Critical Behavior of Anisotropic Heisenberg Mixed-Spin Chains in a Field

Tōru Sakai
Faculty of Science, Himeji Institute of Technology, Ako, Hyogo 678-1297, Japan

Shoji Yamamoto
Department of Physics, Okayama University, Tsushima, Okayama 700-8530, Japan
(January 6, 1999)

We numerically investigate the critical behavior of the spin-$(1/2, 1)$ Heisenberg ferrimagnet with anisotropic exchange coupling in a magnetic field. A quantized magnetization plateau as a function of the field, appearing at a third of the saturated magnetization, is stable over whole the antiferromagnetic coupling region. The plateau vanishes in the ferromagnetic coupling region via the Kosterlitz-Thouless transition. Comparing the quantum and classical magnetization curves, we elucidate what are essential quantum effects.

PACS numbers: 75.10.Jm, 75.40.Mg, 75.50.Gg, 75.40.Cx

Quantized plateaux in magnetization curves as functions of a magnetic field for spin chains have been attracting much current interest. The trimerized spin-$1/2$ chain exhibits a massive phase at $m/m_{\text{sat}} = 1/3$, while the dimerized spin-1 chain at $m/m_{\text{sat}} = 1/4$, where $m$ is the magnetization per unit period and $m_{\text{sat}}$ is its saturation value. The presence of finite gap and plateau has further been discussed and actually been observed for various polymerized spin chains and ladders. It may be the Lieb-Schultz-Mattis theorem [12] and its generalization [13,14] in recent years that motivate such rigorous arguments. Oshikawa, Yamanaka, and Affleck (OYA) pointed out that quantized plateaux in magnetization curves may appear satisfying the condition

$$\tilde{S} - m = \text{integer},$$

(1)

where $\tilde{S}$ is the sum of spins over all sites in the unit period.

The OYA argument stimulates us to study quantum mixed-spin chains as well. An arbitrary alignment of alternating spins $S$ and $s$ in a magnetic field, which is described by the Hamiltonian

$$\mathcal{H} = \sum_{j=1}^{N} [(S_j \cdot s_j)_{\alpha} + (s_j \cdot S_{j+1})_{\alpha} - H(S_j^z + s_j^z)],$$

(2)

with $(S \cdot s)_{\alpha} = S_x^\alpha s_x^\alpha + S_y^\alpha s_y^\alpha + \alpha S_z^\alpha s_z^\alpha$, shows ferrimagnetism [13], instead of antiferromagnetism, and is another current topic from both theoretical [15,16] and experimental [17,21] points of view. As $H$ increases from zero to the saturation field

$$H_{\text{sat}} = \alpha(S + s) + \sqrt{\alpha^2(S - s)^2 + 4Ss},$$

(3)

the OYA criterion [1] allows us to expect quantized plateaux at $m = S + s - 1, S + s - 2, \ldots, 0$ (or $S$). Since the low-energy physics of the model [2] is qualitatively the same [17,18,21] regardless of $S$ and $s$ as long as $S \neq s$, here, let us consider the simplest case $(S, s) = (1, 1/2)$. Then a plateau may appear at $m = 1/2$. At the Heisenberg point, the ground state of the Hamiltonian [2] without field is a multiplet of spin $(S - s)N$ [15] and thus has elementary excitations of two distinct types [18,19,21]. The ferromagnetic excitations, reducing the ground-state magnetization, exhibit a gapless dispersion relation, whereas the antiferromagnetic ones, enhancing the ground-state magnetization, are gapped from the ground state. Therefore, at the isotropic point, $m$ as a function of $H$ should jump up to $1/2$ just as the field is applied and remain unchanged until the field reaches the antiferromagnetic excitation gap $1.759$ [21].

FIG. 1. The ground-state magnetization curves for the quantum Hamiltonian (2) at $\alpha > 0$, where QMC calculations at $N = 32$ and $T = 0.08$ are also shown for comparison.

