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Magnetization plateau in an $S=\frac{3}{2}$ antiferromagnetic Heisenberg chain with anisotropy

Tôru Sakai
Faculty of Science, Himeji Institute of Technology, Kamigori, Ako-gun, Hyogo 678-12, Japan

Minoru Takahashi
Institute for Solid State Physics, University of Tokyo, Roppongi, Minato-ku, Tokyo 106, Japan

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The magnetization process of the $S=\frac{3}{2}$ antiferromagnetic Heisenberg chain with 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 $m=\frac{1}{2}$ for $D>D_c=0.93\pm0.01$. The phase transition with respect to D at D_c is revealed to be of the Kosterlitz-Thouless type. The magnetization curve of the infinite system is also presented for some values of D. [S0163-1829(98)51206-4]

One-dimensional (1D) antiferromagnets have various quantum effects observed even in macroscopic measurements. The Haldane gap,[1] which is the lowest excitation gap of the 1D Heisenberg antiferromagnets with integer S, was also detected as a transition from a nonmagnetic state to a magnetic one in high-field magnetization measurements of $Ni(C_2H_8N_2)_2NO_2(ClO_4)$, abbreviated NENP, which is an $S=1$ quasi-1D antiferromagnet.[2,3] Recently Oshikawa, Yamanaka, and Affleck[4] suggested that even for the 1D $S=\frac{3}{2}$ (half-odd integer) antiferromagnet an energy gap is possibly induced by a magnetic field and a magnetization plateau appears at $m=\frac{1}{2}$, which corresponds to $\frac{1}{3}$ of the saturation moment. Their argument is based on the analogy to the quantum Hall effect and the valence bond solid picture for $S=1$.[5] The magnetization plateau is also predicted in some alternating spin chains[6,7], 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 $S=\frac{3}{2}$ antiferromagnetic chain, a variational approach[8] 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 $D\Sigma_j(S_j^z)^2$. Because in the limit $(D\to\infty)$ every site has $S_j^z=\frac{1}{2}$ for the ground state at $m=\frac{1}{2}$ and any magnetic excitations changing it into $S_j^z=\frac{3}{2}$ 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 $m=\frac{1}{2}$, in contrast to the case of $m\neq\frac{1}{2}$, in which the system is proved to be gapless by the Lieb-Schultz-Mattis theorem.[4,9] Thus some numerical tests are important to check the existence of the gap and magnetization plateau at $m=\frac{1}{2}$. The density matrix renormalization group approach[4] revealed that the isotropic $S=\frac{3}{2}$ antiferromagnetic chain is gapless even at $m=\frac{1}{2}$ 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 $m=\frac{1}{2}$ 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 $S=\frac{3}{2}$ antiferromagnetic Heisenberg Hamiltonian with the single-ion anisotropy in a magnetic field

$$\mathcal{H}=\mathcal{H}_0+\mathcal{H}_Z,$$
$$\mathcal{H}_0=\sum_j \mathbf{S}_j\cdot\mathbf{S}_{j+1}+D\sum_j (S_j^z)^2, \tag{1}$$
$$\mathcal{H}_Z=-H\sum_j S_j^z,$$

under the periodic boundary condition. For L-site systems, the lowest energy of $\mathcal{H}_0$ in the subspace where $\Sigma_j S_j^z=M$ (the macroscopic magnetization is $m=M/L$) is denoted as $E(L,M)$. Using Lanczos' algorithm, we calculated $E(L,M)$ $(M=0,1,2,\ldots,3L/2)$ 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 ±1 is given by

$$\Delta_\pm\equiv E(L,M\pm1)-E(L,M)\mp H. \tag{2}$$

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

$$E(L,M+1)-E(L,M)\to H_+\quad(L\to\infty),$$
$$E(L,M)-E(L,M-1)\to H_-\quad(L\to\infty), \tag{3}$$

H_+ and H_- have 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 Δ_+ nor Δ_- 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.

