Magnetization-plateau state of the $S = 3/2$ spin chain with single ion anisotropy

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I. INTRODUCTION

Recently there has been a considerable interest in the magnetization process of one-dimensional quantum spin systems. Extending the Lieb-Schultz-Mattis theorem, et al. gave a necessary condition for the appearance of the magnetization plateau as $p(S - \langle m \rangle) = \text{integer}$, where $S$ is the magnitude of the spin, $p$ is the periodicity of the magnetic ground state in the thermodynamic limit, and $\langle m \rangle$ is the magnetization per site.

As a simple case, the $S = 3/2$ spin chain with single ion anisotropy in a magnetic field $H$,

$$H = \sum_{j=1}^{L} S_j \cdot S_{j+1} + D \sum_{j=1}^{L} (S_j^z)^2 - hM$$

(1)

has been studied. Here $S_j$ is the $S = 3/2$ spin at the $j$-th site, and $M$ is the magnetization $M = \sum S_j^z$. Hereafter, we define the saturation magnetization as $M_S = 3L/2$.

In this model, a magnetization plateau can appear at $M = M_S/3$ ($p = 1$). For $D = 0$ ($S = 3/2$ Heisenberg model), a magnetization plateau does not appear.

On the other hand for large $D$, the spin of each site tend to have $S^z = 1/2$ for $M = M_S/3$, and a magnetization plateau appears. Oshikawa et al. checked that a magnetization plateau appears for $D = 2$. Sakai and Takahashi studied the model with the numerical diagonalization calculation using the phenomenological renormalization group (PRG) analysis, and found that the transition point is $D_c = 0.93 \pm 0.01$. They concluded this point to be the Berezinskii-Kosterlitz-Thouless (BKT) transition point, that is, the plateau and the no-plateau transition point. Although the PRG analysis is a powerful method to study the second order phase transition, this is not sufficient for the BKT transition because of the singular behavior of the energy gap and of the logarithmic size dependence of excitation energies. Thus we think that it is worthwhile to reexamine this problem by use of another numerical approach.

The organization of this paper is as follows. In the next section, we consider an effective continuum model in order to investigate the mechanism of the appearance of the $M = M_S/3$ magnetization. In section 3, we show the numerical method and the results with the numerical diagonalization data. To study the system, we firstly consider the finite-size behavior with conformal field theory and the renormalization group analysis. Next, using them, we determine the boundary of the plateau and the no-plateau regions, and also check the critical behavior. Last section is devoted to summary and discussion.

II. EFFECTIVE CONTINUUM MODEL

For the magnetization $M = M_S/3$, the effective continuum model describing the low energy physics is given by

$$H_{\text{eff}} = \int \frac{dx}{2\pi} \left[ v_S K \frac{d\phi}{dx} \right]^2 + v_S \frac{d\phi}{dx} \int \frac{dx}{2\pi} \cos \sqrt{2} \phi,$$

(2)

where $\phi$ is the momentum density conjugate to $\phi$, $[\phi(x), \Pi(x')] = i \delta(x - x')$, $v_S$ is the sound velocity of the system. The dual field $\theta$ is defined as $\partial_x \theta = \pi \Pi$. The correlation exponents of several operators are governed by the coupling $K$ and the scaling dimension of the operator $\sqrt{2} \cos \sqrt{2} \phi$ is $x = K/2$. Thus the second term in the Hamiltonian is relevant for $K < 4$ and irrelevant for $K > 4$.

The one-loop renormalization group equations of this model are given by

$$dK(L)^{-1} d\ln L = \frac{1}{8} y_{\phi}^2(L), \quad dy_{\phi}(L) d\ln L = \left( 2 - \frac{K(L)}{2} \right) y_{\phi}(L),$$

where $L$ is an infrared cutoff. These are the recursion relations of Kosterlitz. The renormalization group flow is shown in Figure 1. In the region A, the coupling $K$ renormalized to a finite value and $y_{\phi}$ to zero; the system

