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Finite-Size Scaling for Correlations of Quantum Spin Chains at Criticality

Tohru Koma[1] and Nobuyuki Mizukoshi[1,2]

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We study the finite-size scaling behavior of two-point correlation functions of translationally invariant many-body systems at criticality. We propose an efficient method for calculating the two-point correlation functions in the thermodynamic limit from numerical data of finite systems. Our method is most effective when applied to a two-dimensional (classical) system which possesses a conformal invariance. By using this method with numerical data obtained from exact diagonalizations and Monte Carlo simulations, we study the spin–spin correlations of the quantum spin-1/2 and -3/2 antiferromagnetic chains. In particular, the logarithmic corrections to power-law decay of the correlation of the spin-1/2 isotropic Heisenberg antiferromagnetic chain are studied thoroughly. We clarify the cause of the discrepancy in previous calculations for the logarithmic corrections. Our result strongly supports the field-theoretic predicion based on the mappings to the Wess–Zumino–Witten nonlinear σ-model or the sine-Gordon model. We also treat logarithmic corrections and crossover phenomena in the spin–spin correlation of the spin-3/2 isotropic Heisenberg antiferromagnetic chain. Our results are consistent with the Affleck–Haldane prediction that the correlation of the spin-3/2 chain exhibits a crossover to the same asymptotic behavior as in the spin-1/2 chain.

KEY WORDS: Correlation functions; finite-size scaling; conformal invariance; quantum spin chains; logarithmic corrections; crossover.

1. INTRODUCTION

Techniques related to finite-size scaling have become increasingly important in statistical mechanics and related fields. Since Fisher introduced the

[1] Department of Physics, Gakushuin University, Mejiro, Toshima-ku, Tokyo 171, Japan; E-mail: koma@riron.gakushuin.ac.jp.

[2] Present address: NEC ULSI Systems Development Laboratories, Shimonumabe, Nakahara-ku, Kawasaki-shi, Kanagawa 211, Japan; E-mail: mizu@lsi. tmg.nec.co.jp.

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finite-size-scaling hypothesis[1,2] for critical phenomena, it has been applied to various problems in extrapolating quantities for finite systems to those in the thermodynamic limit.[3-6] Although the basic principle of finite-size scaling is simple and universal, it is not obvious how one should apply it in a concrete situation. A number of concrete methods have been proposed to extrapolate thermodynamic quantities from given numerical data for finite systems.[3]

In this paper, we will concentrate on the finite-size scaling behavior of a two-point correlation function of antiferromagnetic quantum spin chains at criticality (zero temperature). Several extrapolation methods[9-11] to treat two-point correlations for such systems have been proposed. One of the main issues in these studies is the logarithmic corrections to power-law decay of the spin–spin correlations at the $SU(2)$ symmetric point.[12-15,11,16,17] However, there is some discrepancy in the different calculations for the logarithmic corrections.

Here we propose an efficient method for extrapolating the correlations for the finite systems to infinity volume, assuming a finite-size scaling hypothesis. In this method, we determine a correlation function for infinite volume by fitting numerical data of the correlations to a finite-size scaling form of the correlation functions for the finite systems. Our method is most effective when applied to a two-dimensional system which possesses a conformal invariance. By using this method with numerical data obtained from exact diagonalizations and Monte Carlo simulations, we study the spin–spin correlations of the quantum spin-1/2 and -3/2 antiferromagnetic chains, which are believed to be conformally invariant.[18]

We first demonstrate the efficiency of our extrapolation method for the spin-1/2 quantum chains. In particular, the logarithmic corrections to power-law decay of the correlation of the spin-1/2 isotropic Heisenberg antiferromagnetic chain are studied thoroughly. We clarify the cause of the discrepancy in previous calculations for the logarithmic corrections. Our results strongly supports the field-theoretic prediction based on mappings to the continuum models such as the Wess–Zumino–Witten nonlinear σ-model[19] or the sine-Gordon model.[20-22]

Second, we treat logarithmic corrections and crossover phenomena in the spin–spin correlation of the spin-3/2 isotropic Heisenberg antiferromagnetic chain. Our results are consistent with the Affleck–Haldane predicion[23,24] that the correlation of the spin-3/2 chain exhibits a crossover to the same asymptotic behavior as in the spin-1/2 chain.

[3] See, for example, refs. 3 and 7 and work cited therein, and recent work.[8]

Although we do not treat a concrete system which does no possess a conformal invariance in this paper, we believe that our method is useful for studying correlations of more general many-body systems numerically. We hope to be able to report about such studies in the near future.

In the rest of the present section, we give a brief overview of the topics studied in this paper. The corresponding details can be found in the body of the paper.

1.1. Finite-Size Scaling for Correlations at Criticality

Before describing our extrapolation method, we briefly review the idea of finite-size scaling. Consider a translationally invariant many-body system on the d-dimensional parallelepiped of common finite side L with periodic boundary conditions in d' ($\leqslant d$) dimensions but of infinite extent in the remaining $d-d'$ dimensions. In the case of the quantum spin chains which we will treat, we take $d'=1$ for the corresponding two-dimensional ($d=2$) classical systems derived by the mapping based on the path integral idea. (See, for example, refs. 25–27.) We assume that, at criticality, there is no characteristic length except for L.

The finite-size scaling hypothesis states[28,4] that a two-point correlation at criticality satisfies[4]

$$\frac{\langle \phi(\mathbf{r}_1)\,\phi(\mathbf{r}_2)\rangle_L}{\langle \phi(\mathbf{r}_1)\,\phi(\mathbf{r}_2)\rangle_\infty} \cong Q(\tau) \tag{1.1}$$

Here $\langle \cdots \rangle_L$ and $\langle \cdots \rangle_\infty$ are the thermal expectations for the systems with finite L and $L=\infty$, respectively, and $r=|\mathbf{r}_2-\mathbf{r}_1|$ is the distance between the two points $\mathbf{r}_1$ and $\mathbf{r}_2$. The scaling function Q is assumed to be a function of a single variable[5] $\tau := r/L$. The finite-size scaling hypothesis (1.1) plays a fundamental role throughout the present work.

Consider a two-point correlation $\langle \phi(\mathbf{r}_1)\,\phi(\mathbf{r}_2)\rangle_L$ at criticality, where we take $(\mathbf{r}_1-\mathbf{r}_2)$ parallel to one of the finite sides of the parallelepiped. We rewrite the scaling relation (1.1) as

$$\langle \phi(\mathbf{r}_1)\,\phi(\mathbf{r}_2)\rangle_L \cong Q(\tau)\langle \phi(\mathbf{r}_1)\,\phi(\mathbf{r}_2)\rangle_\infty \tag{1.2}$$

with

$$Q(\tau) := \left[\frac{\tau}{X(\tau)}\right]^{d-2+\eta} \tag{1.3}$$

[4] Throughout this paper, we use the symbol $\cong$ when we drop higher order corrections.
[5] The symbol $:=$ signifies definition.

where η is the (unknown) critical exponent of power-law decay of the correlation[6] $\langle \phi(\mathbf{r}_1)\, \phi(\mathbf{r}_2)\rangle_\infty \sim \text{const} \times r^{-d+2-\eta}$. Here $X(\tau)$ is a new unknown function. It can be expanded in a Fourier series as

$$X(\tau) = a_1 \sin(\pi\tau) + a_3 \sin(3\pi\tau) + a_5 \sin(5\pi\tau) + \cdots \tag{1.4}$$

because of the translation invariance. When we are dealing with a two-dimensional conformally invariant system of an infinitely long strip with finite width L, the funcion $X(\tau)$ becomes remarkably simple. The well-known result in conformal field theories guarantees that all the Fourier coefficients in (1.4) except for a_1 are vanishing, and the function $X(\tau)$ takes the Cardy form[(29-32)]

$$X(\tau) = \frac{1}{\pi} \sin(\pi\tau) \tag{1.5}$$

with $\tau = r/L$.

1.2. Extrapolation Method of This Paper

Our extrapolation method is as follows. Suppose, for example, that the asymptotic behavior of the correlation function is given (in advance of numerical work) as

$$\langle \phi(\mathbf{r}_1)\, \phi(\mathbf{r}_2)\rangle_\infty \sim \frac{A}{r^{d-2+\eta}} \tag{1.6}$$

where A and η are unknown quantities. By substituting (1.3) and (1.6) into (1.2), the assumed scaling relation becomes

$$\begin{aligned} \langle \phi(\mathbf{r}_1)\, \phi(\mathbf{r}_2)\rangle_L &\cong Q(\tau) \frac{A}{r^{d-2+\eta}} \\ &= A \left[\frac{1}{LX(r/L)} \right]^{d-2+\eta} \end{aligned} \tag{1.7}$$

For a given set of numerical data for $\langle \phi(\mathbf{r}_1)\, \phi(\mathbf{r}_2)\rangle_L$ with various $(\mathbf{r}_1 - \mathbf{r}_2)$ and L, we can determine the unknown quantities[7] A, η, a_1, a_3, a_5,... by fitting the data to the formulas (1.7) and (1.4).

[6] Throughout this paper, we use the symbol $\sim$ for expressing asymptotic form.

[7] That there are infinitely many fitting parameters may be discouraging. We expect, however, that taking only a finite number of the parameters provides a reliable approximation. We hope to be able to report about such approaches in the near future.

An obvious advantage of our extrapolation method is that we treat the set of numerical data as a whole, and the desired quantities (such as η) are extracted through a *single* fitting formula (1.7). This should be compared with most of the existing extrapolation methods, in which one has to go through more than one fitting procedure.[8]

When applied to a two-dimensional conformally invariant system at criticality, our method becomes extremely effective. By substituting (1.5), the scaling relation (1.7) becomes

$$\langle \phi(\mathbf{r}_1)\, \phi(\mathbf{r}_2) \rangle_L \cong A \left[\frac{\pi}{L \sin(\pi r/L)} \right]^{\eta} \tag{1.8}$$

Since the only unknown quantities in the right-hand side are A and η, we can read off these two quantities from given numerical data of $\langle \phi(\mathbf{r}_1)\, \phi(\mathbf{r}_2) \rangle_L$ for various $(\mathbf{r}_1 - \mathbf{r}_2)$ and L. Let us again stress that all we have to perform here to get the critical exponent η is a simple two-parameter fitting of the given numerical data. There is no need of extrapolating finite-volume correlations to infinite volume and then estimating η by a log–log plot.

