Correlation amplitudes for the spin-$\frac{1}{2}$ XXZ chain in a magnetic field

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We present accurate numerical estimates for the correlation amplitudes of leading and main subleading terms of the two- and four-spin correlation functions in the one-dimensional spin-1/2 XXZ model under a magnetic field. These data are obtained by fitting the correlation functions, computed numerically with the density-matrix renormalization-group method, to the corresponding correlation functions in the low-energy effective theory. For this purpose we have developed the Abelian bosonization approach to the spin chain under the open-boundary conditions. We use the numerical data of the correlation amplitudes to quantitatively estimate spin gaps induced by a transverse staggered field and by exchange anisotropy.

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I. INTRODUCTION

The one-dimensional spin-1/2 XXZ model is a basic and well-studied model in statistical physics. In some parameter range its ground state is critical and spin-spin correlation functions exhibit quasi-long-range order. The model represents a typical example of Tomonaga-Luttinger (TL) liquids in which elementary excitations are gapless collective modes rather than single-particle excitations, in contrast to three-dimensional systems. These features are uncovered by extensive theoretical studies over the years which have employed various powerful methods including the Bethe ansatz,[1] bosonization technique,[2] and the conformal field theory.[3] One-dimensional spin chains are also important from the experimental viewpoint, as they are relevant to many quasi-one-dimensional magnets in which couplings along one direction are considerably stronger than those in the other two directions.

In this paper, we discuss long-distance asymptotes of equal-time correlation functions in the spin-1/2 XXZ chain in a magnetic field. The Hamiltonian is

$$\mathcal{H}_0=J\sum_l (S_l^xS_{l+1}^x+S_l^yS_{l+1}^y+\Delta S_l^zS_{l+1}^z)-H\sum_l S_l^z, \quad (1)$$

where $J>0$ and $\boldsymbol{S}_l=(S_l^x,S_l^y,S_l^z)$ is an $S=1/2$ spin operator on the lth site of the chain. The anisotropy parameter Δ is assumed to satisfy the inequality $\Delta>-1$ such that the system is in the critical regime for a certain range of magnetic fields, i.e., $0\leqslant|H|<H_{c2}$ for $-1<\Delta\leqslant 1$ and $H_{c1}<|H|<H_{c2}$ for $\Delta>1$, where H_{c1} and H_{c2} are the lower and upper critical fields, respectively. The spins partially polarized by the field H have a finite magnetization per site, M, where $-1/2<M<1/2$. The low-energy excitations of $\mathcal{H}_0$ in the critical regime are free massless bosons. They are governed by the Gaussian theory,

$$\tilde{\mathcal{H}}_0=\frac{v}{2}\int dx\left[\left(\frac{d\phi}{dx}\right)^2+\left(\frac{d\tilde{\phi}}{dx}\right)^2\right], \quad (2)$$

where v is the renormalized spin-wave velocity and the bosonic fields $\phi(x)$ and $\tilde{\phi}(x)$ obey the commutation relation $[\phi(x),\tilde{\phi}(y)]=-(i/2)[1+\mathrm{sgn}(x-y)]$. We take the lattice spacing $a=1$ and identify the site index l with the continuous space variable x. For a better description of low-energy physics, one needs to add to $\tilde{\mathcal{H}}_0$ an irrelevant operator $\cos(2\phi/R)$: This operator becomes marginal at $\Delta=1$ and $H=0$ yielding logarithmic corrections, while it is relevant and opens a spin gap for $\Delta>1$ and $0<|H|<H_{c1}$. We ignore this term in this paper, however. This may introduce systematic errors in our analysis for $\Delta\gtrsim 1$ and small M. The spin operators are related to the bosonic fields[3–5] as

$$S_l^z=M+\frac{1}{2\pi R}\frac{d\phi}{dx}-a_1(-1)^l\sin\left(Ql+\frac{\phi(l)}{R}\right)+\cdots, \quad (3)$$

$$S_l^+=e^{i2\pi R\tilde{\phi}(l)}\left[b_0(-1)^l+b_1\sin\left(Ql+\frac{\phi(l)}{R}\right)+\cdots\right], \quad (4)$$

where $Q=2\pi M$ is incommensurate wave number, and a_n and b_n are nonuniversal constants which depend on Δ and M. The TL liquid parameter (or the compactification radius) R characterizes the asymptotic behavior of correlation functions and its exact value is readily obtained by solving the Bethe ansatz integral equations.[6–8] Essentially all the low-energy properties of the spin chain (1) follow from Eqs. (2)–(4). For example, the ground-state two-spin correlation functions are found to decay algebraically,[9,10]

$$\langle S_l^xS_{l'}^x\rangle=A_0^x\frac{(-1)^{l-l'}}{|l-l'|^\eta}-A_1^x\frac{\cos[Q(l-l')]}{|l-l'|^{\eta+1/\eta}}+\cdots, \quad (5)$$

$$\langle S_l^zS_{l'}^z\rangle=M^2-\frac{1}{4\pi^2\eta|l-l'|^2}+A_1^z(-1)^{l-l'}\frac{\cos[Q(l-l')]}{|l-l'|^{1/\eta}}+\cdots. \quad (6)$$

The decay exponent $\eta=2\pi R^2$ is a function of Δ and M. For $-1<\Delta\leqslant 1$, $\eta=1-\cos^{-1}(\Delta)/\pi$ at $M=0$, while $\eta=2$ at $M\to+0$ for $\Delta>1$. As M increases, η varies monotonically and approaches the universal value 1/2 in the limit $M\to 1/2$. The amplitudes A_n^x and A_n^z are related to the coefficients a_n and b_n. Recently Lukyanov and co-workers[11–13] have obtained exact formulas of the correlation amplitudes in Eqs. (5) and (6) at $M=0$ and $-1<\Delta\leqslant 1$. Nevertheless their values at $M\neq 0$ are not known analytically.

The aim of this paper is to numerically determine the nonuniversal coefficients a_n and b_n with high accuracy for arbitrary M. We first extend the bosonic representation of the spin operators (3) and (4) to a more general form of infinite series, and calculate the spin polarization $\langle S_l^z \rangle$ and the two-spin correlation functions $\langle S_l^x S_{l'}^x \rangle$ and $\langle S_l^z S_{l'}^z \rangle$ within the bosonization theory. The analytic formulas so obtained are used to fit numerical data which we compute by using the density-matrix renormalization group (DMRG) method.[14,15] The fitting parameters are the coefficients a_n and b_n. This scheme is basically the same as the one used in our previous studies,[16,10] and in this paper we provide more accurate numerical data of the coefficients a_1, b_0, and b_1 for wider range of parameters.

The information on the coefficients is crucial for quantitative analysis on effects of perturbations to which the critical ground state of the spin-1/2 XXZ model has instabilities. Such perturbations include bond alternation,[17,18] next-nearest-neighbor coupling,[19–21] and transverse staggered magnetic field.[22–25] In the bosonization approach, a perturbation written in the original spin operators is translated into bosonic operators through Eqs. (3) and (4). The impact of the perturbation on the ground state, the vacuum state of the Gaussian model (2), can be qualitatively estimated from scaling dimension of the perturbation operators, which depends only on the TL liquid parameter R. It is, however, necessary to know the exact values of the nonuniversal coefficients a_n and b_n as well, to quantitatively analyze effects of the perturbation, e.g., to estimate magnitude of an energy gap induced by the perturbation or to compute correlation functions in the presence of the perturbation. As an example of such quantitative analysis we calculate the spin gap induced by the staggered transverse field[22–25] from the numerical data of the coefficients.

There are often cases when perturbations are composite operators of two (or more) spins, such as exchange interactions. In this case one must consider fusion of two operators. In general, fusing two spin operators at short distances may generate operators which are not present in each single-spin operator which is fused. Consequently, the leading term of the correlator of the composite operator may be different from a product of the leading terms of the correlators of the single-spin operators. We illustrate this by taking the nearest-neighbor coupling $S_l^x S_{l+1}^x$ as an example. We examine operators generated by the fusion of S_l^x and S_{l+1}^x. From a numerical fitting of four-spin correlation functions, we estimate the amplitude of a leading uniform term of the correlation function. The results are used to analyze the spin gap induced by the perturbation of exchange anisotropy.[26,27]

The paper is organized as follows. We briefly review the Abelian bosonization approach to the model (1) in the following section. The bosonic representation of spin operators in the form of infinite series is introduced in Sec. II A. We then use it to derive the analytic formulas of the two- and four-spin correlation functions in Secs. II B and II C. In Sec. III, we present the numerical results on the correlation functions obtained from the DMRG calculation. The numerical data of amplitudes of the two- and four-spin correlation functions are presented in Secs. III A and III B, respectively. We show that the numerical results are in excellent agreement with analytical predictions available for various limiting cases. Furthermore, we discuss the spin gaps induced by the perturbations of staggered transverse field and exchange anisotropy in Sec. III C. Finally, we summarize the results in Sec. IV. The Appendix explains bosonization of spin operators.