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is critical and this corresponds to the no-plateau region in the spin system. In the regions B and B', $K$ renormalized to 0 and $|y_0|$ to $\infty$; these regions are massive phases and the field $\phi$ is locked to $\pi$ and 0 for B and B' respectively. There is a separatrix $32K^{-1} - 8 \ln K^{-1} - y_0^2 = 8 + 8 \ln 4$ which separates the infrared stable region (A) from the infrared unstable regions (B and B'). On this separatrix the BKT transition takes place. Near $(K, y_0) = (4, 0)$, and with the notation $K = 4 (1 + y_0/2)$, the BKT transition point is on the line $|y_0| = y_0$ and we obtain

$$y_0(L) = \frac{y_0}{y_0 \ln (L/L_0) + 1}. \tag{3}$$

where $y_0$ and $L_0$ are the bare values.

According to the numerical calculation by Oshikawa et al. for the $S = 3/2$ Heisenberg chain $(D = 0)$ at the magnetization $M = M_S/3$, this Gaussian coupling $K$ is $K \approx 4.4$, (in the notation of ref.11 the compactification radius is given by $R = (2\pi K)^{-1/2} = 0.95/\sqrt{8\pi}$), and the system is gapless (no plateau). This value is slightly larger than the BKT critical (fixed point) coupling $K = 4$.

### III. NUMERICAL APPROACH AND RESULTS

#### A. Finite size behavior

In order to study numerically, let us consider the finite-size behavior of the effective model (2) based on the conformal invariance.1 The scaling dimension of the primary field $\phi$ is given by $\Delta = \frac{\Delta}{2} e^{-2\phi}$, which is locked to $\pi$ and 0 for B and B'. According to the conformal field theory, the state of the finite-size system have a correspondence to the operator in the infinite-size system, and the excitation energy of the finite-size system is given by

$$\Delta E_{m,n}(L) = E_{m,n}(L) - E_g(L) = \frac{2\pi v_S}{L} x_{m,n}, \tag{5}$$

where $E_g(L)$ is the ground state energy of $L$-site with PBC.

The BKT transition takes place between the gapless and gapful regions, and the PRG analysis is affected by several irrelevant corrections sensitively. Moreover, on the transition point, there exists a logarithmic size correction in the excitation energy. PRG analysis does not suppose these features. In order to determine the BKT transition point, we apply the method proposed by Nomura and Kitazawa (see also ref.11 and 12), which is free from the logarithmic size correction. If we can have the half-integer for the “magnetic” charge $m$, which is not permitted for PBC by the translational symmetry, we have the following finite size spectrum for $m = \pm 1/2$,

$$x_{\pm 1/2,0}^c(L) = \frac{L}{2\pi v_S} \Delta E_{\pm 1/2,0}^c(L) = \frac{K(L)}{8} + \frac{1}{y_0(L)}, \tag{6}$$

$$x_{\pm 1/2,0}^s(L) = \frac{L}{2\pi v_S} \Delta E_{\pm 1/2,0}^s(L) = \frac{K(L)}{8} - \frac{1}{y_0(L)}, \tag{6}$$

where the energies $\Delta E_{\pm 1/2,0}^c(L)$ correspond to the operators $\sqrt{2} \cos \phi/\sqrt{2}$ and $\sqrt{2} \sin \phi/\sqrt{2}$ respectively. The term with $y_0$ comes from the first order perturbation and from the operator product expansions.13

$$\sqrt{2} \cos \sqrt{2} \phi \left( \sqrt{2} \cos \frac{1}{\sqrt{2}} \phi \right) \sim \sqrt{2} \cos \frac{1}{\sqrt{2}} \phi,$$

$$\sqrt{2} \cos \sqrt{2} \phi \left( \sqrt{2} \sin \frac{1}{\sqrt{2}} \phi \right) \sim \sqrt{2} \sin \frac{1}{\sqrt{2}} \phi.$$

