Magnetization plateau in $S = 3/2$ antiferromagnetic Heisenberg chain with anisotropy

Tōru Sakai$^1$ and Minoru Takahashi$^2$

$^1$Faculty of Science, Himeji Institute of Technology, Kamigori, Ako-gun, Hyogo 678-12, Japan
$^2$Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo 106, Japan

(October 97)

The magnetization process of the $S=3/2$ antiferromagnetic Heisenberg chain with the single-ion anisotropy $D$ at $T = 0$ is investigated by the exact diagonalization of finite clusters and finite-size scaling analyses. It is found that a magnetization plateau appears at $m = 1/2$ for $D > D_c = 0.93 \pm 0.01$. The phase transition with respect to $D$ at $D_c$ is revealed to be the Kosterlitz-Thouless-type. The magnetization curve of the infinite system is also presented for some values of $D$.

PACS Numbers: 75.10.Jm, 75.40.Cx, 75.45.+j

One-dimensional antiferromagnets have various quantum effects observed even in macroscopic measurements. The Haldane gap [3], which is the lowest excitation gap of the 1D Heisenberg antiferromagnets with integer $S$, was also detected as a transition from a non-magnetic state to magnetic one in high-field magnetization measurements of Ni(C$_2$H$_8$N$_2$)$_2$NO$_2$(ClO$_4$), abbreviated NENP, which is an $S=1$ quasi-1D antiferromagnet. Recently Okazaki, Yamanaka and Affleck [4] suggested that even for the 1D $S = 3/2$ (half-odd integer) antiferromagnet an energy gap is possibly induced by a magnetic field and a magnetization plateau appears at $m = 1/2$, which corresponds to 1/3 of the saturation moment. Their argument is based on the analogy to the quantum Hall effect and the valence bond solid picture for $S = 1$. The magnetization plateau is also predicted in some alternating spin chains [5], but the mechanism depends on the structure of the unit cell and the argument for them is not necessarily valid for uniform chains.

For the anisotropic $S = 3/2$ antiferromagnetic chain, a variational approach [6] gave the phase diagram of the nonmagnetic ground state, while few works were done on the magnetic state. However, it is easy to understand that it should have a magnetization plateau at least when the system has the positive and infinitely large single-ion anisotropy $D \sum_j (S_j^z)^2$. Because in the limit ($D \to \infty$) every site has $S_j^z = 1/2$ for the ground state at $m = 1/2$ and any magnetic excitations changing it into $S_j^z = 3/2$ at a site have a gap proportional to $D$. For finite $D$, however, there is no rigorous proof on the existence of the gap at $m = 1/2$, in contrast to the case of $m \neq 1/2$ in which the system is proved to be gapless by the Lieb-Schultz-Mattis theorem. Thus some numerical tests are important to check the existence of the gap and magnetization plateau at $m = 1/2$. The density matrix renormalization group approach [7] revealed that the isotropic $S = 3/2$ antiferromagnetic chain is gapless even at $m = 1/2$ and a critical value $D_c$ should exist as a boundary between the gapless and massive phases.

In this paper, using the exact diagonalization of finite clusters up to the system size $L = 14$ and finite-size scaling analyses, we investigate the $S = 3/2$ antiferromagnetic Heisenberg chain with the single-ion anisotropy and estimate the critical value $D_c$ at $m = 1/2$ and determine the universality class of the phase transition with respect to $D$. In addition we present the ground-state magnetization curve extrapolated to the thermodynamic limit for some typical values of $D$.

Consider the 1D $S = 3/2$ antiferromagnetic Heisenberg Hamiltonian with the single-ion anisotropy in a magnetic field