II. BOSONIZATION

A. Spin operators

In this section, we summarize the Abelian bosonization technique applied to the spin-1/2 XXZ chain in a magnetic field. Let us first express the original spin operators S_l^x and S_l^z in terms of the bosonic fields. To this end, we follow and extend the scheme of Refs. 3 and 4. We begin with the bosonic representation of electron operators in the Hubbard model with the on-site repulsion U. At half filling we have a gapped charge mode and a gapless spin mode. After constructing spin operators from the electron operators, we integrate out the gapped charge mode to obtain a bosonic representation of the spin operators in the Heisenberg chain. We then generalize the result to the XXZ case. A detailed derivation is presented in the Appendix, and here we show only the final results,

$$S_l^z = \frac{1}{2\pi R}\frac{d\phi}{dx} - \sum_{n=0}^{\infty} a_{2n+1}(-1)^l \sin\left[(2n+1)\frac{\phi(x)}{R}\right], \tag{7}$$

$$S_l^+ = e^{i2\pi R\tilde{\phi}(x)} \sum_{n=0}^{\infty} \left\{ b_{2n}(-1)^l \cos\left[2n\frac{\phi(x)}{R}\right] + b_{2n+1}\sin\left[(2n+1)\frac{\phi(x)}{R}\right]\right\}, \tag{8}$$

where a_n and b_n are nonuniversal constants. They depend on the short-distance regularization of the Gaussian theory as well as on the parameters Δ and M. Equations (3) and (4) are just the first few terms of Eqs. (7) and (8) with the shift of the field $\phi(x) \to \phi(x) + QRx$. In principle the right-hand side of Eqs. (7) and (8) should contain descendant fields as well. It follows from Eq. (8) that

$$\begin{aligned} S_l^x &= \tfrac{1}{2}(S_l^+ + S_l^-) = \tfrac{1}{2}[S_l^+ + (S_l^+)^\dagger] \\ &= \sum_{n=0}^{\infty} \left\{ b_{2n}(-1)^l \cos[2\pi R\tilde{\phi}(x)] \cos\left[2n\frac{\phi(x)}{R}\right] + i b_{2n+1} \sin[2\pi R\tilde{\phi}(x)] \sin\left[(2n+1)\frac{\phi(x)}{R}\right]\right\}. \end{aligned} \tag{9}$$

Here we have used the commutator $[\phi(x), \tilde{\phi}(x)] = -i/2$. An equivalent bosonic representation of the spin operators is recently derived in Ref. 13 from global symmetry analysis of the lattice and field operators. Our derivation in Appendix is complementary to Ref. 13.

B. Two-spin correlation functions

The two-spin correlation functions are readily calculated by the bosonization method. Let us first consider the thermodynamic limit where the correlation functions depend only on the distance between the two spins. In this case we expand the bosonic fields $\phi(x)$ and $\tilde{\phi}(x)$ as

$$\phi(x)=\int_0^\infty dk\frac{e^{-\lambda k/2}}{\sqrt{4\pi}}\left[\frac{e^{ikx}}{\sqrt{k-i\delta}}(\alpha_k+\alpha_{-k}^\dagger)+\frac{e^{-ikx}}{\sqrt{k+i\delta}}(\alpha_k^\dagger+\alpha_{-k})\right]+QRx, \tag{10}$$

$$\tilde{\phi}(x)=\int_0^\infty dk\frac{e^{-\lambda k/2}}{\sqrt{4\pi}}\left[\frac{e^{ikx}}{\sqrt{k+i\delta}}(-\alpha_k+\alpha_{-k}^\dagger)+\frac{e^{-ikx}}{\sqrt{k-i\delta}}(-\alpha_k^\dagger+\alpha_{-k})\right], \tag{11}$$

where α_k and $\alpha_k^\dagger$ are boson operators obeying the commutation relation $[\alpha_k,\alpha_{k'}^\dagger]=\delta(k-k')$, λ is a short-distance cutoff, and δ is a positive infinitesimal. The fields $\phi(x)$ and $\tilde{\phi}(x)$ defined by Eqs. (10) and (11) satisfy the commutation relation $[\phi(x),\tilde{\phi}(y)]=-i\Theta(x-y)$ in the limit $\lambda\to 0$, where $\Theta(x)$ is the step function. The Gaussian Hamiltonian (2) defined on the whole real x axis now reads

$$\tilde{\mathcal{H}}_0=\int_0^\infty vk(\alpha_k^\dagger\alpha_k+\alpha_{-k}^\dagger\alpha_{-k})dk+\text{const.} \tag{12}$$

Thus, the ground state $|0\rangle$ of the Hamiltonian (1) corresponds to the vacuum for the bosons α_k, i.e., $\alpha_k|0\rangle=0$. Substituting Eqs. (10) and (11) to Eqs. (7) and (9), we obtain the equal-time two-point correlators in the thermodynamic limit,

$$\langle S_l^x S_{l'}^x\rangle=\sum_{n=0}^\infty\left\{A_{2n}^x(-1)^{l-l'}\frac{\cos[2nQ(l-l')]}{|l-l'|^{\eta+(2n)^2/\eta}}-A_{2n+1}^x\frac{\cos[(2n+1)Q(l-l')]}{|l-l'|^{\eta+(2n+1)^2/\eta}}\right\}, \tag{13}$$

$$\langle S_l^z S_{l'}^z\rangle=M^2-\frac{1}{4\pi^2\eta|l-l'|^2}+\sum_{n=0}^\infty A_{2n+1}^z(-1)^{l-l'}\frac{\cos[(2n+1)Q(l-l')]}{|l-l'|^{(2n+1)^2/\eta}}, \tag{14}$$

where $\langle\cdots\rangle=\langle 0|\cdots|0\rangle$ represents the expectation value in the lowest-energy state in the sector with magnetization M. If we adopt the regularization

$$\int_0^\infty dk\frac{e^{-\lambda k}}{k}(1-\cos kx)=\ln x, \tag{15}$$

then the correlation amplitudes are related to the coefficients in Eqs. (7) and (9) by

$$A_n^x=\frac{b_n^2}{4}(1+\delta_{n,0}),\quad A_n^z=\frac{a_n^2}{2}. \tag{16}$$

For $M=0$ and $-1<\Delta<1$, the values of the amplitudes A_0^x, A_1^x, and A_1^z are obtained by analytical[28,11–13] and numerical[16] methods. We note that in principle the long-distance expansions (13) and (14) should also include contributions from the descendants ignored in Eqs. (7) and (9) and those from the irrelevant operators discarded in $\tilde{\mathcal{H}}_0$.[13]

As mentioned in the Introduction, we determine the coefficients a_n and b_n by fitting numerically computed correlation functions to appropriate formulas. Since the numerical DMRG method works best for finite-size systems with open boundaries, we need to calculate the correlation functions under the open-boundary conditions. For this purpose we employ the open-boundary bosonization scheme developed in Refs. 16 and 10. Suppose that the XXZ spin chain of our interest consists of L spins $\boldsymbol{S}_l$ $(l=1,2,\ldots,L)$. This is equivalent to assuming $\boldsymbol{S}_0=\boldsymbol{S}_{L+1}=0$. In the bosonic representation this amounts to having the Gaussian model (2) defined in the finite region $0<x<L+1$ with Dirichlet boundary conditions at $x=0$ and $x=L+1$. Our convention is that

$$\phi(0)=0,\quad \phi(L+1)=2\pi RLM. \tag{17}$$

These boundary conditions are consistent with Eqs. (7)–(9). Once we fix the boundary conditions (17) and the regularization scheme, the coefficients a_n are uniquely determined whereas the coefficients b_n are determined only up to a phase factor. Instead of Eqs. (10) and (11), we now have the mode expansion[5,10,16]

$$\phi(x)=\frac{x}{L+1}\phi_0+\sum_{n=1}^\infty\frac{\sin(q_nx)}{\sqrt{\pi n}}(\tilde{\alpha}_n+\tilde{\alpha}_n^\dagger), \tag{18}$$

$$\tilde{\phi}(x)=\tilde{\phi}_0+i\sum_{n=1}^\infty\frac{\cos(q_nx)}{\sqrt{\pi n}}(\tilde{\alpha}_n-\tilde{\alpha}_n^\dagger), \tag{19}$$

where $q_n=\pi n/(L+1)$, $[\tilde{\phi}_0,\phi_0]=i$, and $\tilde{\alpha}_n$ and $\tilde{\alpha}_n^\dagger$ are boson operators satisfying $[\tilde{\alpha}_n,\tilde{\alpha}_{n'}^\dagger]=\delta_{n,n'}$. The Gaussian model (2) becomes

$$\tilde{\mathcal{H}}_0=\sum_{n=1}^\infty vq_n\tilde{\alpha}_n^\dagger\tilde{\alpha}_n+\frac{v\phi_0^2}{2(L+1)}-\frac{\pi v}{24(L+1)}. \tag{20}$$