Near the BKT transition point $|y_0| = y_0 (K = 4 (1 + y_0/2))$, defining $y_0 = \pm y_0 (1 + t)$ where $t$ measures the distance from the transition point, we have for $y_0 > 0$

$$x_{\pm 1/2,0}^c(L) = \frac{1}{2} + \frac{3}{4} y_0(L) \left( 1 + \frac{2}{3} t \right),$$

$$x_{\pm 1/2,0}^s(L) = \frac{1}{2} - \frac{1}{4} y_0(L) (1 + 2t), \tag{7}$$

and for $y_0 < 0$,

$$x_{\pm 1/2,0}^c(L) = \frac{1}{2} - \frac{1}{4} y_0(L) (1 + 2t),$$

$$x_{\pm 1/2,0}^s(L) = \frac{1}{2} + \frac{3}{4} y_0(L) \left( 1 + \frac{2}{3} t \right). \tag{8}$$

On the other hand, for $(m, n) = (0, \pm 2)$ we have

$$x_{0,\pm 2}^E(L) \equiv \frac{L}{2\pi v_S} \Delta E_{0,\pm 2}(L) = \frac{2}{K} = \frac{1}{2} - \frac{1}{4} y_0(L). \tag{9}$$

From eqs. (3), (8) and (9), energy differences $\Delta E_{\pm 1/2,0}^c(L)$ and $\Delta E_{0,\pm 1}$ cross linearly at the BKT transition point $t = 0$ for $y_0 > 0$ $(y_0 < 0)$, and this behavior can be used to determine the BKT critical point. From eqs. (3), (8) and (9), $\Delta E_{\pm 1/2,0}^c(L)$ and $\Delta E_{0,\pm 1}$ cross at $y_0 = 0$. This is the Gaussian fixed point. For $K < 4$, the operator $\sqrt{2} \cos \sqrt{2} \phi$, which is in the second term of the Hamiltonian (2), is relevant and a second order phase transition occurs at this point. On this transition point, we have $\Delta E_{\pm 1/2,0}^c < \Delta E_{0,\pm 2}$.

The “electric charge” $n$ in eq. (3) relates to the variation of the magnetization from $M = M_S/3$, and the excitation energy $\Delta E_{0,\pm 2}$ in the spin system is described as

$$\Delta E_{0,\pm 2}(L) = \frac{E(M_S/3 + 2, L) + E(M_S/3 - 2, L) - 2E(M_S/3, L)}{2}, \tag{10}$$
where \( E(M, L) \) is the lowest energy for the magnetization \( M \) with the PBC. The excitation energies corresponding to the operator \( \sqrt{2}\cos \phi / \sqrt{2} \) and \( \sqrt{2}\sin \phi / \sqrt{2} \) are obtained by the two lowest energies with the twisted boundary condition (TBC) [3, 4].

\[
\Delta E_{\pm 1/2,0}(L) = E_{TBC}(M S/3, L, 1) - E(M S/3, L) \quad (11)
\]

where \( E_{TBC}(M S/3, L, P) \) is the lowest energy with the magnetization \( M = M S/3 \) and the parity \( P : S_j \rightarrow S_{L-j+1} \).

### B. Numerical results

Here we show our numerical results. We calculate the energy of finite-size systems \( L = 8, 10, 12, 14 \) with the numerical diagonalization calculation. In the region \( D > 0 \), the lowest energy state with the magnetization \( M \) and with PBC has the parity \( P = (-1)^{M+L/2} \) and the momentum \( q = (M + L/2) \times \pi \). Figure 2 shows the energy differences \( \Delta E_{\pm 1/2,0} \), \( \Delta E_{\pm 1/2,0} \) for \( L = 14 \) systems. We find that among these three energies, the lowest one is \( E_{0, \pm 2} \) for small \( D (0 < D < D_{c1}) \) and \( \Delta E_{\pm 1/2,0} \) for large \( D (D_{c2} < D) \). In the intermediate region \( D_{c1} < D < D_{c2} \), \( \Delta E_{\pm 1/2,0} \) is lower than \( \Delta E_{0, \pm 2} \) and \( \Delta E_{0, \pm 2} \). In Figure 1, the small \( D \) region \( 0 < D < D_{c1} \) should correspond to the region A, the intermediate region \( D_{c1} < D < D_{c2} \) to B, and the large \( D \) region to B'.

