Universal Temperature Dependence of the Magnetization of Gapped Spin Chains

Yoshitaka Maeda,[1] Chisa Hotta,[2] and Masaki Oshikawa[3]

[1]Department of Physics and Astronomy, The University of British Columbia, Vancouver, British Columbia, V6T 1Z1 Canada
[2]Physics Department, Kyoto Sangyo University, Kyoto 603-8555, Japan
[3]Institute of Solid State Physics, University of Tokyo, Kashiwa 277-8581, Japan

(Received 27 March 2007; revised manuscript received 30 May 2007; published 31 July 2007)

A Haldane chain under applied field is analyzed numerically, and a clear minimum of magnetization is observed as a function of temperature. We elucidate its origin using the effective theory near the critical field and propose a simple method to estimate the gap from the magnetization at finite temperatures. We also demonstrate that there exists a relation between the temperature dependence of the magnetization and the field dependence of the spin-wave velocity. Our arguments are universal for general axially symmetric one-dimensional spin systems.

DOI: 10.1103/PhysRevLett.99.057205 PACS numbers: 75.10.Jm, 75.10.Pq

Discovery of the Haldane gap [1] established an important paradigm followed by the extensive studies on gapped spin chains. In particular, recent remarkable progress in high magnetic-field experiments provide numerous data on the closing of these gaps. Once the system becomes gapless, the low-energy physics of the system is expected to be similar to that of the intrinsically gapless $S = 1/2$ Heisenberg antiferromagnetic (HAF) chain. However, there are some aspects unique to *the gapless phase induced by the applied magnetic field* on the gapped spin chains, which have not been clarified.

In this Letter, we focus on one of the most fundamental physical quantities—magnetization—in the gapless phase of the $S = 1$ Haldane chain under an applied field. We demonstrate that, in the gapless regime slightly above the critical field, the magnetization has a minimum as a function of temperature. Such temperature dependence follows a universal function determined from an effective theory. Our findings turn out to be quite universal and applicable to general gapped one-dimensional (1D) spin systems with axial symmetry (rotational symmetry along the magnetic-field direction).

Many one-dimensional quantum systems in the low-energy limit can be described by a relativistic field theory. In particular, the relativistic free boson field theory, also known as the Tomonaga-Luttinger liquid (TLL) theory, applies to a wide range of gapless one-dimensional systems including the gapless phase of the Haldane chain and the $S = 1/2$ HAF chain. In a "true" relativistic theory, the space and time coordinates are related by the speed of light, a universal constant. However, when the relativistic theory is applied to condensed-matter physics, the "speed of light" is given by the velocity of collective excitations (which is often called a spin-wave velocity in spin-chain problems) and is, in practice, a variable. We find that the magnetic-field dependence of the spin-wave velocity is related to the interesting temperature dependence of the magnetization and that it classifies *the field-induced gapless* and the intrinsically gapless phases.

The magnetization minimum discussed in this Letter appears to be similar to the magnetization cusp originated from the Bose-Einstein condensation (BEC) of magnons. However, in our purely 1D case, there is no phase transition at finite temperatures. The minimum rather represents a nonsingular crossover from the relativistic TLL regime to the high-temperature regime governed by the nonrelativistic dispersion relation.

The Hamiltonian of the Heisenberg spin chain is

$$\mathcal{H} = J\sum_{j=1}^{N} \boldsymbol{S}_j \cdot \boldsymbol{S}_{j+1} - h\sum_{j=1}^{N} S_j^z, \qquad (1)$$

where $J > 0$ and N is the system size. The ground state of the $S = 1$ case (the Haldane chain) at zero field is a nonmagnetic singlet state and has a finite energy gap $\Delta = 0.410J$ [2]. The system undergoes a quantum phase transition at finite magnetic field $h = h_c (= \Delta)$. The gapless phase which appears at $h > h_c$ can be described by the TLL [3] as in the $S = 1/2$ HAF chain. Therefore, one might expect that its magnetization also follows that of the $S = 1/2$ case, which is well known as the Bonner-Fisher curve [4]. This turns out not to be the case.