The lowest-energy state of the spin chain (1) with magnetization M corresponds to a vacuum of bosons $\tilde{\alpha}_n|0\rangle=0$ with $\phi_0|0\rangle=2\pi RLM|0\rangle$. To calculate the zero-temperature correlation functions, we substitute Eqs. (18) and (19) into Eqs. (7) and (9) and take average with respect to the state $|0\rangle$. (The readers interested in the detailed calculation should refer to Ref. 10.) We obtain

$$\langle S_l^x S_{l'}^x\rangle = \frac{f_{\eta/2}(2l) f_{\eta/2}(2l')}{f_\eta(l-l') f_\eta(l+l')} \sum_{n,n'=0}^{\infty} \frac{s(n,n';l,l') b_n b_{n'}}{4 f_{n^2/2\eta}(2l) f_{n'^2/2\eta}(2l')} \times \left\{ \cos[q(nl+n'l')] \frac{f_{nn'/\eta}(l-l')}{f_{nn'/\eta}(l+l')} + \cos[q(nl-n'l')] \frac{f_{nn'/\eta}(l+l')}{f_{nn'/\eta}(l-l')} \right\}, \tag{21}$$

$$\langle S_l^z S_{l'}^z\rangle = \left(\frac{q}{2\pi}\right)^2 - \sum_{n=1}^{\infty}{}' \frac{q a_n}{2\pi} \left[\frac{(-1)^l \sin(nql)}{f_{n^2/2\eta}(2l)} + \frac{(-1)^{l'} \sin(nql')}{f_{n^2/2\eta}(2l')} \right] - \frac{1}{4\pi^2\eta} \left[\frac{1}{f_2(l-l')} + \frac{1}{f_2(l+l')} \right]$$
$$+ \sum_{n,n'=1}^{\infty}{}' \frac{(-1)^{l-l'} a_n a_{n'}}{2 f_{n^2/2\eta}(2l) f_{n'^2/2\eta}(2l')} \left\{ \cos[q(nl-n'l')] \frac{f_{nn'/\eta}(l+l')}{f_{nn'/\eta}(l-l')} - \cos[q(nl+n'l')] \frac{f_{nn'/\eta}(l-l')}{f_{nn'/\eta}(l+l')} \right\}$$
$$- \frac{1}{2\pi\eta} \sum_{n=1}^{\infty}{}' n a_n \left\{ \frac{(-1)^l \cos(nql)}{f_{n^2/2\eta}(2l)} [g(l+l') + g(l-l')] + \frac{(-1)^{l'} \cos(nql')}{f_{n^2/2\eta}(2l')} [g(l+l') - g(l-l')] \right\}, \tag{22}$$

$$\langle S_l^z \rangle = \frac{q}{2\pi} - \sum_{n=1}^{\infty}{}' a_n \frac{(-1)^l \sin(nql)}{f_{n^2/2\eta}(2l)}, \tag{23}$$

where $q = 2\pi ML/(L+1)$,

$$f_\nu(x) = \left[\frac{2(L+1)}{\pi} \sin\left(\frac{\pi|x|}{2(L+1)} \right) \right]^\nu, \tag{24}$$

$$g(x) = \frac{\pi}{2(L+1)} \cot\left(\frac{\pi x}{2(L+1)} \right), \tag{25}$$

and the sum Σ' is taken over odd n only. We have used the regularization $\Sigma_{n=1}^{\infty}[1-\cos(q_n x)]/n = \ln[f_1(x)]$ as in our previous studies.[16,10] The factor $s(n,n';l,l')$ in Eq. (21) is

$$s(n,n';l,l') = \begin{cases} (-1)^{(n+1)l+(n'+1)l'+(n+n')/2} & \text{if } n+n' = \text{even} \\ (-1)^{(n+1)l+(n'+1)l'+(n'-n+1)/2} \operatorname{sgn}(l-l') & \text{if } n+n' = \text{odd}. \end{cases}$$

In the thermodynamic limit ($L \to \infty$ with $|l-L/2| \ll L$, and $|l'-L/2| \ll L$) the correlators (21) and (22) reduce to Eqs. (13) and (14).

C. Four-spin correlation functions

In this section, we discuss fusion of two operators taking $S_l^x S_{l+1}^x$ as an example. To find bosonic representation of the composite operator $S_l^x S_{l+1}^x$, we need operator product expansion of the operators in Eq. (9). We explicitly write down the product of S_l^x and S_{l+1}^x as

$$S_l^x S_{l+1}^x = \frac{1}{16} \sum_{\epsilon_1,\epsilon_2,\epsilon_1',\epsilon_2' = \pm 1} \sum_{n_1,n_2=0}^{\infty} X(\{\epsilon_i,\epsilon_i',n_i\};l), \tag{26}$$

where

$$X(\{\epsilon_i,\epsilon_i',n_i\};l) = b_{n_1} b_{n_2} t(\{\epsilon_i,\epsilon_i',n_i;l\}) \times \exp\{i2\pi R[\epsilon_1 \tilde{\phi}(l) + \epsilon_2 \tilde{\phi}(l+1)]\} \times \exp\left\{ \frac{i}{R} [n_1 \epsilon_1' \phi(l) + n_2 \epsilon_2' \phi(l+1)] \right\}, \tag{27}$$

and $t(\{\epsilon_i,\epsilon_i',n_i;l\})$ is defined by $t=-1$ ($n_1,n_2=$ even), $t=-\epsilon_1\epsilon_2\epsilon_1'\epsilon_2'$ ($n_1,n_2=$ odd), $t=-i(-1)^l\epsilon_2\epsilon_2'$ ($n_1=$ even and $n_2=$ odd), $t=i(-1)^l\epsilon_1\epsilon_1'$ ($n_1=$ odd and $n_2=$ even). To find the first few leading operators in the expansion (26), we make each exponential operator in Eq. (27) in normal order and expand the fields $\phi(l+1)$ and $\tilde{\phi}(l+1)$ as $\phi(l+1) = \phi(l) + d\phi(l)/dl + \cdots$. It turns out that the leading operators in Eq. (26) come from the following three contributions.

(i) $\epsilon_1+\epsilon_2=0$ and $n_1\epsilon_1' + n_2\epsilon_2' = 0$. In this case X is expanded as a sum of a constant (identity operator) term, $d\phi/dx$ and $d\tilde{\phi}/dx$ with scaling dimension 1, and higher-order terms.

(ii) $\epsilon_1+\epsilon_2=0$ and $n_1\epsilon_1'+n_2\epsilon_2'=\pm 1$. The leading operators in the expansion of X are $(-1)^l\exp[\pm i\phi(l)/R]$, whose scaling dimension is $1/(2\eta)$.

(iii) $\epsilon_1+\epsilon_2=\pm 2$ and $n_1\epsilon_1'+n_2\epsilon_2'=0$. The leading operators in this case are $\exp[\pm i4\pi R\tilde{\phi}(l)]$, which have dimension 2η.

We thus find that the operator $S_l^xS_{l+1}^x$ has the expansion

$$S_l^xS_{l+1}^x=c_0+c_0'\frac{d\phi(l)}{dl}+c_0''\frac{d\tilde{\phi}(l)}{dl}+c_1(-1)^l\sin\frac{\phi(l)}{R}+c_1'(-1)^l\cos\frac{\phi(l)}{R}+c_2\cos[4\pi R\tilde{\phi}(l)]+\cdots. \tag{28}$$

Apart from the constant term c_0, the leading term in $S_l^xS_{l+1}^x$ is the oscillating one with the coefficients c_1 and c_1' if $\Delta>0$ ($\eta>1/2$), while it is the nonoscillating term with c_0' and c_0'' if $\Delta<0$ ($\eta<1/2$). We note that, for both signs of Δ, the leading term in the expansion of $S_l^xS_{l+1}^x$ is not simply given by the product of the leading operators in S_l^x and S_{l+1}^x. In fact, the higher-order terms with large n in Eq. (9), which can be ignored in the calculation of long-distance asymptotes of two-point correlation functions, give contributions to the leading operator in the operator product expansion of $S_l^xS_{l+1}^x$. The same observation can be made for the other subleading terms in $S_l^xS_{l+1}^x$. This result illustrates that when one fuses two (or more) operators at short distances, information on only a few leading terms of each operator is, in general, not enough to determine the leading terms in the bosonic representation of the fused operator. Instead, one must survey contributions from all higher-order terms.

