Two-step Quantum Spin Flop Transition in Spin Ladders

T Sakai\textsuperscript{1}, K Okamoto\textsuperscript{2} and T Tonegawa\textsuperscript{3}

\textsuperscript{1}Japan Atomic Energy Agency (JAEA), SPring-8, Hyogo 679-5148, and Department of Material Science, University of Hyogo, Kamigori, Hyogo 678-1297, Japan
\textsuperscript{2}Department of Physics, Tokyo Institute of Technology, Tokyo 152-8551, Japan
\textsuperscript{3}Department of Mechanical Engineering, Fukui University of Technology, Fukui 910-8505, Japan

E-mail: sakai@spring8.or.jp

Abstract.

The magnetization process of the $S = 1/2$ spin ladder system with ferromagnetic rung exchange interaction is investigated by the numerical exact diagonalization of finite-size clusters. It is found that in the presence of an easy-axis anisotropy the system exhibits a two-step field induced phase transition corresponding to the spin flop. Due to large quantum fluctuation, each step is a second-order transition and the second step occurs between two different Tomonaga-Luttinger liquid phases. Some phase diagrams are also presented.

It is well known that the antiferromagnet with easy-axis anisotropies exhibits a field-induced first-order phase transition, the so-called spin flop. In one-dimensional quantum spin systems, instead of it, a second-order phase transition occurs because of large quantum fluctuations [1]. Particularly the $S=1$ antiferromagnetic chain with the easy-axis single-ion anisotropy was revealed to exhibit two successive field-induced second-order transitions by our previous numerical analysis [2]. However, such transitions have not been observed yet. Recently a two-step spin flop transition was observed in the spin ladder system IPA-CuCl$_3$ [3], which has ferromagnetic rung coupling. In order to clarify the mechanism of the two-step field-induced transition, we investigate the anisotropic spin ladder using the numerical diagonalization and the finite-size scaling analysis. As a result, we revealed that two different field-induced second-order quantum phase transitions possibly occur. Several phase diagrams will be also presented. Such a two-step spin flop transition was also predicted in the spin alternating chain [4] which is a theoretical model of the compound [Mn(saltmen)Ni(pao)$_2$(bpy)]PF$_6$ [5].

We consider the $S = 1/2$ spin ladder system described by the Hamiltonian

$$\mathcal{H} = J_1 \sum_{i=1,2} \sum_{j=1}^L \vec{S}_{i,j} \cdot \vec{S}_{i,j+1} - \sum_{j=1}^L [\gamma (S_{1,j}^x S_{2,j}^x + S_{1,j}^y S_{2,j}^y) + S_{1,j}^z S_{2,j}^z] - H \sum_{i=1,2} \sum_{j=1}^L S_{i,j}^z,$$  \quad (1)$$

where $\gamma$ is an anisotropy parameter of the ferromagnetic rung exchange interaction.

In the absence of an external magnetic field, the system has a spin gap for $\gamma \sim 1$, while the Néel order along $z$-axis appears for $\gamma \sim 0$. The critical point $\gamma_c$ can be estimated by the phenomenological renormalization. According to the method, the size-dependent critical point
\( \gamma_{c,L} \) is determined by the form of the scaled gaps

\[
(L + 2)\Delta_{L+2}(\gamma_{c,L}) = L\Delta_L(\gamma_{c,L}),
\]

where \( \Delta_L(\gamma) \) is the lowest excitation gap with \( k = \pi \). The scaled gap \( L\Delta_L(\gamma) \) is plotted versus \( \gamma \) for \( J_1 = 0.5 \) and 1.0 in Figs. 1 (a) and (b), respectively. The critical point \( \gamma \) is estimated by an extrapolation of \( \gamma_{c,L} \) to the infinite length limit.