The magnetization of the $S = 1$ gapless phase has already been studied in many articles. Hida, Imada, and Ishikawa discussed the winding number induced by the chemical potential in the sine-Gordon model [5], which has a close relation to our problem. Konik and Fendley [6] discussed the field dependence of susceptibility $\chi(h)$ of the Haldane chain on the basis of the exact solution of the nonlinear sigma (NLσ) model. However, these approaches are not applicable to h significantly larger than the gap. The field dependence of the magnetization was also given numerically at several fixed values of temperature [7–9]. However, characteristic features of the temperature dependence were apparently overlooked; the full systematic understanding of the magnetization over the entire gapless regime $h_c < h < h_s$ is still lacking.

To clarify the issue, we first adopt the quantum Monte Carlo (QMC) simulation to the $S = 1$ Haldane chain under a finite field. The QMC simulation is performed for $N = 512$ with the maximum 1.2×10^6 Monte Carlo steps using the stochastic series expansion [10–12] code of the Algorithms and Libraries for Physics Simulations project [13–15]. The results in the thermodynamic limit after the finite-size scaling converges within 10^{-5} to the high-temperature expansion results. In the gapped phase $h < h_c$, we find that the magnetization decreases and vanishes exponentially toward $T = 0$ as expected. However, in the gapless phase $h > h_c$, the magnetizations shows a nontrivial characteristic minimum at low temperature $T = T_m$, which is clearly detected numerically as shown in Fig. 1(a). We also find that T_m decreases toward $T = 0$ as h approaches h_c. In the $S = 1/2$ case given in the inset in Fig. 1(a), the overall behavior of M is consistent with that of the classical spin [16]. In contrast, in the $S = 1$ case, such similarity with the classical case holds only at the high-temperature region. This indicates the difference between the intrinsically gapless $S = 1/2$ and the present case.

Let us discuss the characteristic behavior in Fig. 1 in terms of the generic effective theory applicable at slightly above the critical field $h \gtrsim h_c$. The first excited states above a gap from a singlet ground state generally consist of a triplet massive boson state with $S^z = \pm 1, 0$, which usually has repulsive short-range interactions. Low-energy states of these particles may be approximated by a nonrelativistic dispersion relation:

$$E(k) \approx \Delta + k^2/2m - hS^z, \tag{2}$$

where $1/m$ is a band curvature, and $v_0 = \sqrt{\Delta/m}$ corresponds to the relativistic speed of light. In the low-energy regime, the higher-energy $S^z = 0, -1$ magnons may be ignored. On the other hand, the $S^z = 1$ magnon branch intersects with the ground state at $h = h_c = \Delta$, a quantum phase transition point. In the gapless regime a quasi-long-range order appears [3]. Then the remaining $S^z = 1$ magnon in its low density limit $h = h_c$ is exactly mapped onto the free-fermion theory with the dispersion equation (2) [3,17,18]. The low but finite magnon density regime $h \gtrsim h_c$ is still approximated by the free fermion since the residual interactions are only proportional to $h - h_c$. Here the magnetization is equal to the number of the particles as

$$\frac{M}{L} = \sqrt{\frac{m}{2\pi^2}} \int_0^\infty d\epsilon D(\epsilon) f(\epsilon - \mu), \tag{3}$$

where $\epsilon = k^2/2m$, $\mu = h - \Delta$, and $f(\epsilon - \mu) = (e^{[\beta(\epsilon-\mu)]} + 1)^{-1}$ is the Fermi distribution function. Near zero temperature, its temperature dependence is given by the Sommerfeld expansion [19]. The leading term in the expansion is $\propto D'(\mu)T^2$. In one dimension, $D(\epsilon) \propto 1/\sqrt{\epsilon}$ is monotonically decreasing so that $D'(\mu) < 0$. Thus, the magnetization (3) near $T = 0$ must be a decreasing function of T. This implies the existence of the magnetization minimum found in Fig. 1.

