Metamagnetism of antiferromagnetic $XXZ$ quantum spin chains

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The magnetization process of the one-dimensional antiferromagnetic Heisenberg model with the Ising-like anisotropic exchange interaction is studied by the exact diagonalization technique. It results in the evidence of the first-order spin flop transition with a finite magnetization jump in the Néel ordered phase for $S \geq 1$. It implies that the $S = \frac{1}{2}$ chain is an exceptional case where the metamagnetic transition becomes second-order due to large quantum fluctuations.

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Metamagnetism is one of interesting topics in the field of the magnetism. The spin flopping of the antiferromagnets with the Ising-like anisotropic exchange interaction is a simple mechanism of the field-induced metamagnetic transition. In the process the spins abruptly changes directions from parallel to perpendicular with respect to the easy axis of the sublattice magnetization at some critical magnetic field. In the classical spin systems it is easily understood that the transition is first-order and accompanied by a finite magnetization jump independently of the lattice dimension. In the quantum systems, however, the process is not so trivial because the sublattice magnetization shrinks or vanishes due to quantum fluctuation even at zero temperature. Such quantum effect is expected to be larger in lower dimensions. In one dimension (1D) the $S = \frac{1}{2}$ Ising-like $XXZ$ model was proved by the Bethe ansatz exact solution to exhibit a second-order metamagnetic transition at some critical magnetic field. In contrast the recent numerical analysis suggested that the corresponding transition is first-order for the same model in two and three dimensions (2D, 3D), while the magnetization jump has a quantum spin reduction. It implies that the quantum fluctuation plays such an important role as to change the order of the phase transition in low dimension. As far as we restrict us on the $S = \frac{1}{2}$ model, the critical dimension seems to lie between one and two. On the other hand, the strength of the quantization also depends on the spin value $S$. Since the quantum effect is smaller for larger $S$, the second-order transition discovered for the $S = \frac{1}{2}$ chain is not necessarily a common feature for all the values of $S$. At least the transition is first-order in the infinite $S$ limit. Thus it is important to investigate the critical value $S_c$ between the second- and first-order transitions, for understanding the quantum effect on the metamagnetism in 1D. In this paper, we study the magnetization process of the $S = 1$ and $\frac{1}{2}$ $XXZ$ spin chains, particularly on the possibility of the first-order spin flopping transition.

The magnetization process of the 1D $XXZ$ model is described by the Hamiltonian

$$\mathcal{H} = \mathcal{H}_0 + \mathcal{H}_Z,$$

$$\mathcal{H}_0 = \sum_j \gamma (S_j^z S_{j+1}^z + S_j^x S_{j+1}^x) + S_j^y S_{j+1}^y,$$

$$\mathcal{H}_Z = -H \sum_j S_j^z,$$

under the periodic boundary condition. We restrict us on the Ising-like anisotropy $0 < \gamma < 1$ to consider the metamagnetic transition from the Néel ordered ground state, induced by the external magnetic field along the easy axis of the sublattice magnetization. In the $S = \frac{1}{2}$ chain a second-order transition occurs at some critical field $H_c$ for $0 < \gamma < 1$. The asymptotic behavior has the form

$$m \sim (H - H_c)^{1/2}.$$

The magnetization curves in the thermodynamic limit for $\gamma = 0.3$ and 0.5 calculated by the Bethe ansatz are shown as solid lines in Fig. 1, where $H_s$ is the saturation field ($H_s = 2S(1 + \gamma)$). On the other hand, in the limit of $S \to \infty$ we know that the spin flop occurs at $H_c = H_s[(1 - \gamma)/(1 + \gamma)]^{1/2}$. This is the first-order transition and the magnetization jumps from 0 to $S[(1 - \gamma)/(1 + \gamma)]^{1/2}$, as shown in Fig. 1. In order to investigate the corresponding transition for finite $S$ larger than 1/2, we perform the exact diagonalization technique applied to the finite clusters with the system size $L$, because there is no exact solution available here. Using the Lanczos algorithm, we calculate the lowest eigenvalue of $\mathcal{H}_0$ in the subspace with $\sum_j S_j^z = M$ for the $L$-site system, defined as $E(L, M)$. To derive the magnetization curve, the magnetic field $H$ to bring about the magnetization $m = M/L$ and $m' = m + \frac{1}{2}$ is estimated by $[E(L, M+1) - E(L, M)]/2$ and $E(L, M+1) - E(L, M)$, respectively. To demonstrate the validity of the method, we show the results of the $S = \frac{1}{2}$ chain by the diagonalization for $L = 20$ and 24 as circles, together with the Bethe ansatz solution in Fig. 1. The bulk property is revealed to be well understood even in such small systems.