Once we turn on the exchange-coupling anisotropy, the plateau is not so trivial any more. We show in Fig. 1 the zero-temperature magnetization curves of the anisotropic chains, which have been calculated by the numerical diagonalization technique combined with a finite-size scaling analysis [30]. In order to verify the reliability of our scal-
ing analysis, which is briefly explained later, we have carried out quantum Monte Carlo (QMC) calculations \[31\] as well as at \(N = 32\) and \(N = 16\), where, due to the small correlation length \[18,19\] of the system, the data show no size dependence beyond the numerical uncertainty. Although the QMC findings are obtained at a sufficiently low but finite temperature, they fully suggest that the present diagonalization-based calculations well describe the thermodynamic-limit properties. As the model approaches the Ising limit (\(\alpha \to \infty\)), the plateau monotonically grows and ends up with a stepwise magnetization curve. On the other hand, the introduction of the \(XY\)-like coupling anisotropy reduces the plateau. Thus we take great interest in where and how the plateau vanishes. Alcaraz and Malvezzi \[17\] showed that the ground state of the model \[2\] without field is in the critical phase over the whole region \(-1 \leq \alpha < 1\). At the Heisenberg point, the model still lies in the massless phase but the low-energy dispersion as a function of momentum is quadratic \[21\]. For \(\alpha > 1\), the model is in the massive phase \[22\] and its low-energy structure is well understood by the spin-wave dispersions

\[
\omega_k^\pm = \sqrt{\alpha^2(S + s)^2 - 4s^2 \cos^2 \frac{k}{2} \mp \alpha(S - s)},
\]

(4)

which describe the sector of the magnetization \(\sum_j (S_j^z + s_j^z)\) \(\equiv M < (S - s)N\) and that of \(M > (S - s)N\), respectively. Thus the introduction of the anisotropy essentially changes the nature of the model \[2\] and a fascinating physics must lie especially in the \(XY\)-like coupling region. In the present article, we clarify how the quantized plateau of the \((1, \frac{1}{2})\) model behaves as a function of the anisotropy and aim to reveal critical phenomena inherent in quantum ferrimagnets.

In order to investigate the quantum critical behavior, we carry out a scaling analysis on the numerically calculated energy spectra of finite clusters up to \(N = 12\). Let \(E(N, M)\) denote the lowest energy in the subspace with a fixed magnetization \(M\) for the Hamiltonian \[3\] without the Zeeman term. The upper and lower bounds of the field which induces the ground-state magnetization \(M\) are, respectively, given by

\[
H^+(N, M) = E(N, M + 1) - E(N, M),
\]

(5)

\[
H^-(N, M) = E(N, M) - E(N, M - 1).
\]

(6)

If the system is massive at the sector labeled \(M\), \(H^\pm(N, M)\) should exhibit exponential size corrections and result in different thermodynamic-limit values \(H^\pm(m)\), which can precisely be estimated through the Shanks’ extrapolation \[32\]. For the critical system, on the other hand, \(H^\pm(N, M)\) are expected to converge to the same value as \[33\]

\[
H^\pm(N, M) \sim H(m) \pm \frac{\pi v_c \eta}{N},
\]

(7)

where \(v_c\) is the sound velocity and \(\eta\) is the critical index defined as \(\langle \sigma^+ \sigma^- \rangle \sim (-1)^r r^{-\eta}\) for the relevant spin operator \(\sigma\), which may here be an effective combination of \(S\) and \(s\).

Figure 1 was thus obtained, where we smoothly interpolated the raw data \(H(m)\). The model is trivially gapless at all the sectors of \(M\) for \(\alpha \leq -1\) and should therefore encounter a massive-massless phase transition in the \(XY\)-like coupling region. Now we present in Fig. 1 the magnetization curves at \(\alpha \leq 0\) so as to detect the transition. Surprisingly, the plateau still exists at the \(XY\) point (\(\alpha = 0\)) and the transition occurs in the ferromagnetic-coupling region. At a naive idea of relating the massive state with the staggered Néel-like order in the direction of the external field, we are never able to understand why the plateau is so stable against the \(XY\)-like anisotropy.
The plateau length $\Delta_N = H_+(N, M) - H_-(N, M)$ is a relevant order parameter to detect the phase boundary. When the system is critical, $\Delta_N$ should be proportional to $1/N$ because of the scaling relation (7). We plot in Fig. 3(a) the scaled quantity $N\Delta_N$ as a function of $\alpha$. $N\Delta_N$ is almost independent of $N$ in a finite range of $\alpha$, rather than at a point, which exhibits an aspect of the Kosterlitz-Thouless (KT) transition [34]. It is likely that the XY-like anisotropy induces the KT transition [35] followed by the gapless spin-fluid phase whose spin correlation shows a power-law decay. Let us evaluate the central charge $c$ of the critical phase, which is expected to be unity. The asymptotic form of the ground-state energy [33]

