Crossover behavior of the J_1-J_2 model in a staggered magnetic field

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The ground states of the $S=\frac{1}{2}$ Heisenberg chain with the nearest-neighbor and the next-nearest-neighbor antiferromagnetic couplings are numerically investigated in a staggered magnetic field. While the staggered magnetic field may induce the Néel-type excitation gap, and it is characterized by the Gaussian fixed point in the spin-fluid region, the crossover to the behavior controlled by the Ising fixed point is expected to be observed for the spontaneously dimerized state at finite field. Treating a low-lying excitation gap by the phenomenological renormalization-group method, we numerically determine the massless flow connecting the Gaussian and Ising fixed points. Further, to check the criticalities, we perform the finite-size-scaling analysis of the excitation gap.

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Theoretically and experimentally, there have been intensive investigations on critical phenomena observed in low-dimensional quantum spin systems. In particular, recent investigations on this subject have focused not only on critical fixed points and their neighboring regions, but also on the global behaviors of the renormalization-group (RG) flows connecting them. For one-dimensional (1D) quantum systems (also for 2D classical systems), besides the exact solutions available for some cases, the conformal field theory (CFT) provides the most efficient way to characterize the fixed points, where the values of the central charge c specify their universality classes. Further, with respect to the RG flows observed in the continuum and unitary models, Zamolodchikov's c-theorem serves for the explanations of their general properties.[1] Since in investigations of the quantum spin chains and interacting electron systems, the $c=1$ CFT has close relevance to their criticality,[2] it is very important to understand its instability and a crossover to behaviors controlled by other critical fixed points.

In this paper, we shall study the ground states of the $S=\frac{1}{2}$ Heisenberg chain with the nearest-neighbor and the next-nearest-neighbor antiferromagnetic couplings (the so-called J_1-J_2 model) in a staggered magnetic field; the Hamiltonian to be considered is given by $H=H_1+H_2$ with

$$H_1=\sum_{j=1}^{L}\left(2J_1\mathbf{S}_j\cdot\mathbf{S}_{j+1}+2J_2\mathbf{S}_j\cdot\mathbf{S}_{j+2}\right), \tag{1}$$

$$H_2=\sum_{j=1}^{L}-h_{\mathrm{s}}(-1)^j S_j^z, \tag{2}$$

where S_j^ν is the νth component of the spin operator on the jth site $\mathbf{S}_j$ and couplings J_1, $J_2>0$ (we take J_1 as the energy unit in the following). We assume the periodic boundary condition $\mathbf{S}_{L+1}=\mathbf{S}_1$ and an even number of L.

In the zero-field case $(h_{\mathrm{s}}=0)$, there are two special points where the exact ground states have been known: at $J_2=0$ where the Bethe ansatz solution is available, the system is in the spin-fluid phase described by the Gaussian fixed point ($c=1$ CFT); at $J_2=0.5$ (the Majumdar-Ghosh point), the direct products of spin singlet pairs formed either on bonds $\langle 2k,2k+1\rangle$ or $\langle 2k+1,2k+2\rangle$ become twofold degenerated ground states (i.e., spontaneously dimerized states),[3–5] and a finite excitation gap exists there.[6] According to Haldane,[7] and Kuboki and Fukuyama,[8] the gap formation caused by the frustration can be well described by the quantum sine-Gordon model obtained via the bosonization procedure;[9] the effective Hamiltonian of Eq. (1) is given as

$$\mathcal{H}_1=\int dx\,\frac{v}{2\pi}\left[K(\partial_x\theta)^2+\frac{1}{K}(\partial_x\phi)^2\right]+\int dx\,\frac{2g_\phi}{(2\pi\alpha)^2}\cos\sqrt{8}\phi, \tag{3}$$

where the bosonic operator θ is the dual field of ϕ satisfying the commutation relation $\partial_y[\phi(x),\theta(y)]=i\pi\delta(x-y)$. K and v are the Gaussian coupling and the spin-wave velocity, and g_ϕ stands for the spin Umklapp scattering bare amplitude.[10] Although the property of this effective continuum model has been well understood and actually the g_ϕ term may become relevant,[11] for the determination of the fluid-dimer transition point J_2^*, numerical treatments of Eq. (1) were required. By carefully investigating the effect of the marginal g_ϕ term on the critical fixed point through lower-energy excitation levels observed in finite-size systems, Okamoto and Nomura precisely determined $J_2^*\simeq 0.2411$.[12] While it is known that the excitation gap also exists in the case of $J_2>0.5$,[13] we, in the following discussion, restrict ourselves to the region $0\leqslant J_2\leqslant 0.5$ for simplicity.