In the small magnetization limit in the Néel ordered phase, only the state with $M = 2Sn$ $(n = 0, 1, 2, \cdots)$
can contribute the ground-state magnetization process of the spin-$S$ chain. Because states where every site has $S^z_j = +S$ or $-S$ are stabilized better than other states. To explain the reason, we consider the $S = 1$ chain, for example. In the excited state produced by changing $S^z_j$ from $-1$ to 0 in the Néel state ($\cdots \downarrow \uparrow 0 \downarrow \cdots$), the motion of the object 0 to the adjacent site ($\cdots \downarrow \uparrow \uparrow 0 \downarrow \cdots$) will lead to some energy loss in the diagonal element of the exchange Hamiltonian, while it will gain some energy in the off-diagonal element. In contrast the object $\uparrow$ doped in the Néel order ($\cdots \downarrow \uparrow \uparrow \uparrow \uparrow \cdots$) can yield the energy gain due to the motion along the chain with no loss in the diagonal element ($\cdots \downarrow \uparrow \uparrow \uparrow \uparrow \cdots$). Thus smaller magnetic field can excite $\downarrow$ to $\uparrow$, rather than to 0. It implies that states with +1 or −1 at every site are more favorable than states including 0, and the magnetization process starting from the Néel phase consists of the states with $M = 2n$ in the small $m$ limit. The argument is also generalized for arbitrary $S$ and the state with $M = 2Sn$ is stabilized. Thus in the small magnetization region an oscillation with the period of $2S$ in the $M$ dependence of the energy of the spin-$S$ chain in the Ising phase. To avoid the oscillation, we will take only states with $M = 2Sn$ into account in the following analysis, except for the determination of the saturation field $H_s$.

In general, a first-order metamagnetic transition occurs, when the ground state energy per site $\epsilon(m)$ for the Hamiltonian $H_0$ (We choose the origin to set $\epsilon(0) = 0$ here.) has such $m$-dependence as shown in Fig. 3, where the region with $\epsilon''(m) < 0$ lies from the origin to some magnetization. We define $\epsilon_0(m)$ as the intersection of the vertical axis and the tangent line of the curve $\epsilon(m)$, as shown in Fig. 3. The magnetization jump $m_s$ is determined as the solution of $\epsilon_0(m) = 0$. It implies that the sign of $\epsilon_0(m)$ changes at $m_s$ and the magnetization with $\epsilon_0(m) > 0$ does not appear in the ground-state magnetization process. In order to examine the possibility of the magnetization jump in the spin-$S$ chains, we investigate the behavior of $\epsilon_0(m)$ based on the finite cluster calcula-
tion. We assume the size dependence of the ground state energy per site obeys the relation

$$e(L,M) \equiv \frac{1}{L}[E(L,M) - E(L,0)] \sim \epsilon(m) + O(\frac{1}{L^2}),$$

(3)

for $L \to \infty$ with fixed $m = M/L$. Although the relation is predicted by the conformal field theory [3] for massless state, the following argument will be valid even in massive cases, as far as the size correction does not exceed $O(\frac{1}{L^2})$. We also define $h(L,M)$ as

$$h(L,M) \equiv \frac{1}{2S}[E(L,M + 2S) - E(L,M - 2S)]$$

$$\sim \epsilon'(m) + O(\frac{1}{L^2}),$$

(4)

where the size dependence is derived from (3). The quantity $h(L,M)$ should converge to $H$ for $L \to \infty$ in the normal magnetization process. Since $\epsilon_0(m)$ is given by

$$\epsilon_0(m) = \epsilon(m) - \epsilon'(m)m,$$

it can be estimated by the form

$$\frac{1}{L}[e(L,M) - h(L,M)M] \sim \epsilon_0(m) + O(\frac{1}{L^2}).$$

(5)

Since various system sizes with fixed $m = M/L$ are available only for few values of $m$ because of the restriction $M = 2Sn$, we neglect the size correction in (3) in the following analysis. For $S = \frac{1}{2}$ the finite cluster calculation up to $L = 26$ indicates $\epsilon_0(m) < 0$ for $0 < m < 1$ in all the region $0 < \gamma < 1$. It means no first-order transition, which is consistent with the result from the Bethe ansatz. For $S = 1$, however, the calculation up to $L = 20$ detects the region with $\epsilon_0(m) > 0$, which suggests the first-order metamagnetic transition. When we vary $\gamma$ with fixed $M$, a point with $\epsilon_0(m) = 0$ can be found for small $m$. The points for various values of $M$ available for $L = 18$ and 20 are plotted on the $m/S - \gamma$ plane as circles in Fig. 4.

Since $\epsilon_0(m)$ is positive under the points, while negative over them in the plane, the points stand for the magnetization jump $m_s$ for corresponding $\gamma$. In the analysis of 20-site cluster, $\epsilon_0(m)$ is always positive for $M \geq 12$. Thus we think that $m = 0.6$ is an upper bound of $m_s$ in the limit $\gamma \to 0$ denoted as $m_{s,0}$, which is shown as X in Fig. 4. $m_{s,0}$ does not correspond to the value of the Ising model $m_s/S = 1$, which implies that there exists a spin reduction due to the quantum fluctuation, as was found in the 2D and 3D $S = \frac{1}{2}$ model [2]. On the other hand, the $S = 1\ XXZ$ chain has the Haldane phase [13], where the second-order transition described by (2) was revealed to occur in the magnetization process [2, 3], in the large $\gamma$ region. Consulting some previous works [3, 13], we put the boundary between the Haldane and Néel phases at $\gamma_c = 0.84$, as shown in Fig. 4.