Since the ground state is in the Haldane phase for \( \gamma > \gamma_c \), a phase transition occurs at some critical field \( H_{c1} \) and the gapless Tomonaga-Luttinger liquid phase is realized for \( H > H_{c1} \) [6]. On the other hand, starting from the Néel ordered phase for \( \gamma < \gamma_c \), the magnetization process is expected to be similar to the \( S = 1/2 \) Ising-like XXZ chain. In this case the Tomonaga-Luttinger liquid phase is also realized at some critical field \( H_{c1} \). The quasiparticle excitation, however, is different between these two Tomonaga-Luttinger liquids. Each elementary magnon excitation should occur by \( \delta S_z = 2 \) due to strong Ising-like ferromagnetic rung exchange interaction for \( \gamma < \gamma_c \), while \( \delta S_z = 1 \) for \( \gamma > \gamma_c \). The former Tomonaga-Luttinger liquid phase is denoted as TLL2, while the latter TLL1. The \( 2k_F \) soft mode is also different between the two phases; \( 2k_F = m\pi \) in TLL2 and \( 2k_F = 2m\pi \) in TLL1. In general \( \gamma_c \) depends on the magnetization \( m \equiv \sum_{i=1,2} \sum_{j} \langle S_{i,j}^z \rangle / L \). Since the \( \delta S_z = 1 \) \( (2k_F = m\pi) \) excitation is gapless (gapped) in TLL1, while gapped (gapless) in TLL2, the crossing point of the two excitation gaps \( (\Delta_1 \text{ and } \Delta_{2k_F}) \) as functions of \( \gamma \) should correspond to \( \gamma_c \) in the thermodynamic limit. These two scaled gaps \( L\Delta_1 \) and \( L\Delta_{2k_F} \) calculated for \( L = 8 \) and 12 by the numerical diagonalization are plotted versus \( \gamma \) with \( m \) fixed to 1/2 for \( J_1 = 0.5 \) in Fig. 2. It suggests that the \( \delta S_z = 1 \) \( (2k_F = m\pi) \) excitation is gapless in TLL1 (TLL2) and the crossing point of the two gaps gives a good estimation of \( \gamma_c \) because the size dependence is small.

All the intersections of the two gaps \( \Delta_1 \) and \( \Delta_{2k_F} \) with available values of \( m \) for \( L = 8, 10, 12 \) and 14 are shown as a phase boundary between TLL1 and TLL2 in Figs. 3 (a) for \( J_1 = 0.5 \) and (b) for \( J_1 = 1.0 \). The system size dependence of each point is so small that Figs. 3 (a) and (b) are useful as the phase diagrams. The phase boundaries look singular around \( m = 1/2 \), but they may be due to finite-size effects.

The phase diagrams in Figs. 3 (a) and (b) suggest that a field-induced phase transition occurs from TLL2 to TLL1 in a wide region of \( \gamma \). In such a region the system is expected to exhibit a two-step field-induced transition; the first one occurs at \( H_{c1} \) from the Néel state with \( m = 0 \) to the gapless magnetized phase TLL2, and the second one at \( H_{c2} \) to TLL1. Both transitions...
are of the second-order \cite{2}. In contrast, the same model (1) of the classical Heisenberg spins exhibits only a first-order transition, so-called spin flop, from the nonmagnetic ground state to the canted Néel ordered phase corresponding to TLL1 for $\gamma < 1$. Thus we should note that TLL2 is a new phase and the transition at $H_{c2}$ is a new field-induced quantum phase transition induced by large quantum fluctuation.

Finally, the ground-state magnetization curves for several values of $\gamma$ for $J_1 = 0.5$ obtained by the numerical diagonalization of $L = 12$ are shown in Fig. 4. According to the phase diagram in Fig. 3 (a), $H_{c2}$ should be about $m = 0.3$ for $\gamma = 0.4$. There is no jump-like behavior around $H_{c2}$ in the magnetization curve for $\gamma = 0.4$ in Fig. 4. It is consistent with the second-order transition.

In conclusion, it is theoretically predicted that a two-step field induced quantum phase transition occurs in the $S = 1/2$ spin ladder system with ferromagnetic rung couplings in the presence of an easy-axis anisotropy. However, the compound IPA-CuCl$_3$ was reported to be in the Haldane phase. Therefore, the two-step field-induced transition observed on this material
cannot be explained by the present mechanism.

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Figure 4. Ground-state magnetization curves for $\gamma = 0.4, 0.6, 0.8$ and 1.0 with $J_1$ fixed to 0.5.