$$E(N, M) \sim \frac{2}{N} \left[ E_{k_1}(N, M) - E(N, M) \right]$$

(8)

allows us to extract $c$ from the finite-cluster energy spectrum provided $v_s$ is given. Here we calculate $v_s$ as

$$v_s = \frac{N}{2\pi} \left[ E_{k_1}(N, M) - E(N, M) \right]$$

(9)

where $k_1 = 2\pi/N$ and $E_{k_1}(N, M)$ is the lowest energy in the subspace specified by the momentum $k$ as well as by the magnetization $M$. The size correction for the formula (9) is of order $O(1/N^2)$, which is essentially negligible in the present system. In Fig. 3(b) we plot $c$ versus $\alpha$ and find that $c$ approaches unity as the system goes toward the critical region. We further investigate the critical exponent $\eta$ so as to verify the KT universality and to specify the phase boundary. In the critical region the asymptotic formula $\Delta_N \sim 2\pi v_s \eta/N$ enables us to estimate $\eta$. Since the KT transition holds $\eta = \frac{1}{8}$ at the phase boundary, we can evaluate the transition point $\alpha_c$ from $\eta$ as a function of $\alpha$. Figure 3(b) claims that $\alpha_c = -0.41 \pm 0.01$, where $c = 1.00 \pm 0.01$. The phenomenological renormalization-group (PRG) technique [36] is another numerical tool to determine the phase boundary. Taking $\Delta_N$ as the order parameter, we extract the size-dependent fixed point $\alpha_c(N, N + 2)$ from the PRG equation

$$(N + 2)\Delta_{N+2}(\alpha) = N \Delta_N(\alpha).$$

(10)

In Fig. 4 we plot $\alpha_c(N, N + 2)$ as a function of $1/(N + 1)$, which is linearly extrapolated to $\alpha_c = -0.57$. The PRG estimate is somewhat discrepant from the above-obtained phase boundary. Here we should be reminded of Nomura-Okamoto’s enlightening analysis [37] on usage of the PRG method. The PRG equation applied to a gapful-gapful phase transition yields a reliable estimate of the critical point, whereas, for a transition of KT type, the PRG estimate is quite likely to miss the exact solution due to the incidental logarithmic size correction, encroaching upon the KT-phase region. Considering the limited availability of the PRG analysis, we may recognize the present PRG solution as the lower boundary of $\alpha_c$. 

**FIG. 4.** The linear extrapolation of the size-dependent fixed point $\alpha_c(N, N + 2)$.

**FIG. 5.** The ground-state magnetization curves for the classical Hamiltonian (2).

**FIG. 6.** The ground-state spin configurations as functions of the field for the classical Hamiltonian (2).
The quantum spin configuration in the massive state of the quantum system. The plateau appears for \( \alpha > -0.41 \), including a ferromagnetic-coupling region. We note that on the boundary of the plateau phase except for the point \((\alpha, H) = (\alpha_c, H_c) \equiv (0.41, 0.293)\) which is indicated as KT point in Fig. 6, is suggestive in understanding the prompt collapse of the classical plateau with the increase of the XY-like anisotropy. In the classical case, the spin configuration in the massive state of \( M = N/2 \) is stuck to \((S^j_x, s^j_z) = (1, -\frac{1}{2})\). In other words, the plateau can not appear unless the configuration \((S^j_x, s^j_z) = (1, -\frac{1}{2})\) is realized. This is not the case for the quantum system. The quantum spin configuration in the massive state of \( M = N/2 \) generally depends on \( \alpha \) and exhibits a quantum reduction from the classical Néel-like state. At the Heisenberg point, for example, the quantum averages of the sublattice magnetizations per unit cell in the massive state are estimated to be 0.793 and 0.293, respectively. It must be the quantum spin reduction that makes the massive state tough against the XY-like anisotropy.

