Determination of boundary scattering, magnon-magnon scattering, and the Haldane gap in Heisenberg spin chains

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Low-lying magnon dispersion in a S = 1 Heisenberg antiferromagnetic (AF) chain is analyzed using the non-Abelian density-matrix-renormalization-group (DMRG) method. The scattering length a_b of the boundary coupling and the intermagnon scattering length a are determined. The scattering length a_b is found to exhibit a characteristic diverging behavior at the crossover point. In contrast, the Haldane gap Δ , the magnon velocity v, and a remain constant at the crossover. Our method allowed estimation of the gap of the S = 2 AF chain to be $\Delta = 0.0891623(9)$ using a chain length longer than the correlation length ξ .

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I. INTRODUCTION

To form a better understanding of interacting many-body systems, it is very important to determine an effective field theory and to clarify the low-energy physics involved. In the physics of low-dimensional quantum systems, considerable attention has been paid to the one-dimensional antiferromagnetic (AF) integer-spin Heisenberg model following the discovery of the Haldane gap.^{1,2} Precise determination of the gap has been reported by several authors.^{3–7} Its massive elementary excitation, i.e., the magnon, has a relativistic dispersion relation, which is often described by a nonlinear sigma model (NLSM).^{1,2,8,9}

In particular, the S = 1 AF Heisenberg chain has been widely studied both theoretically and experimentally. When open boundary conditions (OBC) are applied to a S = 1 AF chain, owing to the unique effective S = 1/2 spins at the ends, quasidegeneracy appears between the singlet ground state and a low-lying triplet state.¹⁰ Various attempts at boundary tuning,³ as exemplified by attachment of real S = 1/2spins to maintain the high accuracy of the density-matrixrenormalization-group (DMRG) method,^{11,12} have shown that deformation of the boundary conditions can selectively modify the magnon wave function while maintaining the uniformity of the ground state.¹³

To form a better understanding of the physics involved in a finite chain under OBC, we can use the NLSM to describe the low-lying energy dispersion. Lou et al. have proposed usage of a form $\sqrt{\Delta^2 + v^2 \sin^2 k_{\text{eff}}}$ for low-lying magnon dispersions, where $k_{\rm eff}$ is the effective wave number.¹⁴ Here, Δ denotes the Haldane gap and v is the velocity of the quasiparticle. They described the asymptotic effects of boundary scattering and intermagnon interactions in terms of the scattering lengths $a_{\rm b}$ and a, which appear in $k_{\rm eff}$. When boundary tuning is applied by introducing an antiferromagnetic coupling J_{end} between the S = 1 spin chain and the extra real S = 1/2 spin, these scattering lengths might be effected. This idea motivated us to study low-lying elementary excitations using both the DMRG and NLSM methods by describing the bulk properties and the boundary-scattering effects in terms of an effective theory. In this work, using the DMRG method, the energy dispersion of various magnon modes was determined for S = 1Heisenberg systems with up to 2048 spins. Finite-size scaling analysis was performed to determine the boundary-scattering length and the intermagnon scattering length, in addition to Δ and v in the thermodynamic limit. We used a relation of the correlation length $\xi \sim v/\Delta$, which is known to hold approximately in the integer-spin AF Heisenberg chain.^{15,16} We found that $a_{\rm b}$ changed sign around a critical value of $J_{\rm end}$. This value should be identical to that required to make local quantities such as the local bond energy of the ground state and the spin density of long-wavelength magnons uniform.^{3,6,17,18} In addition, a divergence-like behavior of a_b was detected around this critical value denoted as J_{end}^{c} . However, the intermagnon scattering length was found to be constant at $a = -0.383(6)\xi$ irrespective of J_{end} . In this derivation, Δ , v, and ξ were confirmed to be always independent of J_{end} in the thermodynamic limit. This allows the low-lying elementary excitations to be effectively described. The results indicated the presence of both itinerating magnons (IMs) and boundary magnons (BMs) bound at the ends. At J_{end}^c , the diagonal magnetization induced by an IM shows a flat structure around the center of the system when $L \gg \xi$, with L being the number of S = 1 spins. Both the diverging behavior of $a_{\rm b}$ and the uniform distribution of the long-wavelength magnons confirm the realization of bulk characteristics in an elementary excitation at the critical point J_{end}^{c} , where the ground state also has a uniform nature around the center of the system.

