phenomenological renormalization. Since, as already shown in section 3, the critical exponent η should be unity at the KT transition point, our previous result was not

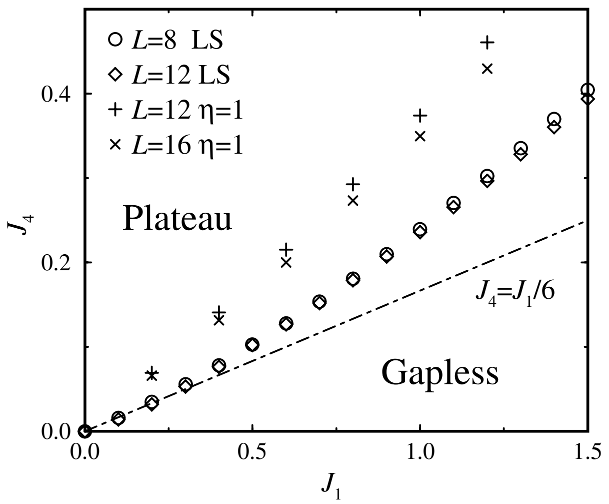

Figure 4. The phase diagram in the magnetized ground state at $m = 1/2$. Circles and diamonds show the critical points determined by LS for $L = 8$ and $L = 12$, respectively. They are almost independent of the system size. The symbols + and $\times$ indicate the points where $\eta = 1$ for $L = 12$ and $L = 16$, respectively. They depend significantly on L. The result from the strong-rung-coupling approach, $J_{4c} \sim J_1/6$, is also displayed.

self-consistent. This inconsistency has been completely resolved by the present analysis. That is, our previous result $J_{4c} = 0.05 \pm 0.04$ for $J_1 = 1$ significantly deviates from the reliable result obtained above. This is consistent with the criticism [38, 39, 41] that phenomenological renormalization leads to serious underestimation of the gapless region for the KT transition.

The phase diagram suggests that, for larger J_1, the critical value J_{4c} becomes larger than the limit for a strong rung coupling. This implies that the quantum fluctuation due to the leg coupling (J_1) suppress plateau formation. In the special case $J_1 = 1$, the critical value is $J_{4c} \simeq 0.24$. Since $Sr_{14}Cu_{24}O_{41}$ is expected to have $J_1 = 1$ and $J_4 \sim 0.14$ as explained in section 1, this is not enough for the appearance of the plateau at $m = 1/2$.

An example of a magnetization curve was already shown in our previous work [32], to which readers should refer. At finite temperatures the magnetization plateau will be smeared. This problem is left for future investigations.

In conclusion, we explained physically the plateau formation scenario of the $S = 1/2$ spin ladder with ring exchange interaction at each plaquette, and also obtained the plateau–gapless phase diagram by both analytical and numerical methods. The present phase diagram is more reliable and covers a wider range of parameters than our previous one [32].

Acknowledgments

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