1.3. Results for Spin-1/2 Anisotropic and Isotropic Chains

1.3.1. *XY* Chain. For the longitudinal correlation $\langle S_i^z S_{i+r}^z \rangle_\infty^{XY}$ of the XY chain, we demonstrate that the scaling relation (1.2) with (1.3) and (1.5) holds exactly as in (3.2) and (3.3) below. In particular, the correlations (3.2) for finite sizes have exactly the form of (1.8) for any finite L and $r > 0$, except for the even–odd oscillation $(-1)^r$. The scaling relation for the transverse correlation $\langle S_i^x S_{i+r}^x \rangle_\infty^{XY}$ is also shown to hold within numerical accuracy, by using the exact numerical values of $\langle S_i^x S_{i+r}^x \rangle_L^{XY}$ for finite L by Kaplan *et al.*[10]

1.3.2. *XXZ* Antiferromagnetic Chain. The scaling function Q of (1.3) with (1.5) for the transverse correlation $\langle S_i^x S_{i+r}^x \rangle_\infty^{XXZ}$ of the XXZ antiferromagnetic chain coincides with numerical one by Kaplan *et al.*[10] when one uses the predicted value by Luther and Peschel[33] or the numerical vale by Takada and Kubo[34,35] as the critical exponent η.

[8] For example, one first extrapolates correlations of finite volumes to infinite volume for each distance r by using the finite-size scaling hypothesis (1.1). Then one estimates the critical exponent η by a log–log plot or by introducing an ad hoc fitting function.

1.3.3. Isotropic Heisenberg Antiferromagnetic Chain. Unlike the above XY and XXZ chains, the spin–spin correlation of the spin-1/2 isotropic Heisenberg antiferromagnetic chain does not exhibit power-law decay because there exists a marginally irrelevant operator in the Hamiltonian. According to the renormalization group analysis,[9] the correlation is believed to behave as

$$\langle S_j^x S_{j+r}^x \rangle_\infty^{XXX} \sim A \times \frac{(-1)^r}{r} \left[\log \left(\frac{r}{r_0} \right) \right]^\sigma - \frac{1}{4\pi^2 r^2} \tag{1.9}$$

for large distance r, where A, r_0, and σ are constants. The existence of such a logarithmic correction was first confirmed numerically by Kubo *et al.*[12] The validity of the second term in (1.9) was confirmed numerically by Sandvik and Scalapino.[11]

As for the value of the exponentσ, however, there a discrepancy arose as follows. According to the renormalization group analysis for effective continuum models such as the Wess–Zumino–Witten (WZW) model[19] or the sine-Gordon model,[20–22] the critical exponent σ is given by 1/2. The numerical works[12–15] based on the finite-size scaling hypothesis (1.1) predicted values of σ which are significantly less than 1/2, or even vanishing. Instead of using the standard scaling hypothesis (1.1), Sandvik and Scalapino[11] introduced a certain relation between correlations for finite volume and that for infinite volume[10] and obtained numerical results which supported the field-theoretic value $\sigma = 1/2$. In recent work[16,17] we obtained a numerical result which also supported $\sigma = 1/2$, where we slightly modified the form of the scaling function Q proposed by Kaplan *et al.*[10]

In this paper, as approximate correlations for finite volume, we propose

$$\langle S_i^x S_j^x \rangle_L^{XXX} \cong A(-1)^r \times \frac{1}{r_L} \times \left[\log \left(\frac{r_L}{r_0} \right) \right]^\sigma - \frac{1}{4\pi^2} \frac{1}{r_L^2} \tag{1.10}$$

which recovers (1.9) in the infinite-volume limit $L \uparrow \infty$, where the right-hand side is given by replacing the distance r in (1.9) by the effective distance $r_L := (L/\pi)\sin(\pi r/L)$ for finite volume, except for the factor $(-1)^r$. This form (1.10) is the extension of the finite-size scaling form (1.8) of finite-volume correlations to the case that there appear logarithmic corrections as deviations from a conformal invariance. We determine the unknown quantities A, r_0, and σ in (1.10) by using numerical data of exact

[9] See, for example, the review in ref. 18.

[10] They argued that the reason for the discrepancy is that the logarithmic correction in the correlation (1.9) makes the finite-size scaling hypothesis (1.1) invalid.

diagonalizations and Monte Carlo simulations. As a result, we obtained $\sigma \cong 0.47$, which strongly supports the field-theoretic value $\sigma = 1/2$.

Further, we propose a new finite-size scaling function

$$Q(\tau, L) := \left[\frac{\pi\tau}{\sin(\pi\tau)} \right]^{\eta_{\text{eff}}(L)} \tag{1.11}$$

where $\tau = r/L$. The relation between this scaling function and the asymptotic form of the correlation (1.10) is stated in Sections 2 and 3.3. The crucial feature of the scaling function (1.11) is that the "effective critical exponent"[36] $\eta_{\text{eff}}(L)$ depends on the finite size L of a system, to take into account the deviations from a conformal invariance. Clearly, unlike the standard scaling form (1.1), the scaling function Q of (1.11) is *not* a function of the single variable $\tau = r/L$. We determined the effective critical exponent $\eta_{\text{eff}}(L)$ from the spectrum of a transfer matrix of the six-vertex model corresponding to the present spin-1/2 isotropic Heisenberg antiferromagnetic chain by assuming a conformal invariance of the spectrum of the transfer matrix. In Section 3.3, we show that, for extrapolating correlation functions for finite volume to infinite volume, our finite-size scaling function (1.11) is more efficient than previous scaling functions with the standard form (1.1). Further, comparing a previous scaling function with our scaling function (1.11), we conclude that the discrepancy in the previous calculations for the exponent σ of the correlation (1.9) is due to ignoring the finite-size corrections of the effective critical exponent $\eta_{\text{eff}}(L)$ in the scaling function (1.11).

1.4. Results for the Spin-3/2 Isotropic Heisenberg Antiferromagnetic Chain

It was conjectured by field-theoretic arguments that the spin–spin correlation of the spin-3/2 isotropic Heisenberg antiferromagnetic chain exhibits the same asymptotic behavior as in the spin-1/2 chain[37,38] but with crossover phenomena.[23,24] Much numerical work has been devoted to examining this conjecture.[14,39–42] However, it is still not clear how the correlation of the spin-3/2 chain behaves.

We apply to the spin-3/2 chain the technique developed for the spin-1/2 chains. Our results appear to be consistent with the Affleck–Haldane conjecture.[23] In particular, we find clear evidence of the crossover that the effective critical exponent η_{eff} varies with distance. Although we cannot give a *conclusive* result, we believe that our formulas and results will be useful for future studies of crossover phenomena, in particular, for experimental observations in a one-dimensional isotropic spin-3/2 antiferromagnetic substance.[43,44]

1.5. Outline of the Paper

The present paper is organized as follows. In Section 2, we describe our method in a general setting. In Section 2.2, we combine our general idea with the conformal invariance. It turns out that the scaling function Q of (1.3) for two-point correlation at criticality can be completely determine as in (1.5). In Section 3, we apply our method to the quantum spin-1/2 antisotropic (XY and XXZ) and isotropic Heisenberg antiferromagnetic chains. In particular, the logarithmic corrections to power-law decay of the spin–spin correlation of the spin-1/2 isotropic Heisenberg antiferromagnetic chain are thoroughly studied with the use of zero-temperature Monte Carlo simulations.[12] The technique developed for the spin-1/2 chains is applied to the spin-3/2 isotropic Heisenberg antiferromagnetic chain in Section 4. The crossover effect in the correlation is discussed.

Appendix A is devoted to a brief review of the zero-temperature Monte Carlo simulation introduced by Kaplan *et al.*[10] The application to the spin-1/2 isotropic Heisenberg antiferromagnetic chain is discussed in Appendix B. We mainly describe some crucial modifications introduced in our earlier work.[16,17] In Appendix C, we summarize some useful techniques in the renormalization group method for calculating logarithmic corrections and a crossover function. Appendix D is devoted to a review of Cardy's transfer matrix argument for a two-dimensional conformally invariant system.[30] In Appendix E, we discuss the relation between a logarithmic correction to power-law decay of a two-point correlation and a logarithmic correction in an energy spectrum from the point of view of conformal field theories. Appendix F is devoted to a calculation of the effective critical exponent $\eta_{\rm eff}$ of the spin–spin correlation of the spin-1/2 isotropic antiferromagnetic Heisenberg chain. In Appendix G, we treat the two-point correlation function of a one-dimensional quantum system at low temperatures under an assumption of conformal invariance.

2. FINITE-SIZE SCALING FOR CORRELATIONS

2.1. General Approach

In the present section, we describe our finite-size scaling method for calculating two-point correlation functions at criticality in a general setting.

Consider a translationally invariant classical system on the d-dimensional parallelepiped of common finite side L with periodic boundary conditions in d' ($\leqslant d$) dimensions but of infinite extent in the remaining $d-d'$ dimensions. We assume that, at criticality, there is no characteristic length except for L.

We first focus on the simplest situation, where the two-point correlation $\langle\phi(0)\,\phi(\mathbf{r})\rangle_\infty$ in the limit $L\uparrow\infty$ at the criticality behaves as

$$\langle\phi(0)\,\phi(\mathbf{r})\rangle_\infty \sim \frac{A}{r^{d-2+\eta}} \tag{2.1}$$

for large distances $r=|\mathbf{r}|$, where A and η are the critical amplitude and the critical exponent, respectively.

For finite size L, consider the two-point correlation $\langle\phi(0)\,\phi(\mathbf{r})\rangle_L$ with $\mathbf{r}$ parallel to one of the finite sides of the parallelepiped. Let us write the correlation in terms of an unknown function $X(\tau, L)$ as

$$\langle\phi(0)\,\phi(\mathbf{r})\rangle_L = A\left[\frac{1}{LX(r/L, L)}\right]^{d-2+\eta} \tag{2.2}$$

where A and η are determined in (2.1). From the translation invariance of $\langle\phi(0)\,\phi(\mathbf{r})\rangle_L$, we find that X should satisfy $X(\tau+1, L)=X(\tau, L)$ and $X(-\tau, L)=X(\tau, L)$ for any τ and L. By comparing (2.2) with the critical decay (2.1), we observe that

$$X(\tau, L)\sim\tau \tag{2.3}$$

should hold for large L and small $\tau\ll 1$.

The relation (2.3) motivates us to state the assumption that, for large enough L, the function $X(\tau, L)$ essentially depends only on the variable τ. We thus drop the L dependence from $X(\tau, L)$ and write it as $X(\tau)$. (We will soon discuss how to take into account a possible L dependence of X as a correction.)