In the case of nonzero field [this is approximately realized in the quasi-1D antiferromagnets with the alternating gyromagnetic tensors, e.g., Cu-benzoate[14] and Yb_4As_3 (Ref. 15) and the field may be also generated as the intrinsic one originated from the Néel ordered sublattice[16]] since the bosonized form of Eq. (2) is given as

$$\mathcal{H}_2=\int dx-\frac{h_{\mathrm{s}}}{\pi\alpha}\cos\sqrt{2}\phi, \tag{4}$$

and the scaling dimension of this perturbation term is $x_2=\frac{1}{2}$ $(1/\nu=2-x_2=3/2)$ on the fixed point,[17] the second-order phase transition occurs for systems in the spin-fluid region $J_2 \leqslant J_2^*$ with the divergence of correlation length $\xi \propto h_s^{-2/3}$ (aside from the logarithmic correction due to the g_ϕ term). On the other hand, for $J_2 > J_2^*$, due to the relevant g_ϕ term, the crossover of the transition driven by the staggered magnetic field occurs. Since the dimer gap may survive in a weak field, the critical point $h_s^*(J_2)$ takes nonzero values depending on J_2, and further the universality class is changed. Recently, Fabrizio *et al.*,[18] on the basis of the double-frequency sine-Gordon (DSG) theory given by Delfino and Mussardo,[19] argued that the system on $h_s^*(J_2)$ is renormalized to the Ising fixed point with $c=\frac{1}{2}$ in accord with the "downhill" condition of the c-theorem, so the criticality in the vicinity of this line is related to the divergent correlation length of the form $\xi \propto [h_s - h_s^*(J_2)]^{-1}$ (explained below) described by the φ^4 theory.

From the viewpoint that the Gaussian fixed point is perturbed by two relevant operators of g_ϕ and h_s, we can qualitatively estimate $h_s^*(J_2)$ around the point according to the crossover argument.[20] However, to evaluate its precise value especially near the Ising fixed point, a numerical treatment of H should be required. Here, it should be noted that the criticality on the Néel-phase boundaries in the $S=1$ bond-alternating XXZ chain also belongs to the Ising universality and they were precisely determined by the numerical method.[21] Thus, we shall perform our calculations by analyzing the lower-energy excitations observed in the finite-size systems. Let us first focus our attention to the excitations in the spin-fluid region described by the Gaussian fixed point,[22,23]

$$\mathcal{O}_1 = \sqrt{2}\sin\sqrt{2}\phi, \tag{5}$$

$$\mathcal{O}_2 = \sqrt{2}\cos\sqrt{2}\phi, \tag{6}$$

$$\mathcal{O}_3 = \exp(\pm i\sqrt{2}\theta). \tag{7}$$

$\mathcal{O}_1$ and $\mathcal{O}_2$ denote dimer and Néel excitations, respectively, while $\mathcal{O}_3$ is the doublet excitation changing an amount of the total spin. According to the finite-size-scaling (FSS) argument based on CFT, corresponding energy levels ΔE_i for these operators (taking the ground-state energy as zero) are expressed by the use of their scaling dimensions x_i as $\Delta E_i \simeq 2\pi v x_i / L$.[24] For the case of $h_s=0$, we can calculate ΔE_i according to the level-spectroscopy method,[23] where discrete symmetries of the lattice Hamiltonian (see below) are utilized to specify excitation levels. On the other hand, for the case of $h_s \neq 0$, the usable symmetry becomes lower, and more importantly, the universality class is changed to the Ising one on the line $h_s^*(J_2)$, so that we should employ other criterion to characterize the levels. Here, we will use the so-called UV-IR (ultraviolet-infrared) operator correspondence,[18,25] i.e., along the critical RG flow the operators on the Gaussian fixed point (UV) are transmuted to those on the Ising fixed point (IR) as