The exact integration of Eq. (3) gives

$$\frac{M}{L} = -\sqrt{\frac{m}{2\pi\beta}} \mathrm{Li}_{n=1/2}(-e^{\beta(h-\Delta)}), \tag{4}$$

where $\mathrm{Li}_n(x) = \sum_{l=1}^\infty x^l/l^n$ is the polylogarithm function. We show in Fig. 1(b) the actual form of Eq. (4) which reproduces well the minimum of M found in Fig. 1(a).

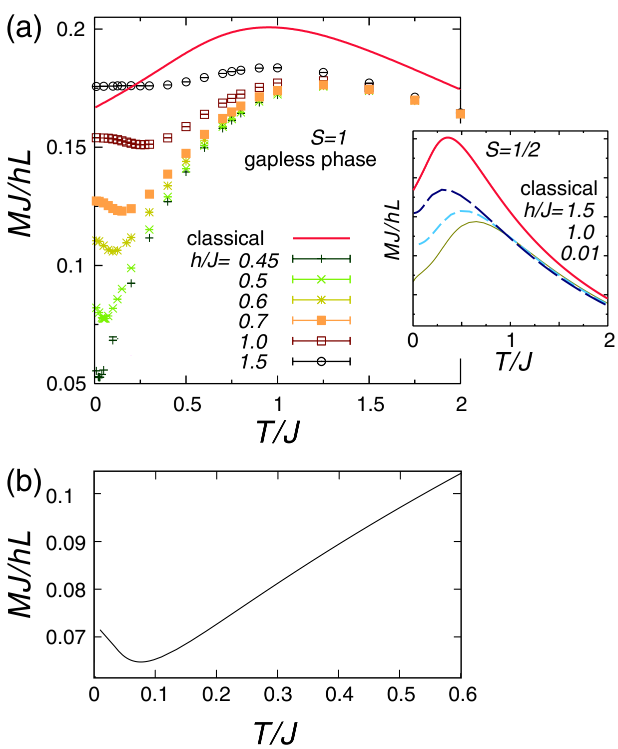

FIG. 1 (color online). (a) Temperature dependence of the magnetization of the $S = 1$ Heisenberg model in the gapless phase ($h > h_c$) at several values of $h/J = 0.45$–1.5, together with the exact susceptibility of the classical spin Hamiltonian. The inset shows the magnetization of $S = 1/2$ for comparison. The error bar of each point is much smaller than the symbol size. (b) Free-fermion result [Eq. (4)] for $h - \Delta = 0.1$, in qualitative agreement with the results in (a).

The analogous mapping between the dilute boson and the free fermion also holds at slightly below the saturation field $h \lesssim h_s$. In this case, the vacuum state is the fully polarized state, and the low-lying excitations consist of the $S^z = 0$ magnon branch instead of the $S^z = 1$ one. Consequently, the magnetization shows a maximum corresponding to the minimum of the magnon density, just the opposite to the case at $h \gtrsim h_c$. Our Monte Carlo results in Fig. 2 are consistent with this argument.

The free-fermion description has thus succeeded in reproducing the minimum and maximum in Figs. 1(a) and 2, respectively. However, it is valid only slightly above h_c and below h_s. On the other hand, the TLL theory should be applicable to the whole gapless regime $h_c < h < h_s$, albeit only in the low-energy limit. In the following, we discuss the temperature dependence of the magnetization from the TLL viewpoint.

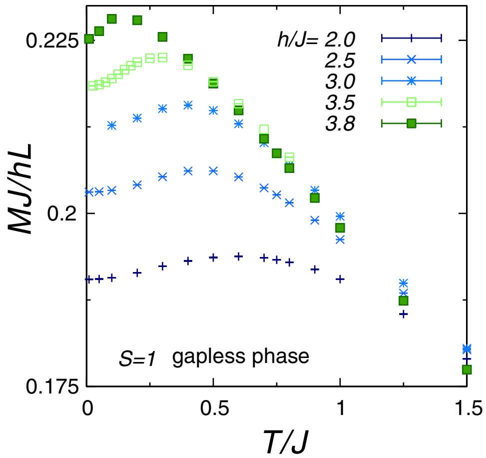

FIG. 2 (color online). Temperature dependence of the magnetization of the $S = 1$ Heisenberg model in the gapless phase near the saturation field ($h \gtrsim h_c = 4J$) at several values of $h/J =$ 2–3.8.