This construction straightforwardly extends to general forms of power-law decay. As an example, let us consider

$$\langle\phi(0)\,\phi(\mathbf{r})\rangle_\infty \sim A_1(-1)^r\frac{1}{r^{d-2+\eta_1}} + A_2\frac{1}{r^{d-2+\eta_2}} \tag{2.4}$$

which is a typical behavior in quantum spin systems. Then the corresponding correlation for finite width L can be written as

$$\langle\phi(0)\,\phi(\mathbf{r})\rangle_L = (-1)^r\,G_L^{(1)}(r) + G_L^{(2)}(r) \tag{2.5}$$

with

$$G_L^{(l)}(r)\cong A_l\left[\frac{1}{LX_l(r/L)}\right]^{d-2+\eta_l} \tag{2.6}$$

for $l=1, 2$. Again we have dropped the possible L dependence of X_l.

Finally we discuss how one can take into account the possible L dependence of $X(\tau, L)$, which has been neglected so far. Since the function $X(\tau, L)$ is expected to be L-independent for large L, we expect that it can be expanded in powers of L^{-1} as

$$X(\tau, L) = X(\tau) + \tilde{X}^{(1)}(\tau) \times L^{-1} + \tilde{X}^{(2)}(\tau) \times L^{-2} + \cdots \tag{2.7}$$

Then the correlation of finite L can be written as

$$\langle \phi(0)\, \phi(\mathbf{r}) \rangle_L = A \left[\frac{1}{LX(\tau)} \right]^{d-2+\eta} \times [1 + X^{(1)}(\tau) \times L^{-1} + X^{(2)}(\tau) \times L^{-2} + \cdots] \tag{2.8}$$

In addition, it is believed from numerical work[45,46,10] that there appear only even powers of L^{-1} in the series (2.8). As we will see later (in Sections 3.1 and 3.3) in concrete examples, this property makes extrapolation procedures based on (2.8) quite efficient.

2.2. Conformal Invariance in Two Dimensions

The function X introduced in the previous section is not universal in general situations. But if we are dealing with a two-dimensional continuum system with conformal invariance,[47–50] then the function X has the universal form

$$X(\tau) = \frac{1}{\pi} \sin(\pi\tau) \tag{2.9}$$

with $\tau = r/L$. This is nothing but the well-known result of Cardy,[29–32] but we discuss its derivation for the sake of completeness.

We begin with a quick review of conformal invariance in two dimensions.[48–50,31,7] We denote the two-dimensional coordinate $\mathbf{r} = (y_1, y_2)$ by the complex number $z = y_1 + iy_2$. We consider a primary field ϕ which transforms covariantly under an arbitrary conformal transformation $w = f(z)$ as[48]

$$\langle \phi(z')\, \phi(z) \rangle = [f'(z')]^h\, [\overline{f'(z')}]^{\bar{h}}\, [f'(z)]^h\, [\overline{f'(z')}]^{\bar{h}}\, \langle \phi(w')\, \phi(w) \rangle \tag{2.10}$$

where $\overline{\cdots}$ indicates complex conjugate, f' stands for the derivative of the function f, and h and $\bar{h}$ are the conformal dimensions. ($\bar{h}$ is *not* neccesarily the complex conjugate of h.)

Following Cardy,[29-31] we consider the conformal mapping

$$w = \frac{L}{2\pi} \log z \tag{2.11}$$

which maps the whole z plane onto the surface of a cylinder. By this mapping, the correlation decaying by a power law[11]

$$\langle \phi(z')\, \phi(z) \rangle_\infty = (z - z')^{-2h} \times (\bar{z} - \bar{z}')^{-2\bar{h}} \tag{2.12}$$

on the whole z plane is transformed into

$$\langle \phi(w')\, \phi(w) \rangle_L = \left(\frac{\pi}{L}\right)^\eta \left\{ \frac{1}{\sinh[\pi(w - w')/L]} \right\}^{2h} \times \left\{ \frac{1}{\sinh[\pi(\bar{w} - \bar{w}')/L]} \right\}^{2\bar{h}} \tag{2.13}$$

where $\eta = 2(h + \bar{h})$.

By setting $w - w' = ir$, the correlation (2.13) becomes

$$\langle \phi(0)\, \phi(\mathbf{r}) \rangle_L = e^{-i\pi(h - \bar{h})} \times \left[\frac{\pi}{L \sin(\pi r/L)} \right]^\eta \tag{2.14}$$

Clearly, in the limit $L \uparrow \infty$ for a fixed r, we recover

$$\langle \phi(0)\, \phi(\mathbf{r}) \rangle_\infty = e^{-i\pi(h - \bar{h})} \times \frac{1}{r^\eta} \tag{2.15}$$

These imply that the function X is given by (2.9) and that we exactly have the scaling law

$$Q\left(\frac{r}{L}\right) := \left[\frac{\pi r/L}{\sin(\pi r/L)} \right]^\eta = \frac{\langle \phi(0)\, \phi(\mathbf{r}) \rangle_L}{\langle \phi(0)\, \phi(\mathbf{r}) \rangle_\infty} \tag{2.16}$$

2.3. Three or Higher Dimensions

For a system in dimensions higher than two, or a system without conformal invariance, the simple scaling law (2.16) is not valid. From the general properties of the periodicity $X(\tau + 1) = X(\tau)$ and the asymptotic behavior (2.3), we can Fourier expand X for $\tau \geqslant 0$ as

$$X(\tau) = a_1 \sin(\pi\tau) + a_3 \sin(3\pi\tau) + a_5 \sin(5\pi\tau) + \cdots \tag{2.17}$$

[11] Because of the conformal invariance, any two-point correlation function for primary fields must take the form (2.12) on the whole plane.[47,48]

with the constraint

$$\sum_{m=1}^{\infty} a_{2m-1} \times (2m-1)\pi = 1 \tag{2.18}$$

Note that there appear only odd terms in the Fourier series.

Although we do not yet have concrete examples, we expect that the representation of X as in (2.17) with the constraint (2.18) provides the basis for an efficient numerical method for calculating two-point correlations.

2.4. Logarithmic Corrections to Power-Law Decay of Correlations

As is well known, the existence of a marginally irrelevant operator in a Hamiltonian leads to a logarithmic correction to power-law decay of correlations as

$$\langle \phi(0)\, \phi(\mathbf{r}) \rangle_\infty \sim \frac{A}{r^{d-2+\eta}} \times \left[\log \left(\frac{r}{r_0} \right) \right]^\sigma \tag{2.19}$$

where A, r_0, and σ are constants. (See Appendix C.2 for details.) Assuming the decay property (2.19), the same strategy as in Section 2.1 yields

$$\langle \phi(0)\, \phi(\mathbf{r}) \rangle_L \cong A \left[\frac{1}{LX(r/L)} \right]^{d-2+\eta} \times \left\{ \log \left[\frac{LX'(r/L)}{r_0} \right] \right\}^\sigma \tag{2.20}$$

where we have dropped the possible L dependence of the functions X and X'. From (2.19) and (2.20), we have

$$\frac{\langle \phi(0)\, \phi(\mathbf{r}) \rangle_L}{\langle \phi(0)\, \phi(\mathbf{r}) \rangle_\infty} \cong \left[\frac{\tau}{X(\tau)} \right]^{d-2+\eta} \times \left[\frac{\tau}{X'(\tau)} \right]^{-\sigma/\log(L/r_0)} \tag{2.21}$$

for a fixed $\tau = r/L$ and large L, where higher orders of logarithmic corrections have been neglected.

Here if $X' = X$, then we have

$$Q(\tau, L) := \left[\frac{\tau}{X(\tau)} \right]^{d-2+\eta_{\rm eff}(L)} \cong \frac{\langle \phi(0)\, \phi(\mathbf{r}) \rangle_L}{\langle \phi(0)\, \phi(\mathbf{r}) \rangle_\infty} \tag{2.22}$$

with

$$\eta_{\rm eff}(L) \cong \eta - \frac{\sigma}{\log(L/r_0)} \tag{2.23}$$

This scaling function Q is no longer a function of a single variable $\tau = r/L$. The exponent $\eta_{\rm eff}(L)$ can be interpreted as the effective critical exponent[36] which appears in the renormalization group analysis when there is a marginally irrelevant perturbation. (See Appendix C.2 for details.) Actually, effective critical exponents $\eta_{\rm eff}(L)$ having the form (2.23) were observed in energy spectra of several systems of infinite L,[51–57,22] based on conformal field theories.[58,19] From these observations, we conjecture $X' = X$.

Under the assumption $X' = X$, the correlation function (2.20) with finite L becomes

$$\langle \phi(0)\, \phi(\mathbf{r}) \rangle_L \cong A \left[\frac{1}{LX(r/L)} \right]^{d-2+\eta} \times \left\{ \log \left[\frac{LX(r/L)}{r_0} \right] \right\}^{\sigma} \qquad (2.24)$$

In particular, in two dimensions, we expect that this function X is given by (2.9) as in Section 2.2. Of course, the existence of logarithmic corrections breaks the conformal covariance (2.10) of a correlation function. This implies that we cannot easily apply the form (2.9) to X of (2.24). But it is believed that deviations from the conformal invariance appear only as logarithmic corrections when a perturbation in the Hamiltonian is marginally irrelevant.[19]

The valicity of the approximation of correlation (2.24) with (2.9) and the scaling function (2.22) with (2.9) will be examined for the spin-1/2 isotropic Heisenberg antiferromagnetic chain in Section 3.3. Our numerical results support these conjectures.

3. APPLICATIONS TO SPIN-1/2 ANISOTROPIC AND ISOTROPIC ANTIFERROMAGNETIC CHAINS

We apply our method to the spin–spin correlations of the Heisenberg antiferromagnetic chains with spin 1/2 and 3/2 in this and the next section, respectively. The Hamiltonian is given by

$$\mathscr{H}_L = \sum_{j=1}^{L} (S_j^x S_{j+1}^x + S_j^y S_{j+1}^y + \Delta S_j^z S_{j+1}^z) \qquad (3.1)$$

where $\Delta \in \mathbf{R}$ is the anisotropy parameter. We assume that L is even, and impose a periodic boundary condition $\mathbf{S}_{L+1} = \mathbf{S}_1$. Here $\mathbf{S}_j$ is the spin operator at site j with $(\mathbf{S}_j)^2 = S(S+1)$ ($S = 1/2, 3/2$). We denote by $\langle \cdots \rangle_L$ and $\langle \cdots \rangle_\infty$ the ground-state expectations for the systems with finite L and $L = \infty$, respectively. As is well known, a one-dimensional quantum system with finite length L at zero temperature is mapped to a two-dimensional classical system of an infinitely long strip with width L by using the path integral idea (see, e.g., refs. 25–27). By using this mapping, we apply our method in the previous section to the two-dimensional classical system corresponding to a quantum spin chain. Then we assume that the long-distance behavior of the correlations of the system can be described by a conformal field theory as in Section 2.2.