Calculating the coefficients c_n from the coefficients b_n is hardly possible not only because each c_n has contributions from infinitely many b_n's but also because of the ambiguity due to the short-distance cutoff. It is thus more practical to estimate the c_n's from the four-spin correlation function $\langle S_l^xS_{l+1}^xS_{l'}^xS_{l'+1}^x\rangle$ and its variants. From Eq. (28) we know the asymptotic behavior of the four-spin correlation functions,

$$\langle S_l^xS_{l+1}^xS_{l'}^xS_{l'+1}^x\rangle=B_0+B_1\frac{(-1)^{l-l'}}{|l-l'|^{1/\eta}}\cos[Q(l-l')]+\frac{B_0'}{|l-l'|^2}+\frac{B_2}{|l-l'|^{4\eta}}+\cdots, \tag{29}$$

$$\langle :(S_l^+S_{l+1}^-+S_l^-S_{l+1}^+)::(S_{l'}^+S_{l'+1}^-+S_{l'}^-S_{l'+1}^+):\rangle=16B_1\frac{(-1)^{l-l'}}{|l-l'|^{1/\eta}}\cos[Q(l-l')]+\frac{16B_0'}{|l-l'|^2}+\cdots, \tag{30}$$

$$\langle S_l^+S_{l+1}^+S_{l'}^-S_{l'+1}^-\rangle=\frac{8B_2}{|l-l'|^{4\eta}}+\cdots, \tag{31}$$

where $:\mathcal{O}:=\mathcal{O}-\langle\mathcal{O}\rangle$. The correlation amplitudes are related to the coefficients c_n by $B_0=c_0^2$, $B_1=(c_1^2+c_1'^2)/2$, $B_0'=-(c_0'^2+c_0''^2)/2\pi$, and $B_2=c_2^2/2$.

III. NUMERICAL RESULTS

In this section, we present numerical results on the correlation amplitudes in the two- and four-spin correlation functions obtained from the DMRG calculation.[14,15] We calculate the spin polarization $\langle S_l^z\rangle$, the two-spin correlation functions $\langle S_l^xS_{l'}^x\rangle$ and $\langle S_l^zS_{l'}^z\rangle$, and the four-spin correlation functions $\langle :(S_l^+S_{l+1}^-+S_l^-S_{l+1}^+)::(S_{l'}^+S_{l'+1}^-+S_{l'}^-S_{l'+1}^+):\rangle$ and $\langle S_l^+S_{l+1}^+S_{l'}^-S_{l'+1}^-\rangle$ in the open XXZ chain of $L=200$ sites. The correlation functions are calculated for $l=r_0-r/2$ and $l'=r_0+r/2$, where r_0 represent the center position of the chain, $r_0=L/2$ (for even r) or $r_0=(L+1)/2$ (for odd r). The numerical calculation is done using the finite system algorithm, and the number of kept states m is up to 200. We estimate the numerical error due to the DMRG truncation from difference between the data computed with $m=200$ and those with $m=150$. The estimated errors for the spin polarization, two-, and four-spin correlation functions are typically less than 10^{-7}, 10^{-6}, and 10^{-6}, respectively, and sufficiently small for accurate estimation of the amplitudes.

A. Amplitudes of two-spin correlation functions

First, we show the results on the spin polarization $\langle S_l^z\rangle$ and the two-spin correlation functions $\langle S_l^xS_{l'}^x\rangle$ and $\langle S_l^zS_{l'}^z\rangle$. Since the nth-order terms in Eqs. (7) and (9) contribute to the correlators less and less for large n, we may neglect the higher-order terms with $n\geqslant 2$ in the fitting procedure. That is to say, we fit the DMRG data to the analytic formulas (21)–(23) setting $a_n=b_n=0$ for $n\geqslant 2$ and taking b_0, b_1, and a_1 as fitting parameters. We note that this scheme for determining the coefficients is basically the same as those used in our previous studies,[16,10] in one[10] of which the numerical data of A_1^z and A_0^x are reported for several typical values of M and $0\leqslant\Delta\leqslant 1$. However, in that work[10] the decay exponent η as well as the coefficients was taken as a fitting parameter, and this could cause small but avoidable errors in the estimates of the coefficients. In the present work, we use the exact value of η obtained from the Bethe ansatz solutions. We therefore believe that the estimates of the coefficients presented here are even more accurate than the previous ones.

Figure 1 shows the two-spin correlation functions $\langle S_l^xS_{l'}^x\rangle$, $\langle S_l^zS_{l'}^z\rangle$, and the spin polarization $\langle S_l^z\rangle$ at $\Delta=0.5,0,-0.5$ and $M=0.25$. The DMRG data and the fitting results are plotted with the open and solid symbols, respectively. The excellent agreement between them demonstrates that the fitting procedure works extremely well at least for the parameters used in Fig. 1. To determine the correlation amplitudes, we perform the fitting for the data of several ranges, $20\leqslant r\leqslant 140$, $20\leqslant r\leqslant 180$, $60\leqslant r\leqslant 140$, and $60\leqslant r\leqslant 180$ for the two-spin correlation functions, and $20\leqslant l\leqslant 180$, $40\leqslant l\leqslant 160$, and $60\leqslant l\leqslant 140$ for the spin polarization. We then take the mean and the variance of the fitting results as the estimate and the error of the numerical values

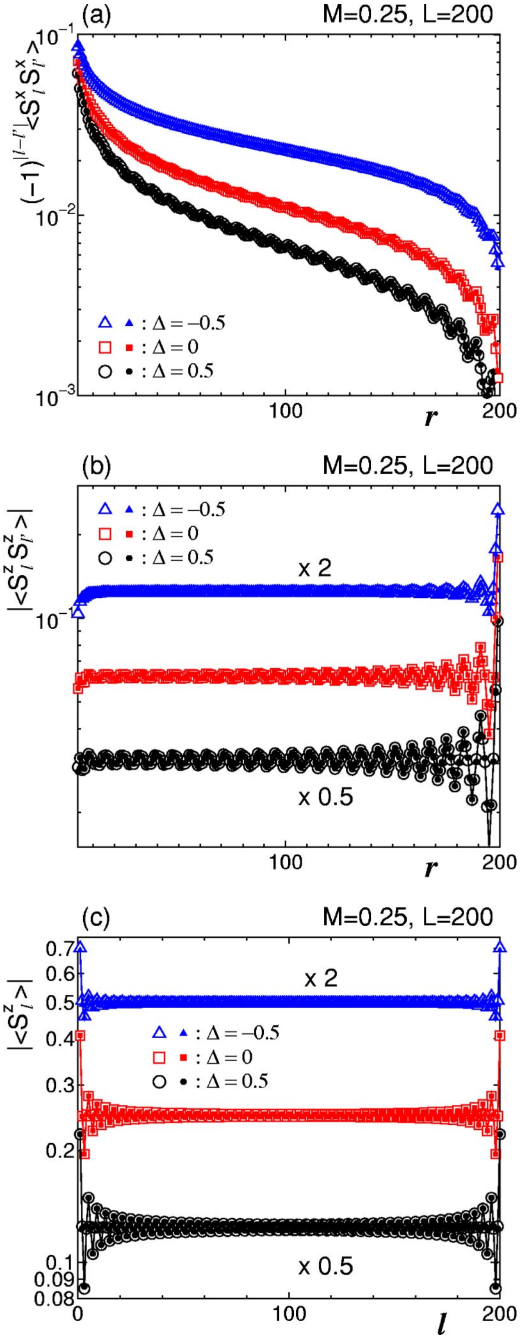

FIG. 1. (Color online) (a) $(-1)^{|l-l'|}\langle S_l^x S_{l'}^x\rangle$ vs $r=|l-l'|$, (b) $|\langle S_l^z S_{l'}^z\rangle|$ vs r, and (c) $|\langle S_l^z\rangle|$ vs l for $\Delta=0.5$, 0, and -0.5 and $M=0.25$. The open symbols are the DMRG data while the small dots are the results of fitting.

of the amplitudes, respectively. The results of $A_0^x=b_0^2/2$, $A_1^x=b_1^2/4$ estimated from $\langle S_l^x S_{l'}^x\rangle$ and $A_1^z=a_1^2/2$ estimated from $\langle S_l^z\rangle$ are plotted in Fig. 2 as functions of M for several typical values of Δ.[29] As shown in the figure, the amplitudes take nonuniversal values at $M=0$ and vary smoothly as M increases. We have confirmed that the data of A_1^z estimated from the correlation function $\langle S_l^z S_{l'}^z\rangle$ coincide with those obtained from $\langle S_l^z\rangle$ within error bars. We note that, for small $\Delta\lesssim -0.8$, the accuracy of the estimated amplitudes A_1^x and A_1^z becomes considerably poor. This difficulty might be due to the fact that, for this parameter range, the subleading terms $\propto A_1^x, A_1^z$ of the correlation functions become considerably smaller than the nonoscillating leading terms. Further studies with a more elaborated scheme will be required for accurate estimation of $A_1^{x,z}$ in this case.