In order to elucidate how far from intuitive the present observation is, we compare it with the classical behavior. Let us consider the classical version of the Hamiltonian (2), where \( S_j \) and \( s_j \) are classical vectors of magnitude 1 and \( \frac{1}{2} \), respectively. We show in Fig. 6 the classical magnetization curves and learn both similarity and difference between the quantum and classical behaviors. In the ferromagnetic and Ising-like antiferromagnetic exchange-coupling regions they are quite alike, which is convincing in that quantum effects are supposed to be less significant in both the regions. However, the quantum behavior is qualitatively different from the classical one in the XY-like coupling region. The classical state of \( M = N/2 \), which is stable enough to form a plateau in the Ising-like coupling region, is no more massive at \( \alpha \leq 0.943 \). The spin configuration as a function of the field, revealed in Fig. 6 is suggestive in understanding the prompt collapse of the classical plateau with the increase of the XY-like anisotropy. In the classical case, the spin configuration in the massive state of \( M = N/2 \) is stuck to \((S^j_x, s^j_z) = (1, -\frac{1}{2})\). In other words, the plateau can not appear unless the configuration \((S^j_x, s^j_z) = (1, -\frac{1}{2})\) is realized. This is not the case for the quantum system. The quantum spin configuration in the massive state of \( M = N/2 \) generally depends on \( \alpha \) and exhibits a quantum reduction from the classical Néel-like state. At the Heisenberg point, for example, the quantum averages of the sublattice magnetizations per unit cell in the massive state are estimated to be 0.793 and 0.293, respectively. It must be the quantum spin reduction that makes the massive state tough against the XY-like anisotropy.

In sum the quantum mixed-spin Heisenberg model (3) with \((S, s) = (1, \frac{1}{2})\) shows the three distinct phases at the sector of \( M = N/2 \); the plateau phase, the gapless spin-fluid phase, and the ferromagnetically ordered phase, as illustrated in Fig. 6. The plateau appears for \( \alpha > -0.41 \), including a ferromagnetic-coupling region. We note that on the boundary of the plateau phase except for the point \((\alpha, H) = (\alpha_c, H_c) \equiv (0.41, 0.293)\) which is indicated as KT point in Fig. 6, the plateau length is generally finite, namely, the relevant correlation length is not divergent. The only point \((\alpha_c, H_c)\) possesses the KT character. The long-lived plateau against the XY-like anisotropy, which is contrastive to the corresponding classical behavior, deserves special remark and further investigation. We expect magnetic measurements on anisotropic systems [8].

It is a pleasure to thank H.-J. Mikeska and U. Schollwöck for helpful discussions. This work was supported by the Japanese Ministry of Education, Science, and Culture through Grant-in-Aid No. 09740286 and by the Okayama Foundation for Science and Technology. The numerical computation was done in part using the facility of the Supercomputer Center, Institute for Solid State Physics, University of Tokyo.