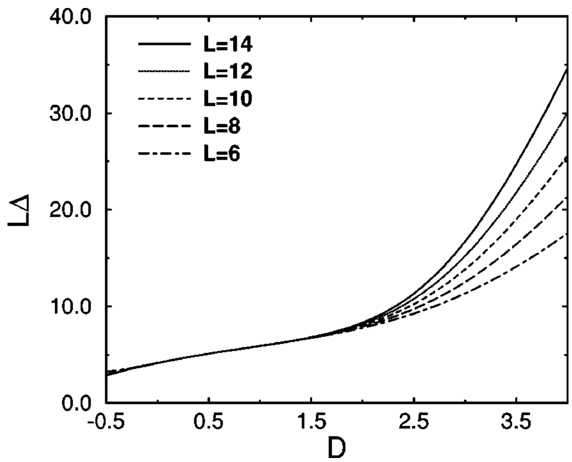

FIG. 1. Scaled gap $L\Delta$ versus the single-ion anisotropy D.

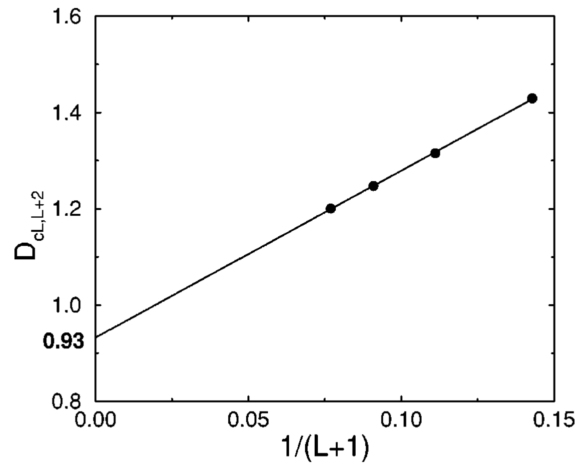

FIG. 2. L-dependent fixed point $D_{cL,L+2}$ is plotted versus $1/L$ to determine D_c in the thermodynamic limit. The estimated value is $D_c=0.93\pm0.01$.

Since $\Delta_\pm$ includes an undecided parameter H in the form (2), we take the sum $\Delta\equiv\Delta_+ +\Delta_-$ for the order parameter of the finite-size scaling, to test the existence of the plateau at $m=\frac{1}{2}$. (In the massive case, the gap Δ leads to the length of the plateau in the magnetization curve in the thermodynamic limit.) The scaled gap $L\Delta$ of finite systems ($L=6\sim14$) at $m=\frac{1}{2}$ 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 $\Delta\sim1/L$ is valid for $0\leqslant D\leqslant0.8$ 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[10]

$$(L+2)\Delta_{L+2}(D')=L\Delta_L(D). \tag{4}$$

We define $D_{cL,L+2}$ as the L-dependent fixed point of Eq. (4) and it is extrapolated to the thermodynamic limit. Fitting the form $D_{cL,L+2}\sim1/(L+1)$ to the data, the extrapolated value is determined as $D_c=0.93\pm0.01$, based on the standard least-square method. Thus for $0\leqslant D<0.93$ the system is gapless in all the region of $0\leqslant m<\frac{3}{2}$, while for $D>0.93$ the energy gap is induced just at $m=\frac{1}{2}$ and the magnetization curve has a plateau.

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

$$\nu_{L,L+2}=\ln\left[\frac{L+2}{L}\right]\bigg/\ln\left[\frac{(L+2)\Delta'_{L+2}(D_{cL,L+2})}{L\Delta'_L(D_{cL,L+2})}\right], \tag{5}$$

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 Δ does not have any algebraic form near D_c. Thus the phase transition is expected to be the Kosterlitz-Thouless (KT) type,[11] 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 $S^z=\frac{3}{2}$, $\frac{1}{2}$, and $-\frac{1}{2}$ (neglecting the state $S^z=-\frac{3}{2}$ because of a large magnetic field) at each site leads to a mapping of the Hamiltonian (1) 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.[8,12]

To determine the universality of the phase boundary D_c at $m=\frac{1}{2}$, we estimate the central charge c in the CFT and the critical exponent η defined as $\langle S_0^+S_r^-\rangle\sim(-1)^r r^{-\eta}$ for $D\leqslant D_c$. The CFT[13] predicts the asymptotic form of the ground state energy per site as

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

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[14]

$$v_s=\frac{L}{2\pi}[E_{k_1}(L,M)-E(L,M)]+O\left(\frac{1}{L^2}\right), \tag{7}$$

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 $D\leqslant D_c$ at $m=\frac{1}{2}$ is shown in Fig. 3. At the boundary $D_c(=0.93)$ our estimation gives $c=1.03\pm0.06$ and other points also have comparable errors. Thus we reasonably conclude $c=1$ for $D\leqslant D_c$.