In the present work, by the analysis of several excitation gaps corresponding to the soft modes of the Luttinger liquid, we checked that the magnetic state for $m_s < m < 1$ consists of a single gapless phase characterized by the dominant spin correlation function $\langle S_0^+ S_r^- \rangle \sim (-1)^r r^{-\gamma}$, in contrast to the magnetization process in the presence of the Ising-like single-ion anisotropy described by $D \sum_j \langle S_j^z \rangle^2$ ($D < 0$), where there appears another massless phase (solid lines) with $\langle S_0^z S_r^z \rangle \sim \cos(2kFr)x^{-\eta'}$. Thus the line of $m_s$ is expected to continue to the unique phase boundary $\gamma_c$ at $m = 0$. The solid line for $S = 1$ in Fig. 4 is the result from the polynomial fitting to the points with $\epsilon_0(m) = 0$ ($L = 18$ and 20) and the boundary $\gamma_c$, also adding $m_{s,0} = 0.6$ because the fitted line excluding it would exceed the upper bound. The points with $\epsilon_0(m) = 0$ for $S = \frac{1}{2}$ are also plotted as squares in Fig. 4, where we use the results of $L = 12$ and 14. Assuming the boundary of the Néel phase lies at $\gamma = 1$, the curve fitted to the points is shown as a solid line in Fig. 4. In this time $m_{s,0}$ is estimated from the fitted curve as $m_{s,0} = 0.70 \pm 0.04$, because it is smaller than the upper bound determined by $m$ for which $\epsilon_0(m)$ is always negative. The spin reduction in the limit $\gamma \to 0$ is smaller than that for $S = 1$. It is consistent with the reasonable assumption that the quantum fluctuation is smaller for larger $S$. The line of the magnetization jump in the classical limit $m_s/S = [(1 - \gamma)/(1 + \gamma)]^{1/2}$ is also plotted as a dashed curve in Fig. 4. These curves suggest that the magnetization jump increases with the spin value increasing from $S = 1$ towards the classical limit. Therefore we conclude that the 1D Ising-like XXZ model ($0 < \gamma < 1$) exhibits the first-order spin flopping transition for $S \geq 1$, except for the Haldane phase. It implies that the $S = \frac{1}{2}$ chain is an exceptional case where the metamagnetic transition from the Néel phase is second-order, that is, the critical spin value $S_c$ lies between $\frac{1}{2}$ and 1.

![Fig. 4. Magnetization jump $m_s/S$ for $S = 1$ and $\frac{1}{2}$ (solid lines) obtained by the polynomial fitting to the points with $\epsilon_0(0) = 0$ for the finite systems (symbols). For $S = 1$ $\gamma_c$ is the boundary between the Néel and Haldane phases, and $x$ is the upper bound of $m_{s,0}$. $m_s/S$ in the classical limit is a dashed line.](https://example.com/fig4.png)
In order to convince of the conclusion, we show the ground-state magnetization curves for $S = 1$ and $\frac{3}{2}$ based on the present finite cluster calculation. We plot $h(L,M)$ as the field $H$ for the magnetization $m = \frac{M}{L}$, and $h'(L,M) \equiv \frac{[E(L,M + 2S) - E(L,M)]/(2S)}{[E(L,M + S)/L - E(L,M)/L]}$ for $m = \frac{(M + S)}{L}$, using the value renormalized by the saturation field $H_s$. The results of the largest two system sizes for $S = 1$ and $\frac{3}{2}$ ($\gamma = 0.3$ and 0.5) are shown as symbols in Figs. 5 and 6, respectively. They all indicate the evidence of the first-order transition, in contrast to the $S = \frac{1}{2}$ in Fig. 1. We determine the magnetization jump $m_s$ from the fitted lines in Fig. 4, and put the fitted curves for $m_s < m$ in Figs. 5 and 6 to complete the magnetization curves. The behaviors of the symbols in Figs. 5 and 6 suggest that the size correction is so small that the magnetization curves given by the solid lines are expected to be of the bulk systems.

The present analysis indicated a numerical evidence of the first-order metamagnetic transition in the 1D XXZ model for $S \geq 1$, based on the finite-cluster calculation. In general the finite system has larger quantum fluctuation, which tends to suppress the magnetization jump, than the infinite system. Thus the present conclusion on the finite jump is expected to be valid even in the thermodynamic limit.

In summary, the exact diagonalization study on the finite cluster suggested that the 1D Ising-like antiferromagnetic XXZ model exhibits the first-order spin flipping transition with a finite magnetization jump for $S \geq 1$, except for the Haldane phase. It implies that only for $S = \frac{1}{2}$ the quantum fluctuation is extremely large and makes the corresponding transition second-order.

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