### References

1. K. Hida, J. Phys. Soc. Jpn. 63, 2359 (1994).
2. K. Okamoto, Solid State Commun. 98, 245 (1995).
3. T. Tonegawa, T. Nakao, and M. Kaburagi, J. Phys. Soc. Jpn. 65, 3317 (1996).
4. K. Totsuka, Phys. Lett. A 228, 103 (1997).
5. H. Nakano and M. Takahashi, J. Phys. Soc. Jpn. 67, 1126 (1998).
6. K. Totsuka, Phys. Rev. B 57, 3454 (1998).
7. D. C. Cabra and M. D. Grynberg, cond-mat/9803368; A. Honecker, cond-mat/9808312.
8. D. C. Cabra, A. Honecker, and P. Pujol, Phys. Rev. Lett. 79, 5126 (1997); Phys. Rev. B 58, 6241 (1998).
9. A. K. Kolezhuk, Phys. Rev. B 59, February 1 (1999).
10. Y. Narumi, M. Hagiwara, R. Sato, K. Kindo, H. Nakano, and M. Takahashi, Physica B 246-247, 509 (1998).
11. W. Shiramura, K. Takatsu, B. Kurniawan, H. Tanaka, H. Uekusa, Y. Ohashi, K. Takizawa, H. Mitamura, and T. Goto, J. Phys. Soc. Jpn. 67, 1548 (1998).
12. E. Lieb, T. Schultz, D. Mattis, Ann. Phys. 16, 407 (1961).
13. I. Affleck, Phys. Rev. Lett. 43, 5186 (1988).
14. M. Oshikawa, M. Yamanaka, and I. Affleck, Phys. Rev. Lett. 78, 1984 (1997).
15. E. Lieb and D. Mattis, J. Math. Phys. 3, 749 (1962).
16. M. Drillon, J. C. Gianduzza, and R. Georges, Phys. Lett. 96A, 413 (1983); M. Drillon, E. Coronado, R. Georges, J. C. Gianduzza, and J. Curely, Phys. Rev. B 40, 10992 (1989).
17. F. C. Alcaraz and A. L. Malvezzi, J. Phys. A 30, 767 (1997).
18. S. K. Pati, S. Ramasesha, and D. Sen, Phys. Rev. B 55, 8894 (1997); J. Phys.: Condens. Matter 9, 8707 (1997).
19. S. Brehmer, H.-J. Mikeska, and S. Yamamoto, J. Phys.: Condens. Matter 9, 3921 (1997).
20. H. Niggemann, G. Uimin, and J. Zittartz, J. Phys.: Condens. Matter 9, 9031 (1997); ibid. 10, 5217 (1998).
21. S. Yamamoto, Int. J. Mod. Phys. C 8, 609 (1997); S. Yamamoto, S. Brehmer, and H.-J. Mikeska, Phys. Rev. B 57, 13610 (1998); S. Yamamoto and T. Sakai, J. Phys.
[22] T. Ono, T. Nishimura, M. Katsumura, T. Morita, and M. Sugimoto, J. Phys. Soc. Jpn. 66, 2576 (1997).
[23] T. Kuramoto, J. Phys. Soc. Jpn. 67, 1762 (1998).
[24] S. Yamamoto and T. Fukui, Phys. Rev. B 57, 14008 (1998); S. Yamamoto, T. Fukui, K. Maisinger, and U. Schollwöck, J. Phys.: Condens. Matter 10, 11033 (1998).
[25] N. B. Ivanov, Phys. Rev. B 57, 14024 (1998).
[26] K. Maisinger, U. Schollwöck, S. Brehmer, H.-J. Mikeska, and S. Yamamoto, Phys. Rev. B 58, 5908 (1998); A. K. Kolezhuk, H.-J. Mikeska, K. Maisinger, and U. Schollwöck, cond-mat/9812326.
[27] S. Yamamoto, Phys. Rev. B 59, 1024 (1999).
[28] O. Kahn, Magnetism of the heteropolymetallic systems, Structure and Bonding 68, 91 (Springer-Verlag, 1987); O. Kahn, Y. Pei, and Y. Journaux, in Inorganic Materials, edited by D. W. Bruce and D. O'Hare (Wiley, New York, 1995), p. 95.
[29] M. Hagiwara, K. Minami, Y. Narumi, K. Tatani, and K. Kindo, J. Phys. Soc. Jpn. 67, 2209 (1998).
[30] T. Sakai and M. Takahashi, Phys. Rev. B 43, 13383 (1991); T. Sakai and M. Takahashi, Phys. Rev. B 57, 3201 (1998).
[31] S. Yamamoto and S. Miyashita, Phys. Rev. B 51, 3649 (1995).
[32] D. Shanks, J. Math. Phys. 34, 1 (1955).
[33] J. L. Cardy, J. Phys. A 17, L385 (1984); H. W. Blöte, J. L. Cardy and M. P. Nightingale, Phys. Rev. Lett. 56, 742 (1986); I. Affleck, Phys. Rev. Lett. 56, 746 (1986).
[34] J. M. Kosterlitz and D. J. Thouless, J. Phys. C 6, 1181 (1973).
[35] J. Sólyom and T. A. L. Ziman, Phys. Rev. B 30, 3980 (1984).
[36] M. P. Nightingale, Physica 83A, 561 (1976).
[37] K. Nomura and K. Okamaoto, J. Phys. Soc. Jpn. 62, 1123 (1993).
[38] P. J. van Koningsbruggen, O. Kahn, K. Nakatani, Y. Pei, J.-P. Renard, Inorg. Chem. 29, 3325 (1990).
$H$-plateau

ferromagnetically ordered

critical

KT point