From the critical properties of the effective model [3, 4], the point \( D_{c1} \) should be a BKT critical point. The size dependence of the crossing points between \( \Delta E_{\pm 1/2,0} \) and \( \Delta E_{0, \pm 2} \) is shown in Figure 3 and the extrapolated value is given by \( D_{c1} = 0.387 \). For small \( D (D_{c1}) \) the excitation spectrum is gapless and there does not exist a plateau in the magnetization curve.

In order to check this, we calculate the averaged scaling dimension [3, 4]

\[
\left(x_{\pm 1/2,0}^c(L) + 3x_{\pm 1/2,0}^c(L)\right) / 4,
\]

at the point \( D = D_{c1} \). From [3, 4], this value cancels the leading logarithmic size correction, and should be 1/2 at \( D = D_{c1} \). To calculate the scaling dimension, we need the sound velocity \( v_S \). This can be calculated using the lowest energy with \( M = M S/3 \) and the wave-number \( q = 2\pi / L \) (corresponding to the U(1) current),

\[
v_S(L) = \frac{E(M S/3, L, q = 2\pi / L) - E(M S/3, L)}{2\pi / L}.
\]

We extrapolate this finite size value in the polynomial of \( 1/L^2 \), and obtain \( 2\pi v_S = 20.06 \). Figure 4 shows the size dependence of the value [4]. We can see that the extrapolated value is very close to the expected one 1/2. We also calculate the conformal anomaly number \(c\) from

\[
\frac{E(M S/3, L)}{L} = \frac{c_{m=1/2} - \pi v_S c + \cdots}{6L^2},
\]

where \( c_{m=1/2} = \pi v_S c + \cdots \) is the energy per site of the limit \( L \rightarrow \infty \), \( c \) is the conformal anomaly number, and \( \cdots \) means the higher size correction. We estimate \( c \) at \( D = D_{c1} \) as \( c = 0.97 \), which is close to the expected value \( c = 1 \).

Thus we can conclude that the point \( D = D_{c1} \) is the BKT critical point. The width of the plateau near the transition point behaves singularly as \( \Delta h \sim \exp(-\text{const.}/\sqrt{D - D_{c1}}) \).

According to (3), the crossing point \( D_{c2} \) between \( \Delta E_{\pm 1/2,0} \) and \( \Delta E_{0, \pm 2} \) should be a second order phase transition point \( (K < 4 \text{ and } y_0 = 0) \). For large \( D (D_{c2} < D) \), the system is in the large-\( D \) region and a plateau appears in the magnetization curve at \( M = M S/3 \). Thus we have another massive phase in the region \( D_{c1} < D < D_{c2} \). As a possibility, this intermediate region should be characterized by the following partially magnetized valence-bond-solid (VBS) state,

\[
|mVBS, PBC\rangle = a_L^\dagger (a_L^0 b_L^1 - b_L^0 a_L^1) \prod_{j=0}^{L-1} a_j^0 (a_j^1 b_{j+1}^0 - b_{j+1}^0 a_j^1)|0\rangle.
\]

where we describe the spin state by the Schwinger bosons, that is, \( a_j^0 (b_j^0) \) creates the \( S = 1/2 \uparrow (\downarrow) \) spin at the \( j \)-th site, and \( |0\rangle \) is the vacuum of the Schwinger bosons. Here we assume PBC. This partially magnetized VBS state had firstly been discussed by Oshikawa [3] for another model (see also [4]).

Let us consider the crossing behavior near the point \( D = D_{c2} \) on another point of view. The large-\( D \) phase is characterized by the state

\[
|\text{large-}D\rangle = \prod_{j=1}^{L} a_j^0 (a_j^1 b_j^0)|0\rangle.
\]

With the twisted boundary condition \( a_{L+1}^0 = a_L^0, b_{L+1}^0 = -b_L^0 \), the magnetized valence-bond-solid state is described as

\[
|mVBS, TBC\rangle = a_L^\dagger (a_L b_L^0 + b_L^0 a_L^0) \prod_{j=1}^{L-1} a_j^0 (a_j^1 b_{j+1}^0 - b_{j+1}^0 a_j^1)|0\rangle,
\]

while the large-\( D \) state is also characterized by (13). The state \( |mVBS, TBC\rangle \) has the parity of the space inversion \( P = -1 \), while the large-\( D \) state has \( P = 1 \). This explains the level crossing between \( \Delta E_{\pm 1/2,0} \) and \( \Delta E_{0, \pm 2} \) in Figure 2.