Using another prediction of the CFT $\Delta_\pm\sim\pi v_s\eta/L$ $(L\to\infty)$, the exponent η can be estimated by the form[14]

$$\eta=\frac{E(L,M+1)+E(L,M-1)-2E(L,M)}{E_{k_1}(L,M)-E(L,M)}+O\left(\frac{1}{L^2}\right). \tag{8}$$

The calculated η is shown in Fig. 3. Our estimation $\eta=0.26\pm0.01$ at $D=0.93$ suggests $\eta=\frac{1}{4}$ just at the phase boundary. In addition the estimated η gradually decreases with decreasing D. Thus the analysis on η also supports the KT transition.

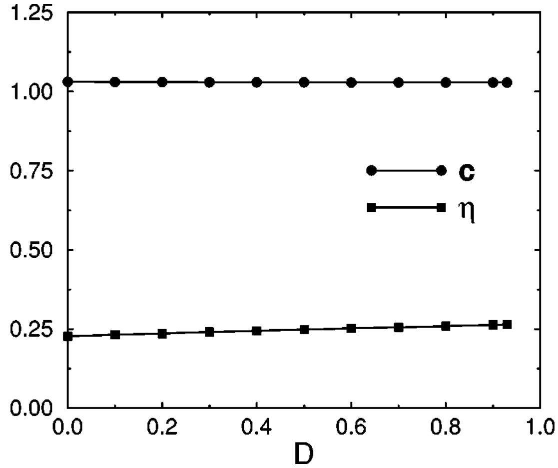

FIG. 3. Estimated central charge c and exponent η for $D \leqslant D_c$. At $D=D_c$ ($=0.93$) our estimation gives $c=1.03\pm0.06$ and $\eta=0.26\pm0.01$. We conclude $c=1$ for $D\leqslant D_c$ and $\eta=1/4$ at $D=D_c$.

The critical behavior for $D>D_c$ can be tested by the Roomany-Wyld approximation for the Callen-Symanzik β function[15]

$$\beta_{L,L+2}(D)=\frac{1+\ln\left(\frac{\Delta_{L+2}(D)}{\Delta_L(D)}\right)\Big/\ln\left(\frac{L+2}{L}\right)}{\left[\frac{\Delta_L'(D)\Delta_{L+2}'(D)}{\Delta_L(D)\Delta_{L+2}(D)}\right]^{1/2}}. \tag{9}$$

When the gap behaves like $\Delta\sim\exp(-a/(D-D_c)^\sigma)$, the function (9) has the form

$$\beta_{L,L+2}(D)\sim(D-D_{cL,L+2})^{1+\sigma}\quad(L\to\infty), \tag{10}$$

in the thermodynamic limit. Fitting the form (10) to the calculated function (9) for each L, σ is estimated as follows: $\sigma_{8,10}=0.46\pm0.06$, $\sigma_{10,12}=0.52\pm0.05$, and $\sigma_{12,14}=0.56\pm0.06$. The results are also consistent with the standard KT transition ($\sigma=\frac{1}{2}$). Therefore we conclude the critical behavior near D_c for $m=\frac{1}{2}$ is characterized by the universality class of the KT transition.

Finally, using the method in Refs. 7 and 16, we present the ground-state magnetization curve in the thermodynamic limit for several values of D; $D=0$, 1, 2, and 3. For $D=0$ the system is isotropic and gapless for $0\geqslant m<\frac{3}{2}$. For other cases, it has the gap at $m=\frac{1}{2}$ and the magnetization plateau appears.

Since the system is gapless except for $m=\frac{1}{2}$, H_+ and H_- of (3) correspond to each other and the common value gives the magnetic field H for given m in the thermodynamic limit. The size correction of (3) is predicted to decay as $\sim O(1/L)$, by the CFT. Thus we can estimate H for given m, using the extrapolation form