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

$$\mathcal{H}_0 = \sum_j S_j \cdot S_{j+1} + D \sum_j (S_j^z)^2,$$

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

under the periodic boundary condition. For $L$-site systems, the lowest energy of $\mathcal{H}_0$ in the subspace where $\sum_j S_j^z = M$ (the macroscopic magnetization is $m = M/L$) is denoted as $E(L, M)$. Using Lanczos’ algorithm, we calculated $E(L, M)$ ($M = 0, 1, 2, \cdots, 3L/2$) for even-site systems up to $L = 14$. For finite systems described by the total Hamiltonian $\mathcal{H}$, the energy gap of the magnetic excitation changing the value of $M$ by $\pm 1$ is given by

$$\Delta_{\pm} \equiv E(L, M \pm 1) - E(L, M) \mp H.$$

If the system is gapless in the thermodynamic limit, the conformal field theory (CFT) gives the asymptotic form of the size dependence of the gap as $\Delta_{\pm} \sim O(1/L)$ with fixed $m = M/L$. If we define $H_+$ and $H_-$ as

$$E(L, M + 1) - E(L, M) \to H_+ \quad (L \to \infty),$$
$$E(L, M) - E(L, M - 1) \to H_- \quad (L \to \infty),$$

$H_+$ and $H_-$ has the same value and it gives the magnetic field $H$ for the magnetization $m$ in the thermodynamic limit. On the other hand, if the system has a finite gap
even in the limit, neither $\Delta_+$ nor $\Delta_-$ vanishes for $L \to \infty$. It implies that $H_+$ and $H_-$ are different. As a result, a plateau appears for $H_- < H < H_+$ at $m = M/L$ in the ground-state magnetization curve.

Since $\Delta_{\pm}$ includes an undecided parameter $H$ in the form \( \delta \), we take the sum $\Delta = \Delta_+ + \Delta_-$ for the order parameter of the finite-size scaling, to test the existence of the plateau at $m = 1/2$. (In the massive case, the gap $\Delta$ leads to the length of the plateau in the magnetization curve in the thermodynamic limit.) The scaled gap $L\Delta$ of finite systems ($L = 6 \sim 14$) at $m = 1/2$ is plotted versus $D$ in Fig. 1 For $D > 2$ the scaled gap obviously increases with increasing $L$, which means that a finite gap exists in the thermodynamic limit. For small $D$ around the region $0 < D < 1$, the scaled gap looks almost independent of $L$. It implies that the system is gapless at a finite region. At least the form $\Delta \sim 1/L$ is valid for $0 \leq D \leq 0.8$ with the relative error less than 0.3% for each point. Our precise analysis, however, indicates that the $L\Delta$ curves for $L$, and $L+2$ have only one intersection in the region $0 < D < 2$ for each $L$. Thus the critical point $D_c$ can be estimated by the phenomenological renormalization group equation \( \Phi \)

$$
(L + 2)\Delta_{L+2}(D') = L\Delta_L(D).
$$

We define $D_{cL,L+2}$ as the $L$-dependent fixed point of \( \Phi \) and it is extrapolated to the thermodynamic limit. Fitting the form $D_{cL,L+2} \sim 1/(L+1)$ to the data, the extrapolated value is determined as $D_c = 0.93 \pm 0.01$, based on the standard least square method. Thus for $0 \leq D < 0.93$ the system is gapless in all the region of $0 \leq m < 3/2$, while for $D > 0.93$ the energy gap is induced just at $m = 1/2$ and the magnetization curve has a plateau.

FIG. 1. Scaled gap $L\Delta$ versus the single-ion anisotropy $D$.

FIG. 2. $L$-dependent fixed point $D_{cL,L+2}$ is plotted versus $1/L$ to determine $D_c$ in the thermodynamic limit. The estimated value is $D_c = 0.93 \pm 0.01$.

The phenomenological renormalization group can also estimate the exponent $\nu$ defined as $\Delta \sim (D - D_c)^\nu$, using the $L$-dependent form

$$
\nu_{L,L+2} = \log \left[ \frac{L + 2}{L} \right] / \log \left[ \frac{(L + 2)\Delta'_{L+2}(D_{cL,L+2})}{L\Delta_L(D_{cL,L+2})} \right],
$$

where $\Delta'_{L}(D)$ is the derivative of $\Delta_L(D)$ with respect to $D$. The result showed a diverging behavior of $\nu_{L,L+2}$ with increasing $L$. It implies that $\Delta$ does not have any algebraic form near $D_c$. Thus the phase transition is expected to be the Kosterlitz-Thouless(KT)-type \( \Phi \), which is also consistent with the existence of a finite gapless region under $D_c$. In addition a naive argument restricting us to three states $S^z = 3/2, 1/2$ and $-1/2$ (neglecting the state $S^z = -3/2$ because of a large magnetic field) at each site, leads to a mapping the Hamiltonian \( \Phi \) to a generalized anisotropic $S = 1$ model without magnetic field, which has the KT phase boundary between the large-$D$ (singlet) and $XY$ (planar) phases \( \Phi \).