Furthermore, this work clearly resolves the problem pointed out by Todo and Kato;⁴ there is disagreement between the DMRG¹⁹ and quantum Monte Carlo (QMC) simulation results⁴ with respect to estimation of the excitation gap in the S = 2 AF Heisenberg model. The reason for this disagreement might be an inappropriate scaling assumption in the DMRG study. This work applies finite-size scaling analysis to the excitation gap in the S = 2 AF chain, and shows that the corrected gap is within the error bar of the QMC value.

II. EFFECTIVE HAMILTONIAN

We consider an S = 1 AF chain with boundary S = 1/2 spins s_j with j = 0 or L + 1, which is described by the following Hamiltonian:

$$H(J_{\text{end}}) = \sum_{i=1}^{L-1} \mathbf{S}_i \cdot \mathbf{S}_{i+1} + J_{\text{end}}(\mathbf{s}_0 \cdot \mathbf{S}_1 + \mathbf{S}_L \cdot \mathbf{s}_{L+1}), \quad (1)$$

where S_i represents the S = 1 operator at the *i*th site.

The low-energy physics of the Hamiltonian (1) can be understood by using an approximate mapping onto the NLSM.^{1,2,8,9} We let $L \rightarrow \infty$, keeping X = Lb constant, with *b* being the lattice spacing. Taking into account the effective S =1/2 boundary modes s_{eff}^{eff} , we obtain the following expression:

$$H_{\text{eff}} = H_{\text{NLSM}} + \lambda_s \left[\boldsymbol{\phi}(0) \cdot \mathbf{s}_1^{\text{eff}} + (-1)^L \boldsymbol{\phi}(X) \cdot \mathbf{s}_L^{\text{eff}} \right] + \lambda_u \left[\mathbf{l}(0) \cdot \mathbf{s}_1^{\text{eff}} + \mathbf{l}(X) \cdot \mathbf{s}_L^{\text{eff}} \right] + \lambda'_s \left[\boldsymbol{\phi}(0) \cdot \mathbf{s}_0 + (-1)^L \boldsymbol{\phi}(X) \cdot \mathbf{s}_{L+1} \right] + \lambda'_u \left[\mathbf{l}(0) \cdot \mathbf{s}_0 + \mathbf{l}(X) \cdot \mathbf{s}_{L+1} \right] + J_{\text{eff}}^{\text{eff}} \left(\mathbf{s}_1^{\text{eff}} \cdot \mathbf{s}_0 + \mathbf{s}_L^{\text{eff}} \cdot \mathbf{s}_{L+1} \right), \qquad (2)$$

with the bulk part of the NLSM expressed as

$$H_{\rm NLSM} = \frac{v}{2} \int_0^X dx \left[g \mathbf{l}^2 + \frac{1}{g} \left(\frac{\partial \boldsymbol{\phi}}{\partial x} \right)^2 \right], \tag{3}$$

where ϕ and $\mathbf{l} \equiv (1/vg)\phi \times \partial_t \phi$ are low-energy Fourier modes of the spin operators with wave vectors near π and 0. The coupling parameter and the velocity are given as $g = \frac{2}{S}$ and v = 2S. Since all the bare couplings are antiferromagnetic, solutions for the bulk fields follow the Neumann boundary conditions (NBC): $d\phi/dx|_{x=0,X} = 0$.¹⁴ The λ_u and λ'_u terms produce an effective boundary repulsive potential on an IM and $J_{\text{end}}^{\text{eff}}$ is a renormalized coupling constant.

The validity of this description is also confirmed by examining the spin density of an IM shown in Fig. 1. When J_{end} is larger than J_{end}^c , the lowest triplet mode has itinerating behavior. Indeed, we see that $\langle S_i^z \rangle$ exhibits a cosine-like behavior for $J_{end} = 1.0$ owing to both strong repulsive coupling via λ_u and λ'_u and the NBC on $\phi(x)$. When J_{end} approaches $J_{end}^c \sim 0.51$, the IM mode becomes uniform around the center of the chain but $\langle S_i^z \rangle$ exhibits damped oscillations near the two ends. This known solution suggests that the mode should continuously change into an end mode $\mathbf{s}_j^{\text{eff}}$ in the low-energy eigenstate when $J_{eff} < J_{eff}^c$.