The size dependence of the crossing point is shown in Figure 5. The estimated critical point between the intermediate and the large-\( D \) regions is \( D_c = 0.943 \), which is
very close to the value \( D_c = 0.93 \pm 0.01 \) obtained by Sakai and Takahashi. However, the phase transition is not of the BKT type but a second order phase transition which is the same universality class as the Haldane-large-\( D \) transition in the \( S = 1 \) anisotropic model.\[16\]

\[
H_{S=1} = \sum_{j=1}^{L} [S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z] + D \sum_{j=1}^{L} (S_j^z)^2.
\]

(18)

Especially, the intermediate region of the model\[1\] corresponds to the \( S = 1 \) Haldane phase in\[18\].

To verify this speculation, we calculate the coupling \( K \). The sound velocity is evaluated as \( 2\pi v_S = 21.87 \). Using this value, we determine \( K \) from \( x_{\pm 1/2,0}^s(L) \), \( x_{\pm 1/2,0}^v(L) \) [eqs.\[3\]], and

\[
\frac{L}{2\pi v_S} \Delta E_{0,\pm 1}(L) = x_{0,\pm 1}(L) = 1/2K,
\]

(19)

\[
\Delta E_{0,\pm 1}(L) = \frac{E(M_S/3 + 1, L) + E(M_S/3 - 1, L) - 2E(M_S/3, L)}{2},
\]

as shown in Figure 6. Extrapolated values of these three are consistent and we obtain \( K = 3.77 \). This is smaller than the BKT fixed point value, and the point \( D_{c2} = 0.943 \) should be a second order phase transition point. We also estimate the conformal anomaly number form eq.\[14\], and check that it is very close to the expected value \( c = 1 \).

In the vicinity of the critical point \( D = D_{c2} \), the width of the magnetization plateau decreases as \( \Delta h \sim |D - D_{c2}|^\nu \), where the critical exponent \( \nu \) is given by \( \nu = 1/(2 - x_{\pm 1,0}) = 8.68 \) mapped the \( S = 3/2 \) model to an \( S = 1 \) generalized anisotropic model with \( h = 0 \). In order to investigate the relation between the \( S = 1 \) with \( h = 0 \) and the \( S = 3/2 \) model in a magnetic field, we further applied the same analysis to the following model,

\[
H_{\Delta} = \sum_{j=1}^{L} [S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z]
\]

\[+ D \sum_{j=1}^{L} (S_j^z)^2 - h \sum_{j=1}^{L} S_j^z, \]

(20)

in the region \( 0 \leq \Delta \leq 1 \). Figure 7 shows the energy differences \( \Delta E_{\pm 1/2,0} \), \( \Delta E_{\pm 1/2,0} \), \( \Delta E_{0,\pm 2} \) for \( L = 14, \Delta = 0.5 \) system. The lowest energy difference is \( \Delta E_{0,\pm 2} \) for small \( D \) and \( \Delta E_{\pm 1/2,0} \) for large \( D \). In this case, there is a transition between the no-plateau and the large-\( D \) regions. [The crossing point of \( \Delta E_{\pm 1/2,0} \) and \( \Delta E_{\pm 1/2,0} \) is the Gaussian fixed point \( y_\phi = 0 \) in the no-plateau region (\( K > 4 \)).]

We show the \( \Delta - D \) diagram in Figure 8. We found that for \( 0.808 < \Delta < 1 \), the \( M = M_S/3 \) phase structure is the same as is of the \( \Delta = 1 \) case and there exists the intermediate magnetic region (\( D_{c1} < D < D_{c2} \)). But for \( 0 < \Delta < 0.808 \), the direct transition (BKT type) occurs between the no-plateau and the large-\( D \) regions. This boundary runs from \( (\Delta, D) = (0, 1.312) \) to the multicritical point (0.808, 0.817). The phase structure is topologically the same as is of the \( S = 1 \) anisotropic model\[12\] with \( h = 0 \)\[13\].