To determine the universality of the phase boundary $D_c$ at $m = 1/2$, we estimate the central charge $c$ in the CFT and the critical exponent $\eta$ defined as $\langle S^z S^z \rangle \sim (-1)^{r-x} \eta$ for $D \leq D_c$. The CFT \( \Phi \) predicts the asymptotic form of the ground state energy per site as

$$
\frac{1}{L}E(L,M) \sim \epsilon(m) - \frac{\pi}{6} v_s \frac{1}{L^2} \quad (L \to \infty),
$$

where $v_s$ is the sound velocity which is the gradient of the dispersion curve at the origin. Thus the central charge $c$ can be numerically determined by estimating the gradient of the plots of $E(L,M)/L$ versus $1/L^2$ and $v_s$. $v_s$ is estimated by the form \( \Phi \)

$$
v_s = \frac{L}{2\pi} (E_{k_1}(L,M) - E(L,M)) + O(\frac{1}{L^2}),
$$

where $k_1 = 2\pi/L$ is the smallest nonzero wave vector for $L$ and $E_{k_1}(L,M)$ is the lowest level in the subspace.
specified by \( M \) and \( k_1 \). The calculated \( c \) for \( D \leq D_c \) at \( m = 1/2 \) is shown in Fig. 3. At the boundary \( D_c (= 0.93) \) our estimation gives \( c = 1.03 \pm 0.06 \) and other points also have comparable errors. Thus we reasonably conclude \( c = 1 \) for \( D \leq D_c \).

Using another prediction of the CFT \( \Delta_{±} \sim \pi v_{±} \eta/L \) (\( L \to \infty \)), the exponent \( \eta \) can be estimated by the form (11)
\[
\eta = \frac{E(L, M + 1) + E(L, M - 1) - 2E(L, M)}{E_k(L, M) - E(L, M)} + O\left(\frac{1}{L^2}\right).
\] (8)

The calculated \( \eta \) is shown in Fig. 3. Our estimation \( \eta = 0.26 \pm 0.01 \) at \( D = 0.93 \) suggests \( \eta = 1/4 \) just at the phase boundary. In addition the estimated \( \eta \) gradually decreases with decreasing \( D \). Thus the analysis on \( \eta \) also supports the KT transition.

The critical behavior for \( D > D_c \) can be tested by the Roemann-Wyld approximation for the Callen-Symanzik \( \beta \)-function (12)
\[
\beta_{\Delta L+2}(D) = \frac{1 + \log \left( \frac{\Delta_{L+2}(D)}{\Delta_{L}(D)} \right)}{\log \left( \frac{L+2}{L+1} \right)}.
\] (9)

When the gap behaves like \( \Delta \sim \exp(-a/(D - D_c)\sigma) \), the function (10) has the form
\[
\beta_{\Delta L+2}(D) \sim (D - D_{cL+2})^{1+\sigma} \quad (L \to \infty),
\] (10)
in the thermodynamic limit. Fitting the form (10) to the calculated function (12) for each \( L \), \( \sigma \) is estimated as follows: \( \sigma_{8,10} = 0.46 \pm 0.06 \), \( \sigma_{10,12} = 0.52 \pm 0.05 \) and \( \sigma_{12,14} = 0.56 \pm 0.06 \). The results are also consistent with the standard KT transition (\( \sigma = 1/2 \)). Therefore we conclude the critical behavior near \( D_c \) for \( m = 1/2 \) is characterized by the universality class of the KT transition.