To further examine the accuracy of the numerical estimates obtained above, we compare them with exact results which are available for some limiting cases.

At $M=0$, the correlation amplitudes A_0^x, A_1^x, and A_1^z for $-1<\Delta<1$ are analytically calculated:[11–13]

$$A_0^x=\frac{1}{8(1-\eta)^2}\left[\frac{\Gamma\left(\frac{\eta}{2(1-\eta)}\right)}{2\sqrt{\pi}\,\Gamma\left(\frac{1}{2(1-\eta)}\right)}\right]^{\eta}\times\exp\left[-\int_0^\infty\frac{dt}{t}\left(\frac{\sinh(\eta t)}{\sinh(t)\cosh[(1-\eta)t]}-\eta e^{-2t}\right)\right], \tag{32}$$

$$A_1^x=\frac{1}{2\eta(1-\eta)}\left[\frac{\Gamma\left(\frac{\eta}{2(1-\eta)}\right)}{2\sqrt{\pi}\,\Gamma\left(\frac{1}{2(1-\eta)}\right)}\right]^{\eta+(1/\eta)}\times\exp\left[-\int_0^\infty\frac{dt}{t}\left(\frac{\cosh(2\eta t)e^{-2t}-1}{2\sinh(\eta t)\sinh(t)\cosh[(1-\eta)t]}+\frac{1}{\sinh(\eta t)}-\frac{\eta^2+1}{\eta}e^{-2t}\right)\right], \tag{33}$$

$$A_1^z=\frac{2}{\pi^2}\left[\frac{\Gamma\left(\frac{\eta}{2(1-\eta)}\right)}{2\sqrt{\pi}\,\Gamma\left(\frac{1}{2(1-\eta)}\right)}\right]^{1/\eta}\times\exp\left[\int_0^\infty\frac{dt}{t}\left(\frac{\sinh[(2\eta-1)t]}{\sinh(\eta t)\cosh[(1-\eta)t]}-\frac{2\eta-1}{\eta}e^{-2t}\right)\right], \tag{34}$$

where $\Gamma(x)$ is the Gamma function. These equations were previously confirmed by numerical calculations,[16,10,12] and here we have found that the numerical estimates of the present work with higher accuracy are even in better agreement with the above exact formulas for $-0.8\lesssim\Delta\lesssim 0.8$.

In the saturation limit $M\to 1/2$, exact asymptotic form of the correlation $\langle S_l^x S_{l'}^x\rangle$ can be obtained from known exact results on the hard-core boson model.[30–32] It follows that near the saturation limit the amplitudes A_0^x and A_1^x should behave as

$$A_0^x=\frac{\rho}{2\sqrt{\pi}}\left(\frac{1}{2}-M\right)^{1/2}, \tag{35}$$

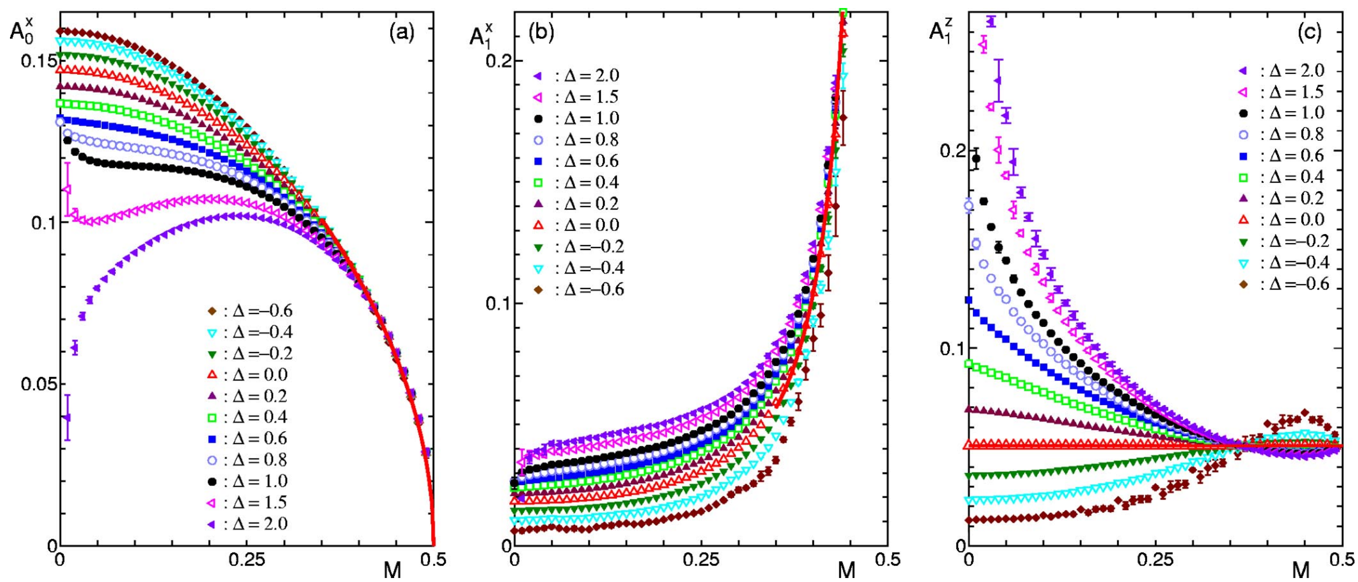

FIG. 2. (Color online) Amplitudes of the two-spin correlation functions as functions of M for several typical values of Δ; (a) A_0^x, (b) A_1^x, and (c) A_1^z. A_0^x and A_1^x shown in (a) and (b) are estimated from $\langle S_l^x S_{l'}^x \rangle$. A_1^z for $M>0$ in (c) are estimated from $\langle S_l^z \rangle$ while A_1^z at $M=0$ are from $\langle S_l^z S_{l'}^z \rangle$. The solid curves plotted for large M in (a) and (b) represent Eqs. (35) and (36), respectively, while the solid line in (c) represents the exact result $A_1^z = 1/(2\pi^2)$ valid at $\Delta=0$.

$$A_1^x = \frac{\rho}{16\pi^{5/2}}\left(\frac{1}{2}-M\right)^{-3/2}, \tag{36}$$

where ρ is a universal constant related to Glaisher's constant A by $\rho=\pi e^{1/2}2^{-1/3}A^{-6}=0.92418\ldots$. We can see in Figs. 2(a) and 2(b) that, for all Δ's shown, the numerical data of A_0^x and A_1^x approach the predicted behavior shown by the solid curves. Note that there is no free parameter in the theoretical predictions (35) and (36).

As for the $\langle S_l^z S_{l'}^z \rangle$ correlation, it is expected from Eq. (14) that the amplitude A_1^z should converge to a universal value $1/(2\pi^2)$ at $M\to 1/2$ for arbitrary Δ, since in this limit η becomes 1/2 and the correlator must take the constant value 1/4. Furthermore, for $\Delta=0$ one can easily calculate $\langle S_l^z S_{l'}^z \rangle$ exactly using the Jordan-Wigner transformation to find $A_1^z = 1/(2\pi^2)$ for arbitrary M. We clearly see that the numerical data of A_1^z in Fig. 2(c) agree with these predictions.

From these observations, we conclude that our estimates for the correlation amplitudes A_0^x, A_1^x, and A_1^z are pretty accurate, except for the following parameter regime: (i) $\Delta \lesssim -0.8$ and (ii) $\Delta \gtrsim 0.8$ and $M=0$. In the latter regime the leading irrelevant operator $\cos(2\phi/R)$ is no longer negligible. We point out that diverging behavior at $M=0$, due to the presence of the (almost) marginal operator, can be clearly seen in the data of A_0^x and A_1^z for $\Delta \gtrsim 0.8$.