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**IV. SUMMARY AND DISCUSSION**

We studied the \( S = 3/2 \) spin chain with the single ion anisotropy in a magnetic field\[1\]. With the numerical approach based on the field theoretical analysis, we found a new region between the no-plateau (small \( D \)) and the magnetized large-\( D \) (large \( D \)) regions. As far as we know, this is the first work in which no-plateau state and two kinds of plateau states are found when the parameter is changed in a simple and realistic model. This intermediate region should have the same character of the partially magnetized valence-bond-solid state, and should be characterized by the string order parameter\[15\] and by the edge states for the open boundary system\[16\] reflecting a hidden discrete symmetry.\[17\] But in our small size calculation, we could not collect evidence, which remains for future study.

Restricting to three states \( S^2 = 3/2, 1/2, \) and \(-1/2, \) (in sufficiently large magnetic field) Sakai and Takahashi

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FIG. 1. Renormalization group flow diagram. The bold lines (separating the regions A and B, and A and B') are the BKT critical lines. On the dotted line between the regions B and B' ($y = 0, K < 4$), a second order phase transition occurs.

FIG. 2. Energy differences $\Delta E_{\pm 1/2,0}^c (\circ), \Delta E_{\pm 1/2,0}^s (\bullet), \Delta E_{0, \pm 1} (\triangledown)$ for the $L = 14$ system. The crossing point of $\Delta E_{\pm 1/2,0}^c$ and $\Delta E_{0, \pm 1}$ is the BKT critical point. The crossing point of $\Delta E_{\pm 1/2,0}^c$ and $\Delta E_{\pm 1/2,0}^s$ is a second order phase transition point.

FIG. 3. Size dependence of the crossing point between the energy differences $\Delta E_{\pm 1/2,0}^c$ and $\Delta E_{0, \pm 2}$. The BKT critical point is estimated as $D_{c1} = 0.387$.

FIG. 4. Size dependence of the averaged scaling dimension $(x_{\pm 1/2,0} + 3x_{\pm 1/2,0})/4$ at the BKT critical point $D_{c1} = 0.387$. 
FIG. 5. Size dependence of the crossing point between the energy differences $\Delta E_{\pm 1/2,0}^c$ and $\Delta E_{\pm 1/2,0}^s$. The critical point between the intermediate and the magnetic large-$D$ regions is estimated as $D_{c2} = 0.943$.

FIG. 6. The parameter $K$ obtained by the data $x_{\pm 1/2,0}^c = K/8$ ($\circ$), $x_{\pm 1/2,0}^s = K/8$ ($\bullet$), and $x_{0,\pm 1} = 1/2K$ ($\Diamond$). The extrapolated value is $K = 3.77$.

FIG. 7. Energy differences $\Delta E_{\pm 1/2,0}^c$ ($\circ$), $\Delta E_{\pm 1/2,0}^s$ ($\bullet$), and $\Delta E_{0,\pm 2}$ ($\Diamond$) for the system with $\Delta = 0.5$ and $L = 14$. The crossing point of $\Delta E_{\pm 1/2,0}^c$ and $\Delta E_{0,\pm 2}$ is the boundary between the no-plateau and the large-$D$ regions. The crossing point of $\Delta E_{\pm 1/2,0}^s$ and $\Delta E_{\pm 1/2,0}^a$ is the Gaussian fixed point in the no-plateau region.

FIG. 8. The boundary of the no-plateau, the large-$D$, and the magnetized VBS (m-v) regions. The boundary between the no-plateau and the large-$D$ regions, and between the no-plateau and the magnetized VBS regions ($\circ$) are the BKT critical lines. The boundary between the large-$D$ and the magnetized VBS regions ($\Diamond$) is a second order critical line. The multicritical point of these regions ($\bullet$) are estimated as $(\Delta, D) = (0.808, 0.817)$. We also show the Gaussian fixed line in the no-plateau region ($\times$).