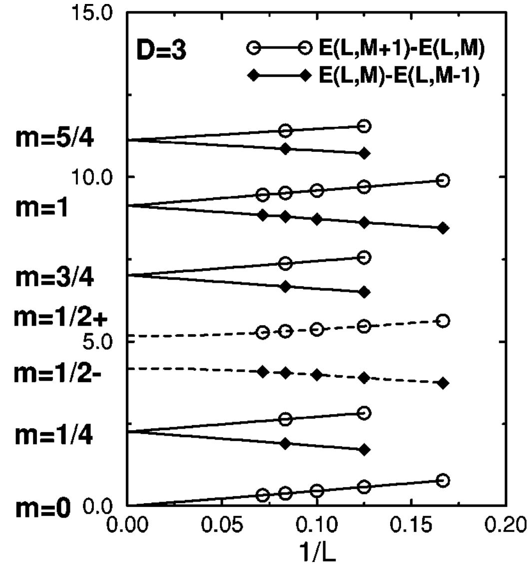

FIG. 4. $E(L,M+1)-E(L,M)$ and $E(L,M)-E(L,M-1)$ plotted versus $1/L$ with fixed m for $D=3$. The dashed curves are guides to the eye. The extrapolated points for $m=1/2-$ and $m=1/2+$ corresponds to the results of the Shanks transformation $H_-=4.17$ and $H_+=5.19$, respectively.

$$E(L,M+1)-E(L,M)\sim H+O(1/L)$$

$$E(L,M)-E(L,M-1)\sim H+O(1/L) \tag{11}$$

with fixed m. For $D=3.0$ the left hand sides of the form (11) calculated for $m=0$, $\frac{1}{4}$, $\frac{1}{2}$, $\frac{3}{4}$, $\frac{1}{2}$ and $\frac{5}{4}$ are plotted versus $1/L$ in Fig. 4. It shows that the form (11) is valid except for $m=\frac{1}{2}$ 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 $m=\frac{1}{2}$ are H_+ and H_- 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 Shanks transformation[17] $P_n'=(P_{n-1}P_{n+1}-P_n^2)/(P_{n-1}+P_{n+1}-2P_n)$ for a sequence $\{P_n\}$. Applying it twice to $E(L,M+1)-E(L,M)$ and

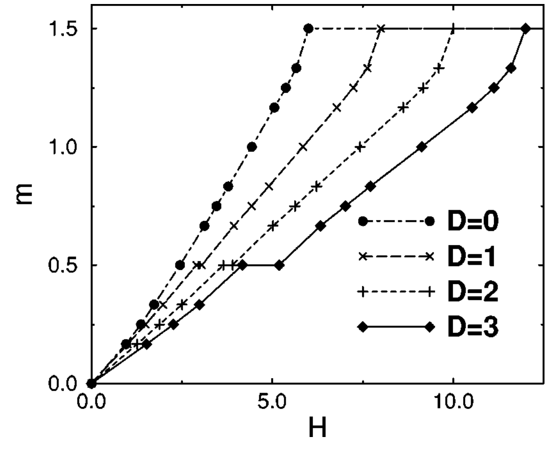

FIG. 5. Ground-state magnetization curves in the thermodynamic limit for $D=0$, 1, 2, and 3.

$E(L,M)-E(L,M-1)$, respectively, for $L=6$, 8, 10, 12, and 14, results in $H_+=5.19\pm0.07$ and $H_-=4.17\pm0.07$, which are indicated as the extrapolated points in Fig. 4. The extrapolated value H for other values of D can be estimated in the same way. Only for $D=0d_0$, H_+ and H_- correspond even at $m=\frac{1}{2}$. 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 $m=\frac{1}{3}$, $\frac{2}{3}$, $\frac{5}{6}$, $\frac{7}{6}$, and $\frac{4}{3}$ which are estimated by the same method as mentioned above. The curve has a plateau at $m=\frac{1}{2}$ $(H_-<H<H_+)$ 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 $S=\frac{3}{2}$ antiferromagnet are $CsVCl_3$ (Ref. 18) and $AgCrP_2S_6$.[19] In particular for $AgCrP_2S_6$ a large anisotropic effect was observed in the magnetization measurement in low fields. Higher-field measurements of those materials would be interesting. Note that for $D>D_c$ the ground state is gapless for $H\leqslant H_-$ and $H\geqslant H_+$, while massive for $H_-<H<_+$. In the quasi-1D systems, some canted Néel orders occur in the 1D gapless phase, due to interchain interactions. Thus a reentrant transition might be observed in the magnetization measurement; with increasing H the Néel order disappears at H_- and appears again at H_+ at sufficiently low temperatures.

In summary the finite cluster calculation and size scaling study showed that the anisotropic $S=\frac{3}{2}$ has the magnetization plateau at $m=\frac{1}{2}$ 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.

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