3.1. Spin-1/2 *XY* Chain

We begin with the simplest case of the spin-1/2 XY chain. The Hamiltonian given by (3.1) with $S = 1/2$ and $\Delta = 0$ is transformed into a free-fermion model on the lattice by using the Jordan–Wigner transformation.[59,60] The continuum limit of the system is a conformally invariant free-fermion model. We can easily calculate the spin–spin correlation function in the z direction as

$$\langle S_j^z S_{j+r}^z \rangle_L^{XY} = \frac{1}{2} \left\{ (-1)^r \left[\frac{1}{L \sin(\pi r/L)} \right]^2 - \left[\frac{1}{L \sin(\pi r/L)} \right]^2 \right\} \tag{3.2}$$

for $r \neq 0$. The above correlation is equivalent to the current–current correlation in the continuum free-fermion model.[18] In the thermodynamic limit $L \uparrow \infty$, the correlation (3.2) reduces to

$$\langle S_j^z S_{j+r}^z \rangle_\infty^{XY} = \frac{1}{2\pi^2} \left[(-1)^r \frac{1}{r^2} - \frac{1}{r^2} \right] \tag{3.3}$$

for $r \neq 0$. In this case, the scaling law (2.16) holds exactly for all the range of r except for $r = 0$. This is not suprising, because in the continuum limit the corresponding free-fermion model is conformally invariant, and the operator S_j^z becomes a current operator. However, the factor $(-1)^r$ is never derived from conformal field theories, because the oscillation is intrinsically a lattice effect.

Next we consider the correlation function $\langle S_j^x S_{j+r}^x \rangle_L^{XY}$ in the x direction, which has the string form in the fermion representation. Lieb *et al.*[59] showed that the correlation is equal to an $r \times r$ Toeplitz determinant. Using the property of the Toeplitz determinant, Wu[61] and McCoy[62] showed that one can obtain the asymptotic form of the correlation function. Following Wu and McCoy, we calculate the asymptotic form of the correlation in the thermodynamic limit $L \uparrow \infty$ as

$$\langle S_j^x S_{j+r}^x \rangle_\infty^{XY} = A(-1)^r \frac{1}{r^{1/2}} \times \exp[-(-1)^r \times w(r)] \tag{3.4}$$

Table I. The Ratio $C_L^{(1)}(r)/\langle S_j^x S_{j+r}^x\rangle_L^{XY}$ in the Spin-1/2 *XY* Chain, Using the Simplest $C_L^{(1)}(r)$ of (3.6) and of the Exact Numerical Values of $\langle S_j^x S_{j+r}^x\rangle_L^{XY}$ Obtained by Kaplan *et al.*[10]

L	$r/L=1/6$	$r/L=1/3$	$r/L=1/2$
6	0.903 115	1.029 329	0.957 899
54	0.998 186	1.000 422	0.999 437
102	0.999 488	1.000 118	0.999 842
150	0.999 763	1.000 055	0.999 927
198	0.999 864	1.000 032	0.999 958

with

$$w(r)=\frac{1}{8}\times\frac{1}{r^2}+\frac{1}{8}\times\frac{1}{r^4}-\frac{17}{48}\times\frac{1}{r^6}+\cdots \tag{3.5}$$

for large r, where A is a constant. But the correlation of a *finite* system cannot be expressed in a compact manner. Kaplan *et al.*[10] calculated $\langle S_j^x S_{j+r}^x\rangle_L^{XY}$ numerically up to $L=1000$ with the help of the symmetry of the Toeplitz determinant.

Following our scheme in Section 2, we introduce the simplest approximate correlation function for finite L

$$C_L^{(1)}(r) := A(-1)^r\left[\frac{\pi}{L\sin(\pi r/L)}\right]^{1/2} \tag{3.6}$$

which is obtained by replacing r in the correlation function (3.4) by $(L/\pi)\sin(\pi r/L)$, and dropping the higher orders.

Table I shows the ratios $C_L^{(1)}(r)/\langle S_j^x S_{j+r}^x\rangle_L^{XY}$. Our approximate correlation function $C_L^{(1)}(r)$ in (3.6) deviates slightly from the exact numerical values of $\langle S_j^x S_{j+r}^x\rangle_L^{XY}$ obtained by Kaplan *et al.*[10]

As a more accurate approximate correlation function for finite L, we take

$$C_L(r) := A(-1)^r\times\left[\frac{\pi}{L\sin(\pi r/L)}\right]^{1/2}$$
$$\times\exp[-(-1)^r\times\tilde{w}(r,L)]\times\left(1+\frac{\mathscr{X}^{(2)}}{L^2}\right) \tag{3.7}$$

Table II. The Ratio $C_L(r)/\langle S_j^x S_{j+r}^x \rangle_L$ in the Spin-1/2 XY Chain, Using the Improved $C_L(r)$ of (3.7) and the Exact Numerical Values of $\langle S_j^x S_{j+r}^x \rangle_\infty^{XY}$ Obtained by Kaplan *et al.*[10]

L	$r/L = 1/6$	$r/L = 1/3$	$r/L = 1/2$
6	1.438 145	0.994 073	1.000 596
54	0.999 997	1.000 002	1.000 000
102	1.000 000	1.000 000	1.000 000
150	1.000 000	1.000 000	1.000 000
198	1.000 000	1.000 000	1.000 000

where $\tilde{w}(r, L)$ is the sum of the first three terms in the expansion (3.5) in which r is replaced by $(L/\pi)\sin(\pi r/L)$. We also have set $X^{(1)} = 0$ in (2.8), and have taken the corrections into account up to the next order $1/L^2$, approximating $X^{(2)}$ in (2.8) by a constant $\hat{X}^{(2)}$. We determined the constant $\hat{X}^{(2)}$ by a least-squares fitting of $C_L(r)$ in (3.7) to the exact numerical values of $\langle S_j^x S_{j+r}^x \rangle_L^{XY}$ with $54 \leqslant L \leqslant 198$ by Kaplan *et al.* As a result, we obtained $\hat{X}^{(2)} = 0.414$. Table II shows the results of this fitting. Although there is only one fitting parameter, the agreement is excellent except for small $r = 1, 2$ of small system size $L = 6$. The reason for the large deviation for $r = 1$ and $L = 6$ is probably that the expansion (3.5) for $w(r)$ gives a *bad* approximation for small r.

3.2. Spin-1/2 *XXZ* Antiferromagnetic Chain

The Hamiltonian of the spin-1/2 XXZ chain is given by (3.1) with a nonvanishing anisotropy Δ and $S = 1/2$. In this section, for the transverse correlation $\langle S_j^x S_{j+r}^x \rangle_L^{XXZ}$, we will examine the consistency between the scaling relation (2.16) and known analytical and numerical results.

To begin with, we shall briefly summarize known results.

From an analysis based on the continuum model, Luther and Peschel[33] predicted that the correlation behaves as

$$\langle S_j^x S_{j+r}^x \rangle_L^{XXZ} \sim A(-1)^r \frac{1}{r^{\eta(\Delta)}} + B\frac{1}{r^2} \tag{3.8}$$

with the critical exponent

$$\eta(\Delta) = \frac{1}{2} + \frac{1}{\pi}\sin^{-1}\Delta \tag{3.9}$$

Table III. Comparison of $\alpha(\Delta)/2$ in the Kaplan *et al.*[10] Scaling Function with the Numerical[34,35] and Analytical[33] Results of the Critical Exponent $\eta(\Delta)$ of the Correlation $\langle S_j^x S_{j+r}^x \rangle_\infty^{XXZ}$ in the Spin-1/2 *XXZ* Heisenberg Chain[a]

		$\eta(\Delta)$	
Δ	$\alpha(\Delta)/2$	Numerical[34,35]	Analytical[33]
0.25	0.564	0.55(1)	0.580
0.50	0.645	0.64(1)	0.667
0.75	0.747	0.746(5)	0.770

[a] Numbers in parentheses indicate the uncertainties in the last digit.

for $-1 < \Delta \leqslant 1$, where A and B are constants. Takada and Kubo[34,35] examined the result (3.9) by employing the quantum transfer matrix method based on the path integral idea. Their numerical results are consistent with (3.9). (See Table III.)

On the other hand, Kaplan *et al.*[10] calculated the scaling functions of the correlation $\langle S_j^x S_{j+r}^x \rangle_L^{XXZ}$ by using the exact numerical diagonalization up to the system size $L = 14$. Their numerical result for the scaling of the correlation functions is represented in the form

$$\frac{\langle S_j^x S_{j+r}^x \rangle_L^{XXZ}}{\langle S_j^x S_{j+r}^x \rangle_\infty^{XXZ}} \cong \left[\frac{\langle S_j^x S_{j+r}^x \rangle_L^{XY}}{\langle S_j^x S_{j+r}^x \rangle_\infty^{XY}} \right]^{\alpha(\Delta)} \tag{3.10}$$

with

$$\alpha(\Delta) \cong 1 + 0.445 \times \Delta + 0.239 \times \Delta^2 + 0.061 \times \Delta^3 \tag{3.11}$$

for $\Delta \in [0, 4]$, where $\langle S_j^x S_{j+r}^x \rangle_L^{XY}$ and $\langle S_j^x S_{j+r}^x \rangle_\infty^{XY}$ are the correlation functions of the spin-1/2 XY chain with finite L and $L = \infty$, respectively.