B. Amplitudes of four-spin correlation functions

Next we discuss numerical results of the four-spin correlation functions. Figure 3 shows the numerical data of the four-spin correlation functions $\langle :(S_l^+ S_{l+1}^- + S_l^- S_{l+1}^+)::(S_{l'}^+ S_{l'+1}^- + S_{l'}^- S_{l'+1}^+): \rangle$ and $\langle S_l^+ S_{l+1}^+ S_{l'}^- S_{l'+1}^- \rangle$ for $\Delta=0.5$, 0, and -0.5 and $M=0.05$. We see that the correlator $\langle :(S_l^+ S_{l+1}^- + S_l^- S_{l+1}^+)::(S_{l'}^+ S_{l'+1}^- + S_{l'}^- S_{l'+1}^+): \rangle$ shows power-law decay with the exponent equal to either $1/\eta$ (for $\Delta \geqslant 0$) or 2 (for $\Delta<0$), while $\langle S_l^+ S_{l+1}^+ S_{l'}^- S_{l'+1}^- \rangle$ always decays with the exponent 4η. We have found the same behavior for other values of Δ and M. These results are consistent with Eqs. (29)–(31).

To estimate the amplitude $B_2 = c_2^2/2$, we fit the numerical data of $\langle S_l^+ S_{l+1}^+ S_{l'}^- S_{l'+1}^- \rangle$ to its analytical formula for finite chains with open boundaries,

$$\begin{aligned}\langle S_l^+ S_{l+1}^+ S_{l'}^- S_{l'+1}^- \rangle &= (2c_2)^2 \langle \exp[i4\pi R\tilde{\phi}(l)] \\ &\quad \times \exp[-i4\pi R\tilde{\phi}(l')]\rangle \\ &= 8B_2 \frac{f_{2\eta}(2l) f_{2\eta}(2l')}{f_{4\eta}(l+l') f_{4\eta}(l-l')},\end{aligned} \tag{37}$$

where we used Eq. (19). We see in Fig. 3 that the data of $\langle S_l^+ S_{l+1}^+ S_{l'}^- S_{l'+1}^- \rangle$ are fitted by the formula extremely well. The estimated values of B_2 from the fitting procedure are shown in Fig. 4. We see that for each Δ the amplitude takes a nonuniversal value at $M=0$, decreases monotonically as M increases, and vanishes eventually at $M\to 1/2$. We note that for $\Delta=0$ the analytic form of $\langle S_l^+ S_{l+1}^+ S_{l'}^- S_{l'+1}^- \rangle$ can be easily calculated, yielding $B_2 = [1+\cos(2\pi M)]/16\pi^2$. Figure 4 shows that the numerical data for $\Delta=0$ are in good agreement with the formula. We also compare the numerical estimate of B_2 at $M=0$ and $-1<\Delta<1$ with the exact formula of B_2 derived recently by Lukyanov and Terras,[13]

$$B_2 = \frac{[\Gamma(\eta)]^4}{2^{3+4\eta}\pi^{2+2\eta}(1-\eta)^2}\left[\frac{\Gamma\left(\dfrac{1}{2-2\eta}\right)}{\Gamma\left(\dfrac{\eta}{2-2\eta}\right)}\right]^{4-4\eta}. \tag{38}$$

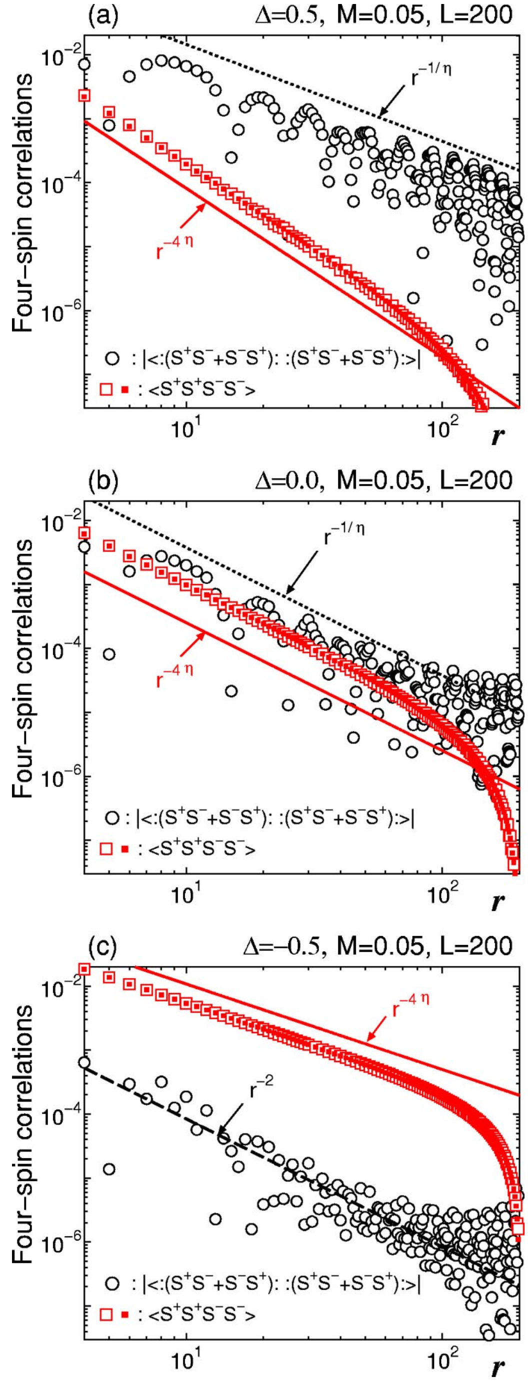

FIG. 3. (Color online) Four-spin correlation functions $|\langle :(S_l^+S_{l+1}^-+S_l^-S_{l+1}^+)::(S_{l'}^+S_{l'+1}^-+S_{l'}^-S_{l'+1}^+):\rangle|$ (open circles) and $\langle S_l^+S_{l+1}^+S_{l'}^-S_{l'+1}^-\rangle$ (open squares) vs $r=|l-l'|$ for $M=0.05$ and (a) $\Delta=0.5$, (b) $\Delta=0$, and (c) $\Delta=-0.5$. The solid, dotted, and dashed lines correspond, respectively, to the algebraic decay of $r^{-4\eta}$, $r^{-1/\eta}$, and r^{-2}. The fitting results for $\langle S_l^+S_{l+1}^+S_{l'}^-S_{l'+1}^-\rangle$ using Eq. (37) are plotted by solid squares.

Here again we find good agreement between the exact result and our numerical data. This is another evidence that our estimates are highly reliable. At $M=0$ and $\Delta\geqslant 1$, B_2 shows a diverging behavior due to the marginal operator, suggesting the breakdown of our analysis.

Unfortunately, we cannot achieve a precise estimation of

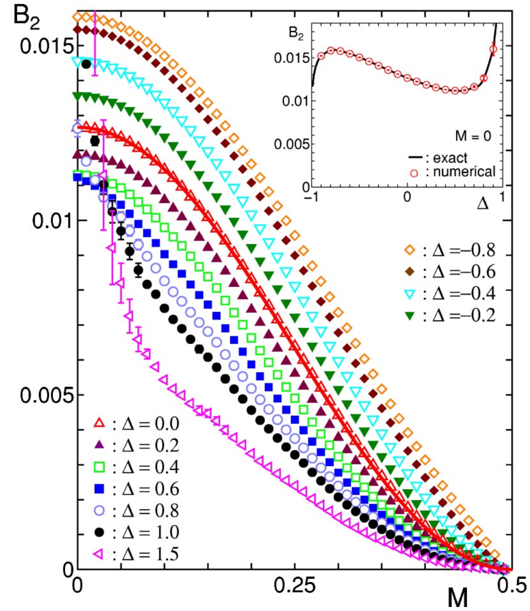

FIG. 4. (Color online) Amplitude B_2 of the four-spin correlation function $\langle S_l^+S_{l+1}^+S_{l'}^-S_{l'+1}^-\rangle$ as functions of M for several typical values of Δ. The solid curve represent the relation $B_2=[1+\cos(2\pi M)]/16\pi^2$ expected for $\Delta=0$. Inset: Numerical estimates of the amplitude B_2 at $M=0$ (open circles) and the analytical prediction Eq. (38) (solid curve).

the amplitude B_1 of the leading oscillating term in $\langle :(S_l^+S_{l+1}^-+S_l^-S_{l+1}^+)::(S_{l'}^+S_{l'+1}^-+S_{l'}^-S_{l'+1}^+):\rangle$ due to the presence of subleading terms which give sizable contributions to the correlation function. This issue of estimating B_1 is left for future studies.

C. Spin gap

The data of the correlation amplitudes obtained in the preceding sections is useful for analyzing effects of perturbations of single-spin type and exchange-coupling type in the bosonization framework. To illustrate how this scheme works, we compute spin gaps induced by such perturbations to the Hamiltonian (1).