Thus the dispersion relation for N itinerating magnon modes at low energies in the dilute limit may be simply



FIG. 1. (Color online) Distribution of local magnetization $\langle S_j^z \rangle$ for a single-magnon state with $S_{tot} = 1$ for various values of J_{end} .

reproduced by a nonrelativistic effective Hamiltonian for N virtual particles:

$$H_{\rm eff}(J_{\rm end}) = \frac{1}{2m} \sum_{i=1}^{N} \frac{d^2}{dx_i^2} + \sum_{\langle i,j \rangle} V(x_i - x_j) + \sum_{i=1}^{N} [V_{\rm b}(J_{\rm end}, x_i) + V_b(J_{\rm end}, X - x_i)], \quad (4)$$

where $0 \le x_j \le X$, with a wave function obeying the Neumann boundary condition: $\partial_j \psi(x_1, \ldots, x_N)|_{x_j=0,X} = 0$. Here, we use the Einstein relation $m \equiv \Delta/v^2$. Effective short-range interactions between IMs and between an IM and a BM are represented by *V* and *V*_b, respectively. We expect they are short-range functions with a range of the order of the correlation length ξ . All of the effects of J_{end} are produced by the boundary potential $V_b(J_{\text{end}},x)$ In the asymptotic region, the effects of *V* and *V*_b appear as scattering phase shifts, which are represented by *a* and a_b .

We now identify low-lying magnon modes. Each mode is specified by a total spin of S_{tot} . When J_{end} is small and positive, since we have two effective S = 1/2 spins creating the bulk low-lying triplet and two real S = 1/2 spins, we need to polarize these four spins before we can create one IM. In this case, the effective chain length for the IM becomes $L - 2a_b$ and $k_{eff} = \pi/(L - 2a_b)$, when the system is about two times longer than the correlation length ξ . Therefore, we have the relation:

$$E_{32} = \sqrt{\Delta^2 + v^2 \sin^2 \frac{\pi}{L - 2a_{\rm b}}},\tag{5}$$

where $E_{ji} = E_j - E_i$ and E_j and E_i are the lowest energy of the $S_{\text{tot}} = j$ and $S_{\text{tot}} = i$ states. The energy spectrum E_{42} for two IMs is given by

$$E_{42} = \sum_{j=1}^{2} \sqrt{\Delta^2 + v^2 \sin^2 \frac{j\pi}{L - 2a_b - a}},$$
 (6)

where we use the small-*k* approximation for the magnonmagnon phase shift. When J_{end} becomes large enough, the effective boundary S = 1/2 modes couple strongly with the real S = 1/2 spins. In this condition, the low-lying magnon states are IMs, and the formulas for E_{10} and E_{20} are, respectively, similar to Eqs. (5) and (6). Thus we can conclude that a crossover value of J_{end}^c exists where the low-energy spectrum changes qualitatively.

III. NUMERICAL RESULTS

We used the non-Abelian DMRG method (NA-DMRG)²⁰ to estimate the energy spectrum of the lowest $S_{tot} = 0, 1, 2, 3$, and 4 states for finite systems. Numerical convergence during finite-system sweeping was accelerated by the use of a wave-function-prediction method.^{21–26} Since the number of kept states for the block spin is up to $m_s = 512$, the truncation error is smaller than 1.0×10^{12} in the lowest $S_{tot} = 4$ state. This corresponds to a number of kept states of $m_{s^z} \sim 2500-2700$ in the standard DMRG. In this case, the numerical cost of the standard DMRG is about 110–140 times higher than that of NA-DMRG because in the DMRG it varies as the cube



FIG. 2. (Color online) Single-magnon energy with $J_{\rm end}$ under the condition $m_s = 512 \ (m_{s^z} \sim 2500)$. The dotted line represents $v^2 \sin^2[\pi/(L-2a_b)]$.

of the number of kept states. The system size L + 2 is up to 2048, where the two extra spins indicate the boundary S = 1/2 spins.