Now we wish to find the relation between the critical exponent $\eta(\Delta)$ of (3.9) and the exponent $\alpha(\Delta)$ of (3.11). Since the scaling relation (3.10) was determined for large distances r of correlations, we may neglect the second term in (3.8). Then one may regard that the scaling relation (3.10) which Kaplan *et al.* found by numerical experiment is a special case of the scaling relation (2.16). In fact, from the scaling relation (2.16) and the critical exponent $\eta = 1/2$ of the XY chain in (3.4), we have

$$\frac{\langle S_j^x S_{j+r}^x \rangle_L^{XXZ}}{\langle S_j^x S_{j+r}^x \rangle_\infty^{XXZ}} \cong \left[\frac{\langle S_j^x S_{j+r}^x \rangle_L^{XY}}{\langle S_j^x S_{j+r}^x \rangle_\infty^{XY}} \right]^{2\eta(\Delta)} \tag{3.12}$$

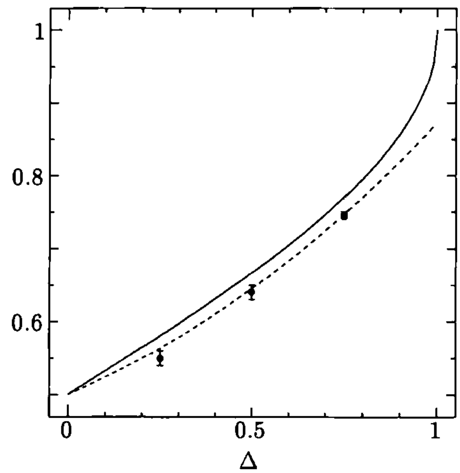

Fig. 1. The exponent $\eta(\Delta)$ of the correlation $\langle S_j^x S_{j+r}^x \rangle_\infty^{XXZ}$ in the spin-1/2 XXZ Heisenberg chain. The dashed line and the solid line are, respectively, $\alpha(\Delta)/2$ of (3.11), from Kaplan *et al.*,[10] and $\eta(\Delta)$ of (3.9), from Luther and Peschel.[33] The solid circles are the numerical results by Takada and Kubo.[34,35]

where $\eta(\Delta)$ is the critical exponent of the XXZ chain. Comparing this with the numerical result (3.10), one finds that the critical exponent $\eta(\Delta)$ of the correlations $\langle S_j^x S_{j+r}^x \rangle_\infty^{XXZ}$ of the XXZ chain must satisfy

$$\eta(\Delta) = \tfrac{1}{2}\alpha(\Delta) \tag{3.13}$$

Let us examine the relation (3.13). That is, we compare $\alpha(\Delta)/2$ with the predicted values (3.9) by Luther and Peschel and the numerical values by Takada and Kubo. As in Table III and Fig. 1, the values $\alpha(\Delta)/2$ are consistent with these values of the critical exponent $\eta(\Delta)$.

Thus the scaling relation (2.16) with this previously obtained critical exponent $\eta(\Delta)$ is consistent with the scaling relation (3.10) obtained numerically by Kaplan *et al.*[12]

3.3. Spin-1/2 Isotropic Heisenberg Antiferromagnetic Chain

In this section, we treat the spin–spin correlation of the spin-1/2 isotropic Heisenberg antiferromagnetic chain. The Hamiltonian is given by

[12] From Fig. 1, it may seem that the two numerical results are systematically smaller than the predicted value (3.9) by Luther and Peschel. But the deviations are within an allowable order of their numerical uncertainties.

(3.1) with anisotropy $\Delta = 1$ and spin $S = 1/2$. It is believed that the spin–spin correlation function behaves as

$$\langle S_j^x S_{j+r}^x \rangle_\infty^{XXX} \sim A(-1)^r \frac{1}{r} \times \left[\log\left(\frac{r}{r_0}\right) \right]^\sigma - \frac{1}{4\pi^2 r^2} \tag{3.14}$$

for a large distance r, where A, r_0, and σ are constants. The logarithmic correction in the first term is due to a marginally irrelevant operator in the Hamiltonian.[19–22] The existence of such a logarithmic correction was first confirmed numerically by Kubo *et al.*[12] The second term in (3.14) can be determined by using the renormalization group analysis.[18] The validity of the second term in (3.14) was confirmed numerically by Sandvik and Scalapino.[11] As for the value of the exponent σ, however, there is a discrepancy as mentioned in Section 1.3.3.

The aims of this section are the following. We first determine the critical exponent σ in (3.14) by using the scheme of Section 2. Then we examine the efficiency of our finite-size scaling function (3.28) below. Such information may be useful when one extrapolates correlations for finite volumes to infinite volume. Finally, we clarify the cause of the discrepancy between the previous calculations for the critical exponent σ of the correlation (3.14).

Our results, in particular, $\sigma = 0.47$ in Section 3.3.2 below, strongly support the field-theoretic prediction $\sigma = 1/2$ based on the mappings to the Wess–Zumino–Witten nonlinear σ-model[18,19] or the sine-Gordon model[20–22]

To begin with, we prepare some notations. Having the asymptotic form of the correlation (3.14) in mind, we write the correlation for finite length L as

$$\langle S_j^x S_{j+r}^x \rangle_L^{XXX} = (-1)^r G_L^{(1)}(r) + G_L^{(2)}(r) \tag{3.15}$$

where $G_L^{(1)}$ and $G_L^{(2)}$ satisfy

$$\lim_{L \uparrow \infty} G_L^{(1)}(r) \sim A \frac{1}{r} \times \left[\log\left(\frac{r}{r_0}\right) \right]^\sigma \tag{3.16}$$

and

$$\lim_{L \uparrow \infty} G_L^{(2)}(r) \sim -\frac{1}{4\pi^2 r^2} \tag{3.17}$$

Following the scheme in Section 2, we approximate the correlation for finite length L as

$$G_L^{(1)}(r) \cong C_L^{(1)}(r) \tag{3.18}$$

and

$$G_L^{(2)}(r) \cong C_L^{(2)}(r) \tag{3.19}$$

where the approximate functions are given by

$$C_L^{(1)}(r) := \frac{A\pi}{L \sin(\pi r/L)} \times \left\{ \log \left[\frac{L}{\pi r_0} \sin \left(\frac{\pi}{L} r \right) \right] \right\}^{\sigma} \tag{3.20}$$

and

$$C_L^{(2)}(r) := -\frac{1}{4} \left[\frac{1}{L \sin(\pi r/L)} \right]^2 \tag{3.21}$$

The former $C_L^{(1)}$ is given by (2.24) with (2.9). Here we note that (3.21) can be rewritten as

$$C_L^{(2)}(r) = -\frac{1}{4\pi^2} \sum_{n=-\infty}^{\infty} \frac{1}{|r+nL|^2} \tag{3.22}$$

because of the well-known formula

$$\frac{1}{\sin^2 z} = \sum_{n=-\infty}^{\infty} \frac{1}{(z+n\pi)^2} \tag{3.23}$$

for $z \in \mathbf{C}$. The right-hand side of (3.22) is nothing but the form obtained by Sandvik and Scalapino.[11] They obtained (3.22) by assuming a certain relation between correlations for finite volumes and that for infinite volume. (See ref. 11 for details).

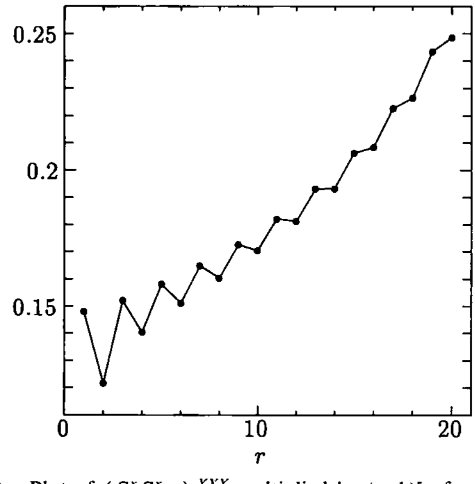

Fig. 2. Plot of $\langle S_j^x S_{j+r}^x \rangle_L^{XXX}$ multiplied by $(-1)^r r$ for $L=40$.

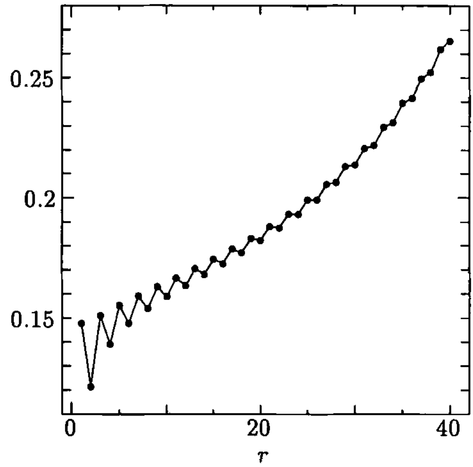

Fig. 3. Plot of $\langle S_j^x S_{j+r}^x \rangle_L^{XXX}$ multiplied by $(-1)^r r$ for $L = 80$.

3.3.1. Extracting the Most Dominant Term from the Correlation. In this section, following Sandvik and Scalapino,[11] we check the validity of (3.19) and subtract the second term $G_L^{(2)}$ from $\langle S_j^x S_{j+r}^x \rangle_L^{XXX}$ of (3.15).

We calculated the correlation function $\langle S_j^x S_{j+r}^x \rangle_L^{XXX}$ for finite L by performing a Monte Carlo simulation at zero temperature (see Appendices A and B for details) which was proposed by Kubo *et al.*[12] to treat directly

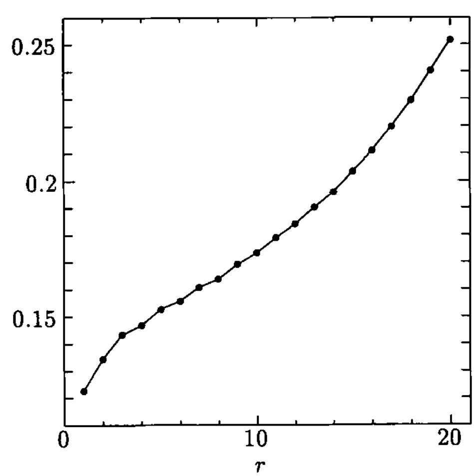

Fig. 4. Plot of $r \times D_L(r)$ for $L = 40$.

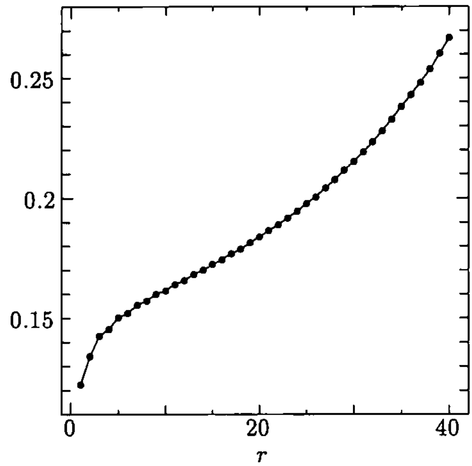

Fig. 5. Plot of $r \times D_L(r)$ for $L = 80$.

a quantum system at zero temperature. Figures 2 and 3 show the Monte Carlo results for the correlation $\langle S_j^x S_{j+r}^x \rangle_L^{XXX}$ multiplied by $(-1)^r r$ for $L = 40$ and $L = 80$, respectively. Clearly the even–odd oscillations in Figs. 2 and 3 should be due to the second term $G_L^{(2)}$ in (3.15).