As an example of the perturbation of the single-spin type, we consider effects of the staggered transverse field. The perturbation to the Hamiltonian (1) is given by

$$\mathcal{H}'=-h_s\sum_l (-1)^l S_l^x. \tag{39}$$

It has been shown that $\mathcal{H}'$ induces a spin gap. This field-induced gap is believed to be the origin of the spin-gap behavior observed in Cu benzoate[22–25,33] and Yb_4As_3[34–36] under a uniform field, in which the staggered field emerges due to the alternating g-tensor and the Dzyaloshinskii-Moriya interaction. In these materials, exchange anisotropy is negligibly small and the staggered transverse field h_s is proportional to the uniform field H. Thus, we may set $\Delta=1$ and $h_s=\gamma H$, where γ is a constant specific to each material.

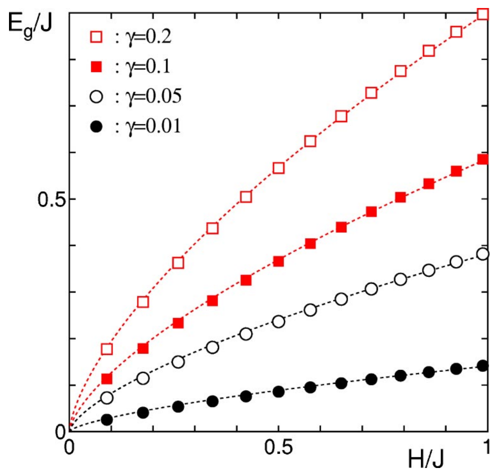

FIG. 5. (Color online) Field dependence of the spin gap in the Heisenberg chain $\mathcal{H}_0(\Delta=1)$ in a uniform field H and a staggered transverse field $h_s=\gamma H$. The dotted curves represent the expected power-law behavior of the gap, $E_g \propto H^{2/3}$.

In the bosonization scheme, the leading uniform term of the perturbing Hamiltonian $\mathcal{H}'$, which is responsible for opening the gap, is a cosine term,

$$\tilde{\mathcal{H}}' = -h_s b_0(H) \int \cos[2\pi R \tilde{\phi}(x)] dx. \tag{40}$$

Effects of the perturbation have been studied in the literature[22–25,37,38] and the induced spin gap is given by[38]

$$\frac{E_g}{J} = \frac{2v(H)}{\sqrt{\pi}} \frac{\Gamma\left(\dfrac{\eta}{8-2\eta}\right)}{\Gamma\left(\dfrac{2}{4-\eta}\right)} \left[\frac{\pi b_0(H)}{2v(H)} \frac{\Gamma\left(\dfrac{4-\eta}{4}\right)}{\Gamma\left(\dfrac{\eta}{4}\right)} \frac{h_s}{J} \right]^{2/(4-\eta)}. \tag{41}$$

Hence, the field-dependence of the spin gap is evaluated by substituting our numerical estimates for $b_0(H)$ as well as the exact values of $v(H)$ and $\eta(H)$ into Eq. (41). The result is shown in Fig. 5 for several typical values of γ. It reproduces the peculiar H dependence of the spin gap observed in experiments, $E_g \sim H^{2/3}$ for small H.

Next, we consider the spin gap induced by the perturbation of exchange anisotropy,

$$\mathcal{H}'' = -J(1-\tilde{\Delta}) \sum_l S_l^x S_{l+1}^x, \tag{42}$$

to the Heisenberg chain $\mathcal{H}_0(\Delta=1)$, where $1-\tilde{\Delta} \ll 1$. Note that by rotating the system around the y axis, the whole Hamiltonian is rewritten as

$$\mathcal{H}_0 + \mathcal{H}'' = J\sum_l (S_l^x S_{l+1}^x + S_l^y S_{l+1}^y + \tilde{\Delta} S_l^z S_{l+1}^z) - H \sum_l S_l^x. \tag{43}$$

Hence, the system can be also viewed as the $S=1/2$ XXZ chain with anisotropy $\tilde{\Delta}$ in a uniform transverse field H. As we have seen in Eq. (28), apart from a constant, the leading operators in the bosonized $\mathcal{H}''$ are $d\phi/dx$ and $d\tilde{\phi}/dx$. Since their main effect is just a small renormalization of the TL liquid parameter R, we can neglect these operators in lowest order in $1-\tilde{\Delta}$. We thus find that the dominant component which is responsible for opening the gap is the cosine term with coefficient c_2,

$$\tilde{\mathcal{H}}'' = -(1-\tilde{\Delta}) c_2(H) \int \cos[4\pi R \tilde{\phi}(x)] dx. \tag{44}$$

The effect of this perturbation has been studied,[26,27] and the spin gap for $H \gg (1-\tilde{\Delta})$ is found to be[27]

$$\frac{E_g}{J} = \frac{2v(H)}{\sqrt{\pi}} \frac{\Gamma\left(\dfrac{\eta}{2-2\eta}\right)}{\Gamma\left(\dfrac{1}{2-2\eta}\right)} \times \left[\frac{\pi(1-\tilde{\Delta})c_2(H)}{2v(H)} \frac{\Gamma(1-\eta)}{\Gamma(\eta)} \right]^{1/(2-2\eta)}. \tag{45}$$

We show in Fig. 6 the field dependence of the spin gap for several typical values of $\tilde{\Delta}$. As shown in the figure, the spin gap opens very slowly with H and closes at the saturation field $H=2J$, reflecting the fact that the coefficient c_2 vanishes as $M \to 1/2$. In contrast to the case of the staggered transverse field, the gap induced by the exchange anisotropy is extremely small. This result is consistent with the observation of the recent numerical study[39] which finds no substantial gap; the spin gap is too small to be detected by the numerical study on finite-size systems. We note that the bosonization scheme with our estimates of c_2 is, at present, the only way to get reliable quantitative results on the spin gap behavior.

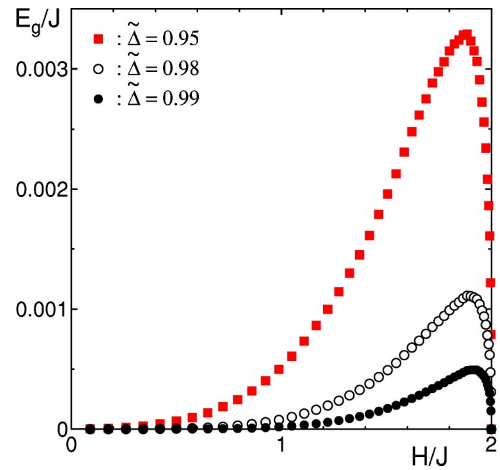

FIG. 6. (Color online) Field dependence of the spin gap in the Heisenberg chain $\mathcal{H}_0(\Delta=1)$ with the perturbation of transverse exchange anisotropy $(1-\tilde{\Delta})$.

IV. SUMMARY

In this paper, we have studied the ground-state correlation functions in the $S=1/2$ XXZ chain in a magnetic field. With the bosonic representation of the spin operators S_l^z and S_l^x for open-boundary conditions, we have calculated the two- and four-spin correlation functions analytically within the effective low-energy theory. We have also calculated the correlation functions numerically using the DMRG method, and estimated correlation amplitudes of the first few leading terms by fitting the numerical results to the analytic formulas. We have thus obtained precise data of nonuniversal coefficients appearing in the bosonic representation of lattice spin operators. Excellent agreement is found in the comparison of the numerical data with the exact known results in various limiting cases.

We believe that the data of the correlation amplitudes presented in this work is suitable for quantitatively studying low-energy properties of perturbed spin chains within the bosonization method. Indeed, it has been shown in Ref. 37 that the data of a_1 and b_0 can be used successfully to explain quantitative features of the dynamical spin structure factor in Cu benzoate. We hope that the data will be applied to a wider variety of problems in one-dimensional spin systems.

ACKNOWLEDGMENTS

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APPENDIX: BOSONIC REPRESENTATION OF SPIN OPERATORS

In this appendix, we briefly overview the derivation of the bosonic representation of the spin operators (7) and (8) in the spin-1/2 XXZ chain. We basically follow the strategy of Refs. 3 and 4. We first bosonize the repulsive Hubbard chain at half filling, in which charge excitations have a Mott-Hubbard gap. We then obtain the spin operators by throwing the gapped charge mode away, and generalize the results to the anisotropic XXZ case.