$$\mathcal{O}_1 \to \mu, \quad \mathcal{O}_2 \to I + \epsilon, \tag{8}$$

where μ is the disorder field (Z_2 odd) and ϵ is the energy density operator (Z_2 even) with scaling dimensions $x_\mu = \frac{1}{8}$ and $x_\epsilon = 1$, respectively. According to this correspondence, we can obtain a relevant excitation in nonzero field by taking the limit $h_s \searrow 0$ and assigning it to one of well-characterized states. From Eqs. (4) and (8), the staggered magnetic field plays a role of the "thermal" scaling variable on $h_s^*(J_2)$, and thus the critical exponent $1/\nu = 2 - x_\epsilon = 1$ as already mentioned (see Ref. 18). On one hand, since the "magnetic" excitation μ stemming from the dimer excitation provides lower energy (i.e., the most divergent fluctuation), we will thus focus attention on it for the determination of $h_s^*(J_2)$.

Now, we shall explain the numerical calculation procedure. Since the system is massive unless it is located on the critical line, the phenomenological renormalization-group (PRG) method is expected to work efficiently for our aim:[26] We numerically solve the PRG equation for the systems of L and $L+2$,

$$(L+2)\Delta E(J_2, h_s, L+2) = L\Delta E(J_2, h_s, L) \tag{9}$$

with respect to h_s for a given value of J_2. Since the equation can be satisfied by the gap having the size dependence of $\Delta E(J_2, h_s, L) \propto 1/L$, the obtained value can be regarded as the L-dependent transition point, say $h_s^*(J_2, L+1)$. Then, extrapolating them to the thermodynamic limit, we estimate $h_s^*(J_2)$. Alternatively, as explained in Refs. 22 and 23—to which we refer the interested readers for a detailed explanation—at $h_s=0$, the dimer excitation is in the subspace of total spin $S_T^z=0$, wave number $k=\pi$, space inversion $P=+1$, and spin reversal $T=+1$ for $L \equiv 0$ (mod 4) [$S_T^z=0$, $k=0$, $P=-1$, and $T=-1$ for $L \equiv 2$ (mod 4)]. Thus, we can calculate $\Delta E(J_2, h_s, L) = E_\mu(J_2, h_s, L) - E_g(J_2, h_s, L)$ from $E_\mu(J_2, h_s, L)$ connecting to the dimer excitation and $E_g(J_2, h_s, L)$, i.e., the ground-state energy.

In Fig. 1, we demonstrate L and h_s dependences of $L\Delta E(J_2, h_s, L)$ at several values of J_2. Systems up to $L=28$ sites are treated, where the Lanczos algorithm is used to obtain eigenvalues of the Hamiltonian in specified subspaces. We can see that the L dependence of the crossing point is almost absent for large value of J_2 (near $J_2=0.5$), while it is visible for the small value case.

After evaluating $h_s^*(J_2, L+1)$, we extrapolate them to $L \to \infty$; here we assume the following formula:

$$h_s^*(J_2, L) = h_s^*(J_2) + aL^{-2}(1 + bL^{-\omega}) \quad (\omega > 0), \tag{10}$$

where the b term stands for a correction to the leading one, and four parameters $h_s^*(J_2)$, a, b, and ω are determined according to the least-square-fitting condition. We used the data of $L=18$–28, and extrapolated them to $h_s^*(J_2)$ as shown in the inset of Fig. 2, where from bottom to top a series of data with fitting curves are given in the increasing order of J_2. Consequently, we obtain the critical line $h_s^*(J_2)$ as shown in the figure. The RG eigenvalue of the scaling variable g_ϕ is "almost zero" (i.e., marginal), while that of the staggered magnetic field is 3/2 on the point $(J_2, h_s) = (J_2^*, 0)$. The phase boundary is thus expected to behave as $h_s^*(J_2) \propto (J_2 - J_2^*)^{1.5/0_+}$, which agrees with a weak J_2 dependence of the line near the point.