Following Sandvik and Scalapino,[11] we subtract the oscillatory part $G_L^{(2)}$ from $\langle S_j^x S_{j+r}^x \rangle_L^{XXX}$ as

$$D_L(r) := (-1)^r \times \{\langle S_j^x S_{j+r}^x \rangle_L^{XXX} - C_L^{(2)}(r)\} \tag{3.24}$$

where we used the assumption (3.19). As shown in Figs. 4 and 5, the even–odd oscillations almost disappear by this subtraction. From this observation, we conclude

$$D_L(r) \cong G_L^{(1)}(r) \tag{3.25}$$

Consequently we have been able to extract the desired term $G_L^{(1)}(r)$ related to the logarithmic correction from the original spin–spin correlation $\langle S_j^x S_{j+r}^x \rangle_L^{XXX}$ of the spin-1/2 isotropic Heisenberg antiferromagnetic chain.

3.3.2. Logarithmic Correction to the Correlation $\langle S_j^x S_{j+r}^x \rangle_L^{XXX}$. Now we shall determine the parameters A, r_0, and σ by fitting $C_L^{(1)}$ of (3.20) directly to numerical results of D_L, (3.24). As numerical data, we used the results of the numerical exact diagonalization for $L \leqslant 24$ from ref. 63 and for $L = 28$ and 30 from ref. 64. Further, for larger lengths $32 \leqslant L \leqslant 80$, we performed the zero-temperature Monte Carlo simulations as mentioned in the preceding section.[13]

[13] Throughout Section 3.3, we use these data.

By using a least-squares fitting, we obtained $A \cong 0.071$, $r_0 \cong 0.039$, and $\sigma \cong 0.47$ with the accuracy

$$\left| \frac{D_L(r) - C_L^{(1)}(r)}{D_L(r)} \right| < 1.21 \times 10^{-2} \tag{3.26}$$

for $1 \leqslant r \leqslant L/2$ and $4 \leqslant L \leqslant 80$. This accuracy (3.26) is comparable to the accuracy 1 % for relatively large distance r in the Monte Carlo simulations.

The result for the critical exponent $\sigma \cong 0.47$ strongly supports the field-theoretic prediction $\sigma = 1/2$ based on the mappings to the Wess–Zumino–Witten nonlinear σ-model[18,19] or the sine-Gordon model.[20–22]

With the critical exponent σ fixed to the field-theoretic value $\sigma = 1/2$, we also determined the parameters A and r_0. As a result, we obtained $A \cong 0.065$ and $r_0 \cong 0.028$ with the accuracy

$$\left| \frac{D_L(r) - C_L^{(1)}(r)}{D_L(r)} \right| < 1.26 \times 10^{-2} \tag{3.27}$$

for $1 \leqslant r \leqslant L/2$ and $4 \leqslant L \leqslant 80$.

These numerical results strongly support our conjecture (3.18) with (3.20), and the field-theoretic prediction $\sigma = 1/2$ of the critical exponent.

3.3.3. Efficiency of a New Finite-Size Scaling Function. So far we have treated the critical exponents η and σ and the critical amplitude A. Unfortunately, by the method in Sections 3.3.1 and 3.3.2, one cannot get a value for an infinite-volume correlatin function itself for a given distance r. For this purpose, one must extrapolate correlation functions for finite volumes to infinite volume. In such a situation, information about finite-size scaling may be useful. But, as Sandvik and Scalapino[11] pointed out, it is not clear whether the standard scaling hypothesis (1.1) holds or not when there exists a logarithmic correction to a correlation as in the correlation (3.14) of the present spin-1/2 isotropic Heisenberg antiferromagnetic chain. Actually, as mentioned in Section 1.3.3., there is a discrepancy among the previous calculations of the exponent σ of the correlation (3.14).

For this problem, we propose a new finite-size scaling function

$$Q(\tau, L) := \left[\frac{\pi\tau}{\sin(\pi\tau)} \right]^{\eta_{\text{eff}}(L)} \tag{3.28}$$

with $\tau = r/L$, whose form is derived from (2.22) and (2.9). Here $\eta_{\text{eff}}(L)$ is an effective exponent to be determined. The aim of this section is to examine

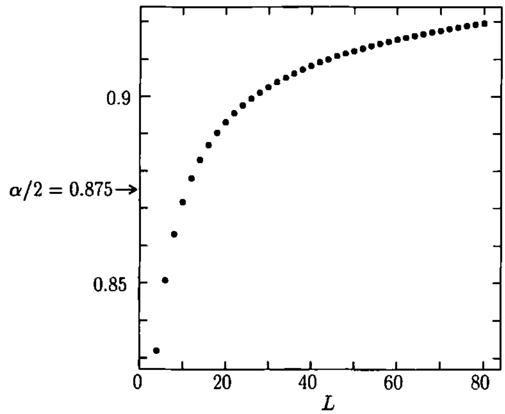

Fig. 6. The effective critical exponent $\eta_{\rm eff}(L)$ of the spin–spin correlation of the spin-1/2 isotropic Heisenberg antiferromagnetic chain. (We use the value of $\alpha/2$ in the discussion at the end of Section 3.3.3.)

the efficiency of our scaling function (3.28) and to clarify the cause of the discrepancy in the previous calculations of the exponent σ of (3.14).

First, to examine the efficiency of the scaling function $Q(\tau, L)$ of (3.28), let us extrapolate $G_L^{(1)}$, (3.16), for finite lengths to $G_\infty^{(1)} := \lim_{L\uparrow\infty} G_L^{(1)}$ by relying on the scaling relation

$$G_L^{(1)}(r) \cong G_\infty^{(1)}(r) \times Q(\tau, L) \tag{3.29}$$

For this purpose, we must determine the effective critical exponent[36] $\eta_{\rm eff}(L)$ in $Q(\tau, L)$, (3.28), as a function of the length L of the chain. Under the assumption of a conformal invariance, we calculated $\eta_{\rm eff}(L)$ numerically from the spectrum of the diagonal-to-diagonal transfer matrix of the six-vertex model,[14] which is the two-dimensional classical system corresponding to the present spin-1/2 isotropic Heisenberg antiferromagnetic chain. (See Appendices D–F for details). The results for $\eta_{\rm eff}(L)$ are shown in Fig. 6.

Combining the scaling relation (3.29) with the result $D_L(r) \cong G_L^{(1)}(r)$, (3.25), we expect

$$\frac{D_L(r)}{Q(\tau, L)} = D_\infty(r) + D^{(1)}(r) \times L^{-2} + D^{(2)}(r) \times L^{-4} + \cdots \tag{3.30}$$

[14] Klümper *et al.*[65] studied the spectrum of the transfer matrix of the six-vertex model by using the Bethe ansatz. As a consequence, they observed a tower structure which is expected from conformal field theories. See also refs. 66–68 and 54 for the tower structure in the energy spectrum of the Heisenberg chain.

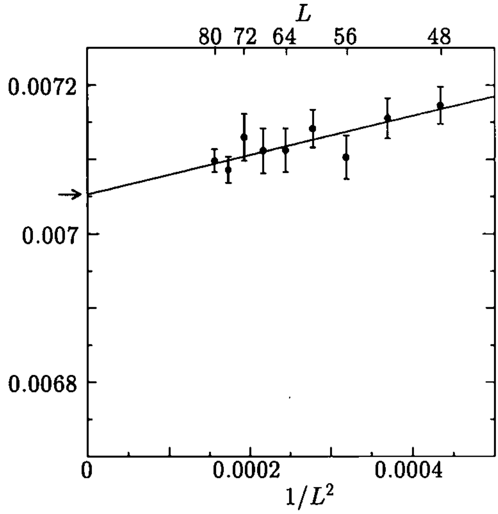

Fig. 7. Plot of D_L/Q with the Kaplan–Horsch–Borysowicz scaling function Q of (3.10) for the distance $r = 24$.

with small correction terms $D^{(l)}(r)$ $(l = 1, 2,...)$ to the extrapolation value

$$D_\infty(r) := \lim_{L \uparrow \infty} D_L(r) \tag{3.31}$$

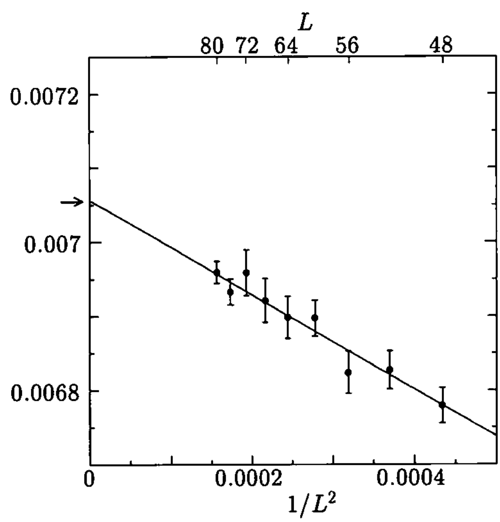

Fig. 8. Plot of D_L/Q with the simple function Q of (2.16) with $\eta = 1$, but without logarithmic correction, for the distance $r = 24$.

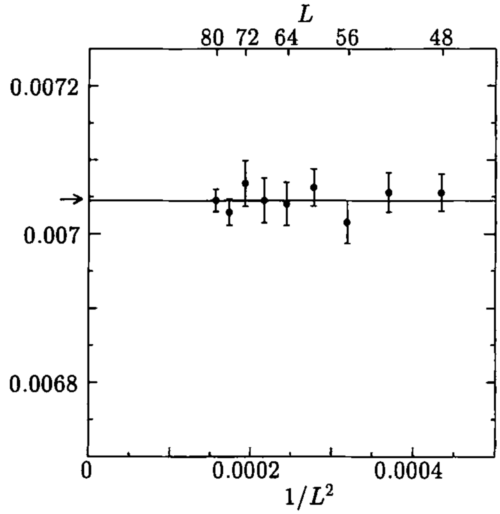

Fig. 9. Plot of D_L/Q with our scaling function Q, (3.28), for the distance $r = 24$.

for a fixed r, where we have used the assumption that there appear only even powers of L^{-1} in the series.[45,46,10] For the fixed distance $r = 24$, Figs. 7–9 show D_L/Q with three different scaling functions Q, i.e., the Kaplan–Horsch–Borysowicz scaling function, the simple form (2.16) with $\eta = 1$, but without logarithmic correction, and our scaling function (3.28), respectively. Here the Kaplan–Horsch–Borysowicz scaling function is given by the right-hand side of (3.10) with (3.11) and $\Delta = 1$.