The energy of a single IM as a function of the system size is shown in Fig. 2. The target energy spectrum is E_{32} when $J_{\text{end}} = 0$, and E_{10} when $J_{\text{end}} = 0.6$ or 1. To estimate Δ , v, and $a_{\rm b}$, we generated sequences $A^*(L_0 + 2)$ for different values of $L = L_0$, where $A^*(L)$ denotes finite values of $A = \Delta$, v, and $a_{\rm b}$ in the thermodynamic limit. The sequences were determined by least-square fitting with the function $\sqrt{\Delta^2 + v^2 \sin^2 \frac{\pi}{L - 2a_b}}$ for IM energies of $L + 2 = 2^{\ell}(L_0 + 2)$, where $\ell = 0, \pm 1$. The value of A was estimated by power-law extrapolation with elements of $A^*(512)$ and $A^*(1024)$. The estimation error was taken to be $|A - A^*(1024)|$. Based on the optimum boundary scattering length $a_{b}(J_{end})$ for each J_{end} , we found a universal finite-size dependence for a fixed energy gap Δ and spin velocity v. As a result, we showed that only the boundary scattering length a_b was affected by changing J_{end} , whereas Δ and v were independent of J_{end} (see Table I). This result is consistent with the effective model in Eq. (4).

The estimated values of Δ , v, and $\xi = v/\Delta$ are consistent to within $\Delta = 0.4104792485(4)$, v = 2.46685(2), and $\xi =$



FIG. 3. (Color online) Boundary-scattering length and intermagnon scattering length as a function of J_{end} . The dotted line represents $J_{end} = 0.50865$.

6.00967(5), respectively, except for a somewhat larger error at $J_{end} = 0.4$ and 0.6, which are closest to J_{end}^{c} . Since our data is obtained by extrapolation using system sizes larger than those treated in former studies,^{3,4} our results show meaningful differences. The reported value of $a_b(J_{end} = 0) =$ -1 in Ref. 14 is about three times larger than our result of $a_{\rm b}(J_{\rm end}=0)=-0.3748(1)$. The value of $a_{\rm b}(J_{\rm end})$ changes rather dramatically with J_{end} (see Fig. 3) with a change in sign even occurring around $J_{end} \sim 0.5$. The values seem to diverge around J_{end}^{c} . When the boundary-scattering length becomes $a_b \to -\infty$, $k_{eff} = \pi/(L - 2a_b)$ approaches zero, and the energy of the lowest IM is almost at its minimum value, Δ , and is independent of J_{end} . This is consistent with the report in Refs. 3 and 17. However, we should note that the above picture holds only when $L \gg a_b$, requiring a high-performance simulation tool such as NA-DMRG.

In the same manner, using the estimated Δ , v, and a_b , we determined the intermagnon scattering length a. The target energy spectrum is E_{42} when $J_{end} < J_{end}^c$, and is E_{20} when $J_{end} > J_{end}^c$. With a common a, universal behavior is observed in the large L region. The estimated values of a are consistent to within $a = -2.30(4) = -0.383(6)\xi$ except for a somewhat larger error at $J_{end} = 0.4$ and 0.6. (See Table I and Fig. 3.) Thus

TABLE I. Results of numerical simulations for a single itinerating magnon, showing magnon energy Δ , magnon velocity v, boundaryscattering length a_b , intermagnon scattering length a, and correlation length $\xi = v/\Delta$, a_b/ξ , and a/ξ .

Jend	Δ	υ	a _b	а	ξ	$a_{\rm b}/\xi$	a/Ę
0	0.4104792487(1)	2.466838(1)	-0.3748(1)	-2.30(2)	6.009654(1)	-0.06237(2)	-0.383(4)
0.1	0.4104792486(1)	2.466844(2)	-0.0836(3)	-2.301(2)	6.009669(4)	-0.01391(5)	-0.3830(4)
0.2	0.4104792487(1)	2.46684(1)	0.540(2)	-2.303(5)	6.00966(3)	0.0898(3)	-0.3833(9)
0.3	0.4104792486(4)	2.46684(4)	2.081(8)	-2.30(4)	6.0096(1)	0.346(1)	-0.384(6)
0.4	0.410479248(2)	2.4668(3)	7.33(5)	-2.3(2)	6.0098(7)	1.220(9)	-0.38(5)
0.6	0.410479248(2)	2.4668(2)	-16.93(2)	-2.3(2)	6.0096(5)	-2.821(6)	-0.38(3)
0.7	0.4104792483(2)	2.46685(3)	-9.586(5)	-2.30(3)	6.00968(7)	-1.5951(9)	-0.382(4)
0.8	0.4104792483(2)	2.46685(2)	-7.317(3)	-2.30(2)	6.00968(4)	-1.2176(5)	-0.383(3)
0.9	0.4104792483(2)	2.46685(2)	-6.233(3)	-2.30(2)	6.00968(4)	-1.0372(5)	-0.383(3)
1.0	0.4104792485(1)	2.46684(1)	-5.605(3)	-2.30(2)	6.00967(4)	-0.9328(5)	-0.383(3)