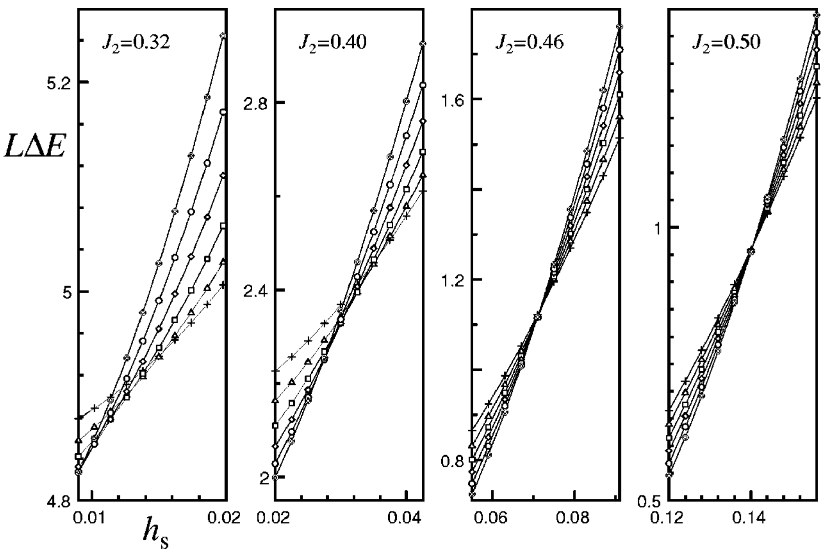

FIG. 1. The L and h_s dependences of $L\Delta E(J_2,h_s,L)$. From left to right, the next-nearest-neighbor coupling $J_2=0.32$, 0.40, 0.46, and 0.5. Data for systems of $L=18$ (crosses), 20 (triangles), 22 (squares), 24 (diamonds), 26 (circles), and 28 (double circles) are plotted with the fitting curves.

At this stage, we shall check the criticalities by the use of the FSS analysis in the vicinity of the boundary lines,[27] i.e., we assume the following one-parameter scaling form of the excitation gaps in the finite system of L:

$$\Delta E(J_2,h_s,L)=L^{-1}\Psi(L(h_s-h_s^*(J_2))^{\nu}), \qquad (11)$$

where $\nu=2/3$ for $J_2\leqslant J_2^*$ and $\nu=1$ for $J_2>J_2^*$. Further, the asymptotic behaviors of the scaling function are expected as $\Psi(x)\propto x$ for large x and $\Psi(x)\simeq\text{const}$ for $x\to 0$. Using the obtained transition points, we plot Eq. (11) for the Gaussian ($J_2=J_2^*$) and the Ising transitions ($J_2=0.46$ and 0.5) in Fig. 3. The results show that the data of different system sizes are collapsed on the single curve in both cases, and the asymptotic behaviors of Ψ agree with the expected ones (dotted lines) despite of the small L. From these plots, we can check the crossover behavior of the transitions driven by the staggered magnetic field in the present frustrated quantum spin chain system and also the accuracy of the phase boundary line in Fig. 2. This good FSS behaviors may rely on the conditions that the marginal operator that brings about the multiplicative logarithmic correction to the pure power-law singularity of ξ is absent on the fluid-dimer transition point,[28] and that the crossover region for $J_2>0.4$ may be large enough to be detected. On the other hand, the FSS nature becomes obscure in the weak and intermediate values of J_2 since our system sizes are too small to reach the region.

Finally, we evaluate the values of the central charge through the L dependence of the ground-state energy:[29]

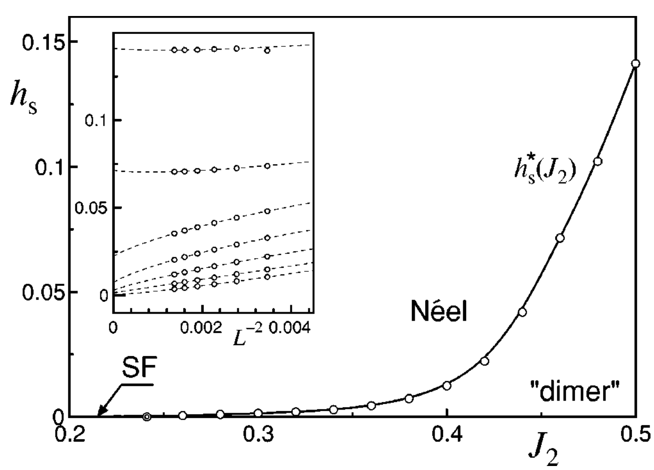

FIG. 2. The boundary line of the Néel and "dimer" phases (for an explanation of "dimer" phase, see Ref. 18). Inset shows some of extrapolations of the L-dependent critical fields to the thermodynamic limit, where fitting curves are given. The double circle shows the fluid-dimer transition point $(J_2,h_s)=(J_2^*,0)$ at which the criticality of the boundary changes from the Gaussian to the Ising type. The spin-fluid (SF) state exists on the x axis of $J_2\leqslant J_2^*$.