Let us begin with the bosonic representation of electron operators ($\sigma=\uparrow,\downarrow$),

$$\psi_\sigma(x)=\psi_{R,\sigma}(x)+\psi_{L,\sigma}(x), \tag{A1}$$

$$\psi_{R,\sigma}(x)=\frac{\kappa_\sigma}{\sqrt{2\pi a}}e^{i\sqrt{4\pi}\varphi_{R,\sigma}(x)+ik_{F\sigma}x}, \tag{A2}$$

$$\psi_{L,\sigma}(x)=\frac{\kappa_\sigma}{\sqrt{2\pi a}}e^{-i\sqrt{4\pi}\varphi_{L,\sigma}(x)-ik_{F\sigma}x}, \tag{A3}$$

where κ_σ are Klein factors obeying $\{\kappa_\sigma,\kappa_{\sigma'}\}=2\delta_{\sigma,\sigma'}$ and the bosonic fields φ obey the commutation relations,

$$[\varphi_{R,\sigma}(x),\varphi_{R,\sigma'}(y)]=(i/4)\delta_{\sigma,\sigma'}\mathrm{sgn}(x-y), \tag{A4}$$

$$[\varphi_{L,\sigma}(x),\varphi_{L,\sigma'}(y)]=-(i/4)\delta_{\sigma,\sigma'}\mathrm{sgn}(x-y), \tag{A5}$$

$$[\varphi_{R,\sigma}(x),\varphi_{L,\sigma'}(y)]=-(i/4)\delta_{\sigma,\sigma'}. \tag{A6}$$

The Fermi wave numbers $k_{F\sigma}$ are functions of the magnetization M, $k_{F\uparrow}=\pi(1/2+M)$ and $k_{F\downarrow}=\pi(1/2-M)$. We introduce fields ϕ and $\tilde{\phi}$ given by

$$\phi_\sigma(x)=\varphi_{L,\sigma}(x)+\varphi_{R,\sigma}(x), \tag{A7}$$

$$\tilde{\phi}_\sigma(x)=\varphi_{L,\sigma}(x)-\varphi_{R,\sigma}(x), \tag{A8}$$

which satisfy $[\phi_\sigma(x),\tilde{\phi}_\sigma(y)]=-(i/2)[1+\mathrm{sgn}(x-y)]\delta_{\sigma,\sigma'}$. It then follows that the electron density becomes

$$\rho_\sigma=\psi^\dagger_{R,\sigma}\psi_{R,\sigma}+\psi^\dagger_{L,\sigma}\psi_{L,\sigma}=\frac{k_{F\sigma}}{\pi}+\frac{1}{\sqrt{\pi}}\frac{d\phi_\sigma}{dx}. \tag{A9}$$

The uniform charge and spin densities are

$$\rho_c=\frac{1}{2}(\rho_\uparrow+\rho_\downarrow)=\frac{1}{2}+\frac{1}{\sqrt{2\pi}}\frac{d\phi_c}{dx}, \tag{A10}$$

$$\rho_s=\frac{1}{2}(\rho_\uparrow-\rho_\downarrow)=M+\frac{1}{\sqrt{2\pi}}\frac{d\phi_s}{dx}, \tag{A11}$$

where the charge and spin fields are defined by

$$\phi_c=\frac{1}{\sqrt{2}}(\phi_\uparrow+\phi_\downarrow),\quad \phi_s=\frac{1}{\sqrt{2}}(\phi_\uparrow-\phi_\downarrow), \tag{A12}$$

$$\tilde{\phi}_c=\frac{1}{\sqrt{2}}(\tilde{\phi}_\uparrow+\tilde{\phi}_\downarrow),\quad \tilde{\phi}_s=\frac{1}{\sqrt{2}}(\tilde{\phi}_\uparrow-\tilde{\phi}_\downarrow). \tag{A13}$$

The charge mode in the Hubbard chain is gapped at half filling when the on-site interaction is repulsive, $U>0$. The charge gap is generated by the umklapp scattering term,

$$\begin{aligned}U[&\psi^\dagger_{R,\uparrow}(x)\psi_{L,\uparrow}(x)\psi^\dagger_{R,\downarrow}(x)\psi_{L,\downarrow}(x)\\&+\psi^\dagger_{L,\uparrow}(x)\psi_{R,\uparrow}(x)\psi^\dagger_{L,\downarrow}(x)\psi_{R,\downarrow}(x)]\\&=-\frac{2U}{(2\pi a)^2}\cos(\sqrt{8\pi}\phi_c),\end{aligned} \tag{A14}$$

which pins the charge field at $\phi_c=n\sqrt{\pi/2}$ (n: integer). At low energies we may treat the field as a classical number, i.e.,

$$\begin{aligned}\cos(\sqrt{8\pi}\phi_c)&=C,\\ \sin(\sqrt{8\pi}\phi_c)&=0,\end{aligned} \tag{A15}$$

where C is a positive nonuniversal constant. At this point, following Ref. 40, we modify Eqs. (A2) and (A3) to

$$\psi_{R,\sigma}(x)=\frac{\kappa_\sigma}{\sqrt{2\pi a}}\sum_{n=0}^{\infty}e^{i(2n+1)(k_{F\sigma}x+\sqrt{\pi}\phi_\sigma)-i\sqrt{\pi}\tilde{\phi}_\sigma},$$

$$\psi_{L,\sigma}(x)=\frac{\kappa_\sigma}{\sqrt{2\pi a}}\sum_{n=0}^{\infty}e^{-i(2n+1)(k_{F\sigma}x+\sqrt{\pi}\phi_\sigma)-i\sqrt{\pi}\tilde{\phi}_\sigma}.$$

Using the equations above, one can derive the bosonic representation for the spin operators. The z component of the spin operator is given by

$$
\begin{aligned}
S^z(x) &= \tfrac{1}{2}[\psi_\uparrow^\dagger(x)\psi_\uparrow(x)-\psi_\downarrow^\dagger(x)\psi_\downarrow(x)] \\
&= \frac{1}{2}[\rho_s(x)+\psi_{R,\uparrow}^\dagger(x)\psi_{L,\uparrow}(x)+\psi_{L,\uparrow}^\dagger(x)\psi_{R,\uparrow}(x) \\
&\quad -\psi_{R,\downarrow}^\dagger(x)\psi_{L,\downarrow}(x)-\psi_{L,\downarrow}^\dagger(x)\psi_{R,\downarrow}(x)] \\
&= M+\frac{1}{\sqrt{2\pi}}\frac{d\phi_s}{dx}-\sum_{n=0}^{\infty} a_{2n+1}(-1)^x \\
&\quad \times \sin[(2n+1)(2\pi M x+\sqrt{2\pi}\phi_s)],
\end{aligned}
\tag{A16}
$$

where a_{2n+1} is a nonuniversal constant. Here we must recall that Eq. (A16) is obtained from the Hubbard chain at half filling, whose low-energy effective spin Hamiltonian is nothing but the antiferromagnetic Heisenberg spin chain, in which $R=1/\sqrt{2\pi}$. To generalize the result to the XXZ chain, what one needs to do is replacing $\sqrt{2\pi}\phi_s$ with ϕ_s/R. We also define $\phi(x)=\phi_s(x)+2\pi RMx$ to obtain

$$
S^z(x)=\frac{1}{2\pi R}\frac{d\phi(x)}{dx}-\sum_{n=0}^{\infty} a_{2n+1}(-1)^x \sin\left[(2n+1)\frac{\phi(x)}{R}\right].
\tag{A17}
$$

Similarly, the operator S^+ in the antiferromagnetic Heisenberg chain is given by

$$
\begin{aligned}
S^+(x) &= [\psi_{R,\uparrow}^\dagger(x)+\psi_{L,\uparrow}^\dagger(x)][\psi_{R,\downarrow}(x)+\psi_{L,\downarrow}(x)] \\
&= e^{i\sqrt{2\pi}\tilde{\phi}_s}\sum_{n=0}^{\infty}\{b_{2n}(-1)^x\cos[2n(2\pi Mx+\sqrt{2\pi}\phi_s)] \\
&\quad + b_{2n+1}\sin[(2n+1)(2\pi Mx+\sqrt{2\pi}\phi_s)]\}.
\end{aligned}
\tag{A18}
$$

By generalizing the equation to the XXZ case, we arrive at the final formula,

$$
\begin{aligned}
S^+(x) &= e^{i2\pi R\tilde{\phi}}\sum_{n=0}^{\infty}\left\{b_{2n}(-1)^x\cos\left[2n\frac{\phi(x)}{R}\right]\right. \\
&\quad \left. + b_{2n+1}\sin\left[(2n+1)\frac{\phi(x)}{R}\right]\right\},
\end{aligned}
\tag{A19}
$$

where we have replaced $\sqrt{2\pi}\tilde{\phi}_s$ with $2\pi R\tilde{\phi}$.

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