we conclude that the value of *a* is independent of J_{end} . The estimated value of *a* is comparable to $a = -0.32\xi$ in Ref. 14. In Fig. 3, the dotted line represents $J_{end} = 0.50865$ determined in Ref. 6.

IV. APPLICATION TO S = 2 HEISENBERG CHAIN AND CONCLUSIONS

We have shown that the energy spectrum modified by the tuning parameter J_{end} can be fitted using an effective massive relativistic dispersion with a boundary-scattering length $a_b(J_{end})$ modified for lattice models. The intermagnon scattering length *a* is constant irrespective of J_{end} as well as other bulk quantities including the Haldane gap, the magnon velocity, and the correlation length. In contrast, $a_b(J_{end})$ drastically changes around $J_{end} \sim 0.5$, representing a crossover point for the physics at the boundary.

Analysis of the boundary-scattering length and intermagnon scattering length was also carried out for an S = 2AF Heisenberg chain, where S_i and s_i in the Hamiltonian in Eq. (1) represent the S = 2 and S = 1 operators, respectively. In addition, we choose $J_{end} = 1$, so that the low-lying magnon states are IMs and a similar formula for E_{10} is obtained to that shown in Eq. (5). Our data was taken using $m_s = 1024$, which corresponds to $m_{s^z} \sim 6000$ and large systems up to L + 2 = 2048. The truncation error is smaller than 1×10^{-11} . Note that the numerical cost using NA-DMRG is about 200 times less than that for the standard DMRG in this case. In contrast to a former report,²⁷ our results suggest a large value of $a_b(J_{end} = 1) = -33(1) = -0.67(2)\xi$. Our calculations give the excitation gap $\Delta = 0.0891623(9)$, the spin velocity v =4.42(1), and the correlation length $\xi = 49.6(1)$. In particular, the value of Δ obtained in the present study is consistent with the value of 0.08917(4) determined by quantum Monte Carlo simulations.⁴ The estimate of the Haldane gap has thus been improved by two more significant digits. This indicates the ability of the effective theory to correctly describe the low-energy physics and the usefulness of the proposed numerical approach is studying such problems.

It would be of interest to apply the approach used in this work to finite-size scaling with different boundary tuning methods such as hyperbolic deformation.^{13,28,29} In such a situation, the excited quasiparticle is weakly confined near the center of the system under the deformation. In Ref. 28, we showed that it is necessary to introduce an additional parameter d and replace L + 1 by L + d in order to reduce higher-order corrections. This replacement is introduced in the effective model shown in Eq. (4) by considering the effective boundary scattering. The boundary-scattering length has an important and universal influence on excitation energy scaling as long as there are chain ends.

In this work, a relation $\xi = v/\Delta$ is used to estimate the correlation length in each spin-*S* chain. If we use an assumption for a relation between the low-energy dispersion curve and the ground-state correlation length, namely $\sinh \xi^{-1} = \Delta/v$ in this case,³⁰ the correlation lengths are evaluated as 6.03720(9) in S = 1 and 49.6(1) in S = 2. In the case of S = 1, we have a meaningful different value from the former estimation. On the contrary, the difference is not confirmed in the case of S = 2. To find correct relation between the low-energy dispersion and the correlation length in each spin-*S* AF Heisenberg chain is a future issue.

For a final development of the low-lying effective field theory to describe the low-lying magnon dispersions, discussions for rigorous results of wave functions and energy dispersions for low-lying states are important. The effective dispersion relation of $\sqrt{\Delta^2 + v^2 \sin^2 k_{\text{eff}}}$ is known to appear in the Haldane phase³¹ and also in the massive phase of the S = 1/2 Heisenberg XXZ model.³² The Bethe-ansatz solutions for OBC suggest that an analogous crossover from an IM with real k_{eff} to a BM with a damping nature can be found as a continuous change from a real to an imaginary rapidity.³³

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