Conformal field theory gives the celebrated low-temperature expansion of the free energy per unit volume [20,21]

$$f = \epsilon_0 - \frac{\pi c}{6 v_F} T^2 + O(T^3), \tag{5}$$

where ϵ_0 is the ground state energy, v_F is the excitation velocity of a fixed point theory, and c is the central charge ($c = 1$ for TLL). The derivative of the free energy with respect to the magnetic field gives the magnetization as

$$\frac{M}{L} = \frac{M_0}{L} - \frac{\pi}{6 v_F^2} \frac{\partial v_F}{\partial h} T^2 + O(T^3). \tag{6}$$

The first and the second terms give the magnetization of the ground state and the leading finite-temperature correction, respectively. We did not discuss explicitly the effect of irrelevant operators in its derivation. However, the leading irrelevant operator just gives a correction of $O(T^2)$, which should be understood as already included in Eq. (6). Equation (6) is, in fact, a generalization of the lowest order Sommerfeld expansion of Eq. (3) to the interacting system.

This equation indicates that whether the magnetization near $T = 0$ increases or decreases is determined by the sign of the gradient of the velocity with respect to the magnetic field $\partial_h v_F$. For the $S = 1/2$ Heisenberg chain, we always have $\partial_h v_F < 0$ (see Fig. 9 in Ref. [22]). In contrast, the gapless TLL regime in the present case has $v_F = 0$ at both end points $h = h_c$ and $h = h_s$. This indeed gives the characteristic behavior observed in Figs. 1(a) and 2.

To obtain the precise values of v_F, we performed a density-matrix renormalization group (DMRG) calculation [23] on the $S = 1$ Haldane chain with the periodic boundary condition [24]. The velocity v_F as a function of the magnetic field is extracted from a finite-size scaling analysis of the energy spectra and is shown in Fig. 3. The velocity increases rapidly just above $h = h_c$, takes a maximum at around $h = h_m \sim J$, and then decreases toward $h = h_s$, as anticipated. At the velocity maximum $h = h_m$, the leading finite-temperature correction starts from $O(T^3)$, so that the magnetization becomes flat. Even when h is away from h_m, v_F depends rather weakly on h for a range of the magnetic field $J \lesssim h \lesssim 2J$, where magnetization should become almost flat at low temperatures. This is indeed consistent with what we find in Figs. 1(a) and 2.

The magnetization minimum/maximum marks the temperature above which the predictions based on the TLL picture break down. Thus, it can be interpreted as a crossover from the TLL with the linear dispersion to the state governed by the nonrelativistic dispersion $\epsilon \propto k^2$, as is indicated by the arrow in Fig. 4(a).

Taking advantage of this finding, we propose a new quantitative way to estimate the gap from T_m near the critical field. Equation (4) takes the minimum under the condition $2x = \mathrm{Li}_{n=1/2}(-e^x)/\mathrm{Li}_{n=-1/2}(-e^x)$, where $x = \mu/T_m$. Its solution $x = x_0 \sim 0.762\,38$ yields

$$T_m = x_0(h - \Delta). \tag{7}$$

The finite-temperature measurement of magnetization at several $h > h_c$ in either experiments or numerical calculations thus provides a useful estimate of Δ. Since Eq. (7) consists only of the universal constant, we can use it without any microscopic information of the system. As a demonstration, we show in Fig. 4(b) the comparison of our Monte Carlo results with Eq. (7). The data asymptotically approach to Eq. (7) when $h \to h_c = \Delta$.

All of the data at $h > h_c = \Delta$ in Fig. 4(b) fall below the exact asymptotics equation (7). Such deviation is understood as an effect of the repulsive interaction between the fermions. The excitations to the higher-energy modes should be enhanced by the interaction so that the band curvature effect is more important than that in the free case. Consequently, the exact value of the crossover temperature T_m must be generally lowered compared to the estimate (7) derived from the free-fermion theory.