Finally using the method in Ref. 3, we present the ground-state magnetization curve in the thermodynamic limit for several values of \( D; D = 0, 1, 2, 3 \). For \( D = 0 \) the system is isotropic and gapless for \( 0 \leq m < 3/2 \). For other cases, it has the gap at \( m = 1/2 \) and the magnetization plateau appears.

\[ E(L, M + 1) - E(L, M) \quad \text{and} \quad E(L, M) - E(L, M - 1) \]
plotted versus \( 1/L \) with fixed \( m \) for \( D = 3 \). The dashed curves are guides to the eye. The extrapolated points for \( m = 1/2 \) and \( m = 1/2+ \) corresponds to the results of the Shank’s transformation \( H_+ = 4.17 \) and \( H_- = 5.19 \), respectively.

Since the system is gapless except for \( m = 1/2 \), \( H_+ \) and \( H_- \) of (10) correspond to each other and the common value gives the magnetic field \( H \) for given \( m \). Using the extrapolation form
\[
E(L, M + 1) - E(L, M) \sim H + O(1/L)
\]
\[
E(L, M) - E(L, M - 1) \sim H + O(1/L)
\] (11)
with fixed \( m \). For \( D = 3.0 \) the left hand sides of the form (11) calculated for \( m = 0.1/4, 1/2, 3/4, 1 \) and \( 5/4 \) are plotted versus \( 1/L \) in Fig. 4. It shows that the form (11) is valid except for \( m = 1/2 \) and the two extrapolated values of \( H \) (the one is extrapolated from \( E(L, M + 1) - E(L, M) \) and the other is from \( E(L, M) - E(L, M - 1) \)) correspond to each other well. Thus we take the mean value of the two for the magnetic field for each \( m \). Only for \( m = 1/2 \), \( H_+ \) and \( H_- \) are obviously different and the size correction decays faster than \( 1/L \), as shown in Fig. 4, because the system has a gap. Then we estimate \( H_+ \) and \( H_- \) by the Shank’s transformation (12) \( P_n = (P_{n-1}P_{n+1} - P_n^2)/(P_{n-1} + P_{n+1} - 2P_n) \) for a sequence \( \{P_n\} \). Applying it twice to \( E(L, M + 1) - E(L, M) \) and \( E(L, M) - E(L, M - 1) \) respectively, for \( L = 6, 8, 10, 12 \) and \( 14 \), results in \( H_+ = 5.19 \pm 0.07 \) and \( H_- = 4.17 \pm 0.07 \), which are indicated as the extrapolated points in
The extrapolated value $H$ for other values of $D$ can be estimated in the same way. Only for $D = 0$ $H_+$ and $H_-$ correspond even at $m = 1/2$. The ground-state magnetization curve in the thermodynamic limit is given by all the extrapolated values of $H$ for each $m$. We present the results for $D = 0, 1, 2$ and 3 in Fig. 5, where we also used the values of $H$ for $m = 1/3, 2/3, 5/6, 7/6$ and $4/3$ which are estimated by the same method as mentioned above. The curve has a plateau at $m = 1/2$ ($H_- < H < H_+$) for $D = 1, 2$ and $3$, in contrast to the case of $D = 0$ which does not have any nontrivial behaviors.

Among those curves in Fig. 5 $D = 1$ is the most important in terms of experiments to detect the plateau, because $D \sim J$ might be realized in some real materials. The candidates of the quasi-1D $S = 3/2$ antiferromagnet are CsVCl$_3$ and AgCrP$_2$S$_6$. In particular for AgCrP$_2$S$_6$ a large anisotropic effect was observed in the magnetization measurement in low fields. Higher-field measurements of those materials would be interesting.

In summary the finite cluster calculation and size scaling study showed that the anisotropic $S = 3/2$ has the magnetization plateau at $m = 1/2$ for $D > D_c = 0.93$ and the phase transition with respect to $D$ belongs to the same universality class as the Kosterlitz-Thouless transition.

We wish to thank Dr. M. Yamanaka and Prof. K. Nomura for fruitful discussions. We also thank the Supercomputer Center, Institute for Solid State Physics, University of Tokyo for the facilities and the use of the Fujitsu VPP500. This research was supported in part by Grant-in-Aid for the Scientific Research Fund from the Ministry of Education, Science, Sports and Culture (08640445).