Clearly, D_L/Q with our scaling function (3.28) gives the smallest correction to the extrapolation values D_∞. Further, with the help of the above three scaling functions, we extrapolate D_L to the limit $L \uparrow \infty$. Figures 10–12 show the results D_∞ so obtained. Clearly, the result with our scaling function (3.28) gives the smallest errors for the whole range of the distance r. The other two results give larger errors for relatively large r. These errors make a calculation of the exponent σ in the correlation $\langle S_j^x S_{j+r}^x \rangle_\infty^{XXX}$ of (3.14) hard. In passing, if we make the extrapolation without scaling, then the results have enormous errors, as in Fig. 13.

We thus conclude that the scaling relation (3.29) with the scaling function (3.28) is quite efficient when there is a logarithmic correction to correlations.

Next we shall check that the above results for D_∞ obtained with the help of our scaling function (3.28) are consistent with the results obtained in Section 3.3.2.

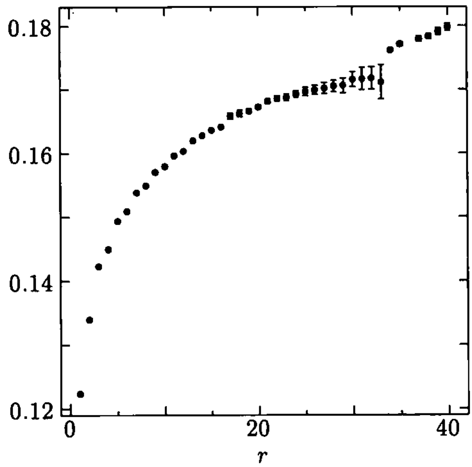

Fig. 10. The extrapolated result $r \times D_\infty$ with the use of the Kaplan–Horsch–Borysowicz scaling function Q. The point for $r = 36$ is not included in the figure because it is off scale.

We note that, from (3.25) and (3.16), we have

$$D_\infty(r) \sim \frac{A}{r}\left[\log\left(\frac{r}{r_0}\right)\right]^\sigma \tag{3.32}$$

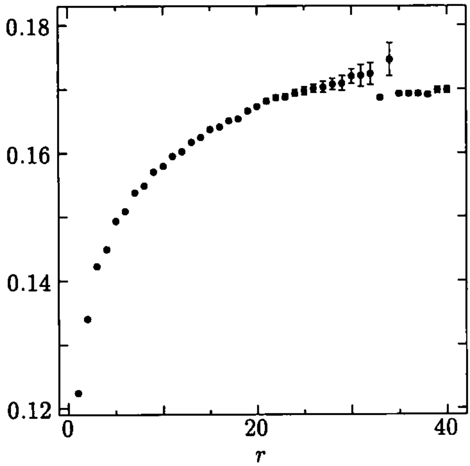

Fig. 11. The extrapolated result $r \times D_\infty$ with the use of the simple function Q with $\eta = 1$, but without logarithmic correction.

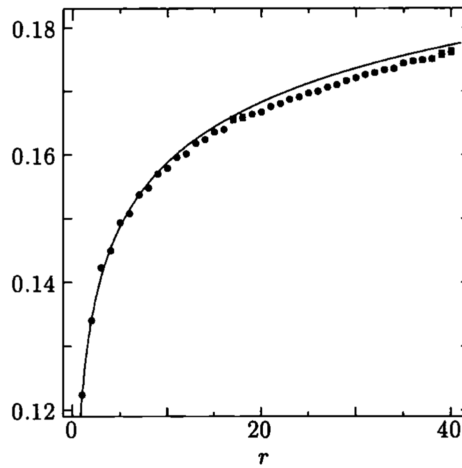

Fig. 12. The extrapolated result $r \times D_\infty$ with the use of our scaling function. The solid line is $A[\log(r/r_0)]^{1/2}$, whose parameters A and r_0 are determined from a least-squares fitting.

Assuming the field-theoretic value $\sigma = 1/2$,[15] we determine the constants A and r_0 by a least-squares fitting to the results D_∞ obtained with the help of our scaling function (3.28). As a consequence, we have obtained $A \cong 0.067$ and $r_0 \cong 0.036$. Clearly, these values are consistent with those in Section 3.3.2. Further, as shown in Fig. 12, the fitting function $A[\log(r/r_0)]^{1/2}$ is in good agreement with the extrapolated values $r \times D_\infty$ in spite of using only two fitting parameters A and r_0.[16]

These observations strongly support the field-theoretic prediction $\sigma = 1/2$ based on the mappings to the Wess–Zumino–Witten nonlinear σ-model[(18,19)] or the sine-Gordon model.[(20–22)]

Let us discuss the relation between our scaling function (3.28) and the Kaplan–Horsch–Borysowicz scaling relation (3.10). To compare these two scaling functions, we rewrite the Kaplan–Horsch–Borysowicz scaling

[15] If we treat σ also as a fitting parameter, we obtain $\sigma \cong 0.5$, which strongly supports the field-theoretic value 1/2.

[16] The curve $A[\log(r/r_0)]^{1/2}$ is systematically larger than the extrapolated values for relatively larger r. This is because the numerical data for small r have smaller errors than those for large r, since we have more data for small r than for large r, i.e., we have data for all distances $r \leqslant L/2$ for a size L. Thus the fitting curve, which is determined by a least-squares fitting with large weight for small distances r and with small weight for large r, often turns out to have large deviations for large r.

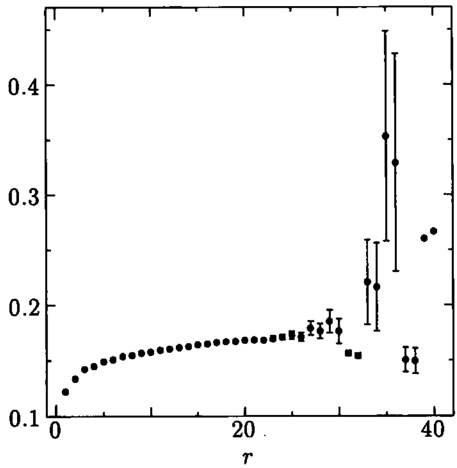

Fig. 13. The extrapolated result $r \times D_\infty$ without scaling.

function Q_{KHB} as follows. The right-hand side of (3.10) with (3.11) and $\Delta = 1$ can be rewritten as

$$Q_{\mathrm{KHB}}(\tau) \cong \left[\frac{\pi\tau}{\sin(\pi\tau)} \right]^{\alpha/2} \tag{3.33}$$

with $\alpha/2 \cong 1.75/2 = 0.875$ and $\tau := r/L$, where we have used the scaling relation (2.16) for the correlation function of the XY chain and the critical exponent $\eta = 1/2$ of the correlation (3.4) of the XY chain. Comparing (3.33) with (3.28), we conjecture that Kaplan *et al.* obtained the value $\alpha/2 \cong 0.875$ as a smeared value of the effective critical exponent $\eta_{\mathrm{eff}}(L)$ for some lengths L. Let us check this conjecture. Actually, from Fig. 6, for the lengths $8 \leqslant L \leqslant 18$ treated by Kaplan *et al.*,[10] the effective critical exponent $\eta_{\mathrm{eff}}(L)$ takes the values 0.86–0.89.

In conclusion, the result by Kaplan *et al.* can be explained in terms of our scaling function (3.28). Further, our scaling function also explains the fact that the optimal value of the parameter α in the Kaplan–Horsch–Borysowicz scaling (3.33) increases slightly with the increase of the system size L as we observed previously.[16,17] Clearly, in a calculation of the exponent σ of the correlation (3.14), one cannot ignore errors which come from the deviation of the value of the parameter α. But many of the previous numerical calculations[12–15] of σ have relied on the Kaplan–Horsch–Borysowicz scaling function (3.33) with $\alpha = 1.75$. We conclude that the discrepancy in the previous calculations is due to ignoring the finite-size corrections of the effective critical exponent $\eta_{\mathrm{eff}}(L)$ in the scaling function (3.28).

4. APPLICATION TO THE SPIN-3/2 ISOTROPIC HEISENBERG ANTIFERROMAGNETIC CHAIN

The Hamiltonian is given by (3.1) with $S = 3/2$ and $\Delta = 1$. The spin–spin correlation has been studied intensively in recent years,[69–71, 38–41, 23, 42, 14, 24] concerning the Haldane conjecture,[37] logarithmic corrections, and crossover phenomena.

Before applying our method to the spin-3/2 isotropic Heisenberg chain, we shall briefly summarize previous work, which will be related to our calculations.

Haldane[37] treated the spin-S antiferromagnetic chains by using a semiclassical large-S approximation, and conjectured that the low-energy theories of the spin chains are described by the $O(3)$ nonlinear σ model with the topological term $\theta = \pi$ or 0 for half-odd integer and integer spin, respectively. This result implies that all half-odd-integer-spin chains behave like the spin-1/2 chain. The same conclusion was reached by Schulz,[38] who used the Jordan–Wigner transformation and an Abelian bosonization. Affleck[71] identified the spin-S Heisenberg antiferromagnetic chain with the Wess–Zumino–Witten nonlinear σ model (WZW model) with topological coupling $k = 2S$ by using a non-Abelian bosonization.[72] The corresponding critical exponent η of the WZW model is given by[73]

$$\eta = \frac{3}{2+k} \tag{4.1}$$

for topological coupling k. For example, one has $\eta = 1$ for the $S = 1/2$ chain, and $\eta = 3/5$ for $S = 3/2$. Moreo[39] diagonalized the Hamiltonian of the spin-3/2 isotropic Heisenberg chain numerically up to length $L = 12$ of the chain, and calculated the critical exponent η of the spin–spin correlation function by relying on the standard finite-size scaling[9] under the assumption that the correlation decays by a power law as[71]

$$\langle S_i^z S_{i+r}^z \rangle_\infty \sim (-1)^r \frac{A}{r^\eta} + \frac{B}{r^2} \tag{4.2}$$

where A and B are constants. As a result, she obtained $\eta = 0.53 \pm 0.03$, which is consistent with $\eta = 0.6$ predicted by Affleck in 1986[71] rather than the $\eta = 1$ expected by Haldane[37] and Schulz.[38]

However, if there exists a marginally irrelevant perturbation in the Hamiltonian of the spin-3/2 chain, then the operator leads to logarithmic corrections to the decay of the correlation, as in the spin-1/2 isotropic Heisenberg antiferromagnetic chain. (See Appendix C.2 for details.) Affleck *et al.*[19] argued by using a conformal field theory that the leading term of the logarithmic correction is universal as

$$\langle S_i^z S_{i+r}^z \rangle_\infty \sim (-1)^r \frac{A}{r^\eta} \times \left[\log \left(\frac{r}{r_0} \right) \right]^{1/2} + \frac{B}{r^2} \tag{4.3}$$

where r_0 is a nonuniversal constant.