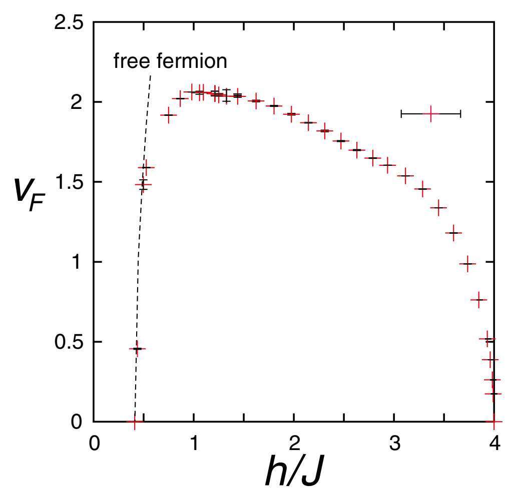

FIG. 3 (color online). Magnetic-field dependence of velocity obtained by DMRG. The dashed line shows the free-fermion result obtained from Eq. (3). The upper bounds of errors are 10^{-5} for ϵ_0 and between $10^{-3} (h \sim h_c)$ and $10^{-5} (h \sim h_s)$ for v_F (see the error bar).

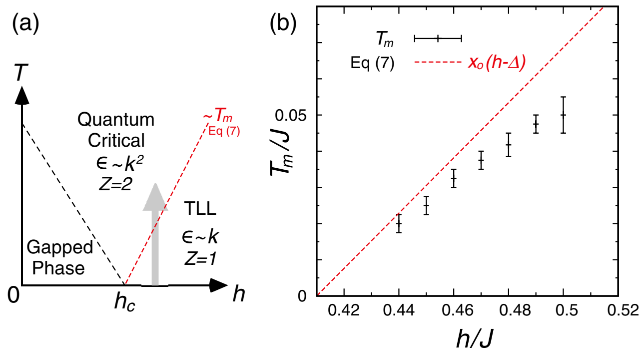

FIG. 4 (color online). (a) Phase diagram for the gapped spin chains. Dashed lines indicate the crossovers. The one between the TLL and the quantum critical regime is given by $T \sim h - h_c \sim T_m$. (b) The fitting of the QMC results with Eq. (7). From this fitting, the gap Δ can be estimated. The error bars come from a discreteness of the numerical data with respect to temperature.

Our argument again describes universal low-energy features of general axially symmetric one-dimensional spin systems, provided that the field-induced gapless phase can be described by a single-component TLL.

The magnetization minimum has often been discussed in terms of BEC. Although the three-dimensional (3D) BEC observed in Ref. [25] gives a similar M-T curve to Fig. 1(a), it differs from our case in several points; the magnetization shows a singular cusplike minimum at the transition temperature $T_c \propto (h - h_c)^{2/3}$ (which is possibly smeared in actual systems due to anisotropies [26]), whereas $T_m \propto h - h_c$ in our model just marks the crossover. The transverse magnetization is finite, namely, the off-diagonal long-range order is present in BEC at $T < T_c$ but is absent in our 1D system at any temperature.

We are not aware of any experimental evidence of the present analysis. However, there might already be some corresponding experiments, which have been interpreted in different inappropriate ways. Actually, the upturn of magnetization at low temperature found in many experiments had been considered as a 3D effect (BEC of magnons). However, our findings indicate that it does occur generally in purely 1D gapped spin systems as well. Therefore, a cautious interpretation is required for the magnetization data. To distinguish these two scenarios, one should examine whether or not the transverse magnetization exists below T_m as well as the presence or absence of the thermodynamic phase transition. In reality, the actual systems generally have finite interchain interactions. However, the effects described in the present Letter are observable if the interchain interactions are sufficiently weak.

We thank I. Affleck, J. Akimitsu, H. Tanaka, C. Yasuda, K. Sakai, K. Hida, and S. Todo for discussions. We thank A. I. Smirnov for help in finding Refs. [27–29]. This work is supported by 21st Century COE Programs at Tokyo Tech and Aoyama Gakuin University, a Grant-in-Aid for Scientific Research (No. 18540341) from MEXT of Japan, and by NSERC of Canada.