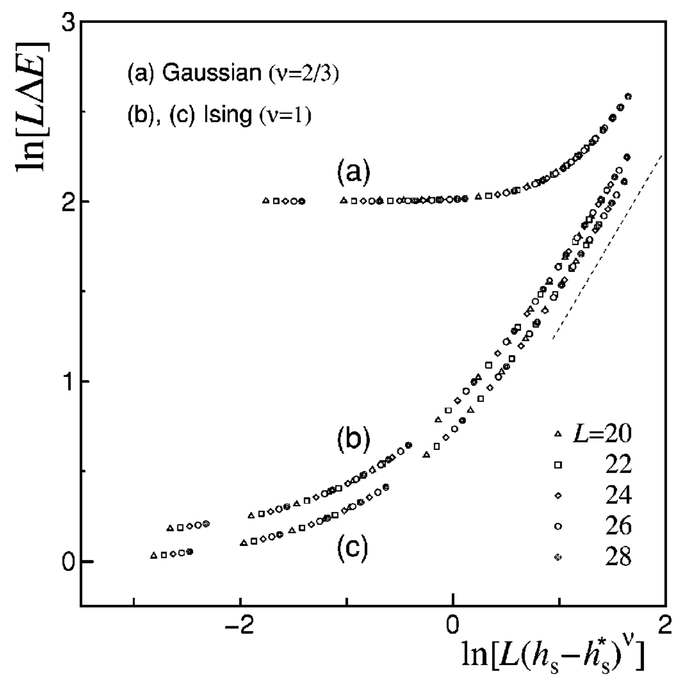

FIG. 3. The FSS plots of the excitation gap for systems of $L=20$–28 in log-log scale. We have used $\nu=2/3$ for the Gaussian transition [(a) $J_2=J_2^*$], and $\nu=1$ for the Ising transition [(b) $J_2=0.46$, (c) $J_2=0.5$]. The slope of the dotted line is 1 showing the expected asymptotic behavior of the scaling functions.

$$E_g(J_2,h_s^*(J_2),L)\simeq e_0L-\frac{\pi v c}{6L} \qquad (12)$$

(e_0 is the energy density in the thermodynamic limit). For this calculation, we should estimate v in advance; here we use the FSS relation $\Delta E_\mu \simeq 2\pi v x_\mu (=\frac{1}{8})/L$ and the least-square-fitting procedure for the data. The obtained results agree well with the Ising one for the considerably large values of J_2, i.e., $(v,c)\simeq(1.439,0.494)$ at $J_2=0.46$ and (1.248,0.491) at $J_2=0.50$. For comparison, we also estimate them at $J_2=J_2^*$ and obtain $(v,c)\simeq(2.365,0.995)$ [here the relation $\Delta E_1 \simeq 2\pi v x_1(=\frac{1}{2})/L$ has been used to estimate v]. Consequently, we can again confirm the universalities of critical systems on the phase boundary line. On the other hand, we could not extract the reliable data using the above procedure in the small and intermediate regions of J_2; this may be due to the finite-size effects on the line so that more detailed analysis might be required in this region.

To summarize, we have numerically investigated the ground-state phase diagram of the one-dimensional J_1-J_2 model in the staggered magnetic field. The crossover behavior of the second-order phase transitions driven by the staggered magnetic field occurs between the Gaussian and the Ising fixed points. According to the operator correspondence between these fixed points and using the level-spectroscopy technique, we have analyzed the Z_2-odd excitation gap by the use of the phenomenological renormalization-group method, and determined the boundary line $h_s^*(J_2)$ representing the massless flow connecting the fixed points. To check the two criticalities, we have performed the finite-size-scaling analysis of the excitation gap for typical parameter values, and we have also evaluated the values of the central charge.

The present investigation has based upon the recent development of the $(1+1)$-dimensional double-frequency sine-Gordon theory, where its very interesting applications in wide areas of researches including condensed matter physics have been pointed out.[18,19] However, as in the present case, numerical treatments of finite-size systems may be required for quantitative discussions on the lattice Hamiltonian models. We think that our numerical approach can also serve for the investigations of more complicated systems such as the correlated electrons;[30,31] we will report on the application results of this approach in the future publications.

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