Note added in proof.—Recently, we became aware that the magnetization minimum was reported in numerical calculations of the $S = 1/2$ two-leg spin ladder [27,28] and possibly in an experiment on the Haldane chain [29]. The present Letter clarifies its origin and universality in one-dimensional spin gap systems.

[1] F. D. M. Haldane, Phys. Lett. **93A**, 464 (1983); for a review, see I. Affleck, J. Phys. Condens. Matter **1**, 3047 (1989).
[2] S. R. White and D. A. Huse, Phys. Rev. B **48**, 3844 (1993).
[3] I. Affleck, Phys. Rev. B **41**, 6697 (1990); **43**, 3215 (1991).
[4] J. Bonner and M. E. Fisher, Phys. Rev. **135**, A640 (1964).
[5] K. Hida, M. Imada, and M. Ishikawa, J. Phys. C **16**, 4945 (1983).
[6] R. M. Konik and P. Fendley, Phys. Rev. B **66**, 144416 (2002).
[7] K. Okunishi, Phys. Rev. B **60**, 4043 (1999).
[8] J. Lou *et al.*, Phys. Rev. B **62**, 3786 (2000).
[9] V. A. Kashurnikov *et al.*, Phys. Rev. B **59**, 1162 (1999).
[10] A. W. Sandvik and J. Kurkijärvi, Phys. Rev. B **43**, 5950 (1991).
[11] A. W. Sandvik, J. Phys. A **25**, 3667 (1992).
[12] O. F. Syljuåsen and A. W. Sandvik, Phys. Rev. E **66**, 046701 (2002).
[13] F. Alet *et al.*, J. Phys. Soc. Jpn. Suppl. **74**, 30 (2005); see also http://alps.comp-phys.org/.
[14] F. Alet, S. Wessel, and M. Troyer, Phys. Rev. E **71**, 036706 (2005).
[15] M. Troyer, B. Ammon, and E. Heeb, Lect. Notes Comput. Sci. **1505**, 191 (1998).
[16] M. E. Fisher, Am. J. Phys. **32**, 343 (1964).
[17] H. J. Schulz, Phys. Rev. B **22**, 5274 (1980).
[18] E. H. Lieb and W. Liniger, Phys. Rev. **130**, 1605 (1963); E. H. Lieb, *ibid.* **130**, 1616 (1963).
[19] N. W. Ashcroft and N. D. Mermin, *Solid State Physics* (Brooks-Cole, Belmont, MA, 1976).
[20] I. Affleck, Phys. Rev. Lett. **56**, 746 (1986).
[21] J. L. Cardy, J. Phys. A **17**, L385 (1984); **17**, L957 (1984); Nucl. Phys. **B240**, 514 (1984).
[22] I. Affleck and M. Oshikawa, Phys. Rev. B **60**, 1038 (1999).
[23] S. R. White, Phys. Rev. Lett. **69**, 2863 (1992).
[24] Although DMRG generally works better for the open boundary condition, we choose the periodic boundary to make the magnetization distribute uniformly in the system, in which case the finite-size scaling analysis on Eq. (5) works more accurately (see Fig. 3). Furthermore, we scaled the numerical data in advance of the finite-size scaling by the truncation error which makes the numerical accuracy quite comparable with the open boundary condition case.
[25] T. Nikuni *et al.*, Phys. Rev. Lett. **84**, 5868 (2000).
[26] J. Sirker, A. Weiße, and O. P. Sushkov, Europhys. Lett. **68**, 275 (2004).
[27] X. Wang and Lu Yu, Phys. Rev. Lett. **84**, 5399 (2000).
[28] S. Wessel, M. Olshanii, and S. Haas, Phys. Rev. Lett. **87**, 206407 (2001).
[29] Z. Honda *et al.*, Phys. Rev. B **63**, 064420 (2001); J. Appl. Phys. **89**, 7338 (2001).