Affleck and Haldane[23] reexamined the relation between quantum spin chains and conformal field theories, and predicted, among other things, that the half-odd-integer-spin ($S > 1/2$) Heisenberg chains exhibit a crossover from the WZW model with topological coupling $k = 2S$ ($=$odd) to the WZW model with $k = 1$ ($\eta = 1$) due to relevant perturbations in the Hamiltonian. In particular, in the case of the spin 3/2, there appear one relevant and one marginally irrelevant perturbations in the Hamiltonian, which are the causes of the crossover and logarithmic corrections, respectively. The numerical results by Ziman and Schulz[40] strongly support the Affleck–Haldane conjecture. They calculated the ground-state energy $E_0(L)$ and the excitation energies $\Delta E_n(L) = E_n(L) - E_0(L)$ for lengths $L = 8$, 10, 12 of the spin-3/2 antiferromagnetic chain, and determined the central charge c and the critical exponent η by using a finite-size correction method based on a conformal field theory.

In the following, we will perform three types of fittings by assuming three types of asymptotic forms of the correlation, i.e., a typical power decay (4.2), a power decay with a logarithmic correction (4.3), and a power decay with a logarithmic correction and with a crossover as was predicted by Affleck and Haldane.

Although we cannot give a conclusive result, our results strongly support the Affleck–Haldane predicion. In fact, from the point of view of the Affleck–Haldane argument, we can give consistent interpretations of the numerical results of the correlation by Moreo[39] and Lin.[64]

4.1. Fitting (i)

First we assume as a trial that the spin–spin correlation decays by a power law as in (4.2). Following our scheme in Section 2, from (2.5), (2.6), and (2.9), we take

$$C_L(r) := A(-1)^r \left[\frac{\pi}{L \sin(\pi r/L)} \right]^\eta + B \left[\frac{\pi}{L \sin(\pi r/L)} \right]^2 \tag{4.4}$$

as an approximate correlation function for $\langle S_i^z S_{i+r}^z \rangle_L$. We determine the constants A, B, and η by a least-squares fitting of $C_L(r)$ to the exact

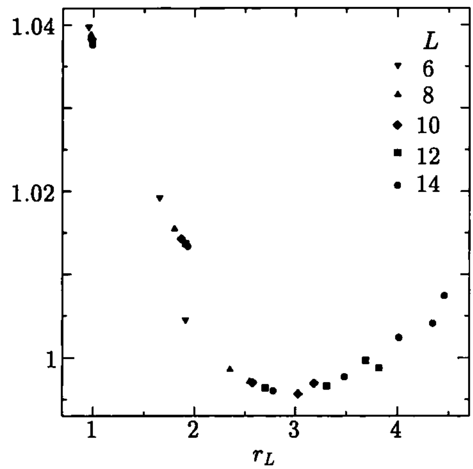

Fig. 14. The ratio $C_L(r)/\langle S_i^z S_{i+r}^z \rangle_L$ versus the effective distance $r_L = (L/\pi)\sin(\pi r/L)$ in the spin-3/2 Heisenberg chain. The fitting function $C_L(r)$ of (4.4) is determined by using a least-squares fitting to exact numerical values $\langle S_i^z S_{i+r}^z \rangle_L$.

numerical values of $\langle S_i^z S_{i+r}^z \rangle_L$ for the distance $3 \leqslant r \leqslant L/2$ in finite chains of length $L = 6$–12 obtained by Moreo[39] and of $L = 14$ by Lin.[64] As a consequence, we obtained $A = 0.92$, $B = -0.06$, and the exponent $\eta = 0.51$. Figure 14 shows the ratio $C_L(r)/\langle S_i^z S_{i+r}^z \rangle_L$ versus the effective distance $r_L := (L/\pi)\sin(\pi r/L)$.

Our result $\eta = 0.51$ for the exponent is in agreement with the result $\eta = 0.53 \pm 0.03$ obtained by Moreo.[39] This value is also in agreement with $\eta = 0.6$ predicted by Affleck in 1986[71] rather than $\eta = 1$ expected by Haldane[37] and Schulz.[38] As in Fig. 14, the fitting results are accurate to the exact values within 4%. But the results for the ratio $C_L(r)/\langle S_i^z S_{i+r}^z \rangle_L$ curve upward with the increase of the effective distance r_L.

4.2. Fitting (ii)

Next we assume the asymptotic behavior (4.3) of the correlation. Following the same procedure as for the spin-1/2 isotropic Heisenberg antiferromagnetic chain in Section 3.3, we put

$$C_L^{\log}(r) := A(-1)^r \left[\frac{\pi}{L\sin(\pi r/L)}\right]^\eta \times \left\{\log\left[\frac{L\sin(\pi r/L)}{r_0 \pi}\right]\right\}^{1/2} + B\left[\frac{\pi}{L\sin(\pi r/L)}\right]^2 \tag{4.5}$$

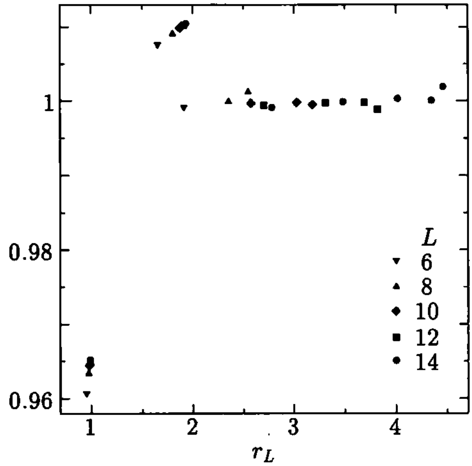

Fig. 15. The ratio $C_L^{\log}(r)/\langle S_i^z S_{i+r}^z \rangle_L$ versus the effective distance, $r_L = (L/\pi)\sin(\pi r/L)$ in the spin-3/2 Heisenberg chain. The fitting function $C_L^{\log}(r)$ of (4.5) is determined by using a least-squares fitting to exact numerical values $\langle S_i^z S_{i+r}^z \rangle_L$.

to trial, and determine the fitting parameters A, B, η, and r_0 in the same way as in Section 4.1. As a result, we obtained $A = 0.77$, $B = -0.05$, $\eta = 0.73$, and $r_0 = 0.29$. Figure 15 shows the ratio $C_L^{\log}(r)/\langle S_i^z S_{i+r}^z \rangle_L$ versus the effective distance $r_L = (L/\pi)\sin(\pi r/L)$. The fitting resuls are accurate to the exact values within 4%. The outstanding feature is the following. The fitting error is within order 10^{-4} for the distance $r \geqslant 3$ of the correlation. However, we obtained a somewhat strange value $\eta = 0.73$, which lies between $\eta = 0.6$ of the $k = 3$ WZW model and $\eta = 1$ of the $O(3)$ nonlinear σ model with topological term $\theta = \pi$. We cannot find a corresponding critical theory with the exponent $\eta = 0.73$ from the point of view of conformal field theories,[18,23] which are believed to describe the low-energy behavior in antiferromagnetic quantum spin chains.

4.3. Fitting (iii)

According to Affleck and Haldane,[23] there appear one relevant and one marginally irrelevant perturbations, which are the causes of the crossover and logarithmic corrections, respectively, in the spin-3/2 isotropic Heisenberg antiferromagnetic chain. In this section, we try to take account of the crossover effect predicted by Affleck and Haldane in our scheme.

Affleck *et al.*[19] showed that the leading term in the logarithmic corrections for large distances is universal, i.e., is independent of the topological coupling k ($=$odd) in the WZW models. This result suggests that the existence of a relevant perturbation leading to the crossover does not affect the leading term of the logarithmic correction to the decay of the correction for large distances. We assume that the crossover occurs only for the exponent of the power-law decay of the correlation but not for the logarithmic corrections.

Under this assumption, we calculate the asymptotic form of the correlation $\langle S_i^z S_{i+r}^z \rangle_\infty$ of the spin-3/2 isotropic Heisenberg chain, following Affleck and Haldane.[23] As a result (see Appendix C.3 for details), we formally obtain

$$\langle S_i^z S_{i+r}^z \rangle_\infty \sim (-1)^r \frac{1}{r^{3/5}} \times \left[\log\left(\frac{r}{r_0}\right)\right]^{1/2} \times Y\left(\frac{r}{r_0}\right) + \frac{B}{r^2} \tag{4.6}$$

with the crossover function Y. Here the exponent $\eta = 3/5$ came from (4.1) for the $k=3$ WZW model, and the crossover function is expected to behave as

$$Y(l) \sim \begin{cases} \text{const} & \text{for small } l \\ \text{const} \times 1/l^{\delta\eta} & \text{for large } l \end{cases} \tag{4.7}$$

with $\delta\eta = 0.4$. This describes a crossover from $\eta = 0.6$ ($k=3$ WZW model) to $\eta = 1$ ($k=1$ WZW model).

Unfortunately, we cannot get an explicit form of the crossover function Y. Therefore we must take a different approach from that in Sections 4.1 and 4.2. We determine the crossover function Y from the exact numerical results of the correlations obtained by Moreo[39] and Lin.[64] That is, we determine Y by

$$\begin{aligned} \langle S_i^z S_{i+r}^z \rangle_L = (-1)^r \left[\frac{\pi}{L \sin(\pi r/L)} \right]^{3/5} \times (\log l_L)^{1/2} \times Y(l_L) \\ + B \left[\frac{\pi}{L \sin(\pi r/L)} \right]^2 \end{aligned} \tag{4.8}$$

with the effective scale.

$$l_L := \frac{L}{r_0 \pi} \sin\left(\frac{\pi r}{L}\right) \tag{4.9}$$

Here, for the values of the parameters B and r_0, we use $B = -0.05$ and $r_0 = 0.29$, which were obtained in Section 4.2. These values are expected to be good estimates for (4.6) because the resulting exponent $\eta = 0.73$ in Section 4.2 can be interpreted as the effective exponent. Figure 16 shows $Y(l_L)$ multiplied by $l_L^{\delta\eta}$ with $\delta\eta = 0.0$–0.6. The results for the predicted $\delta\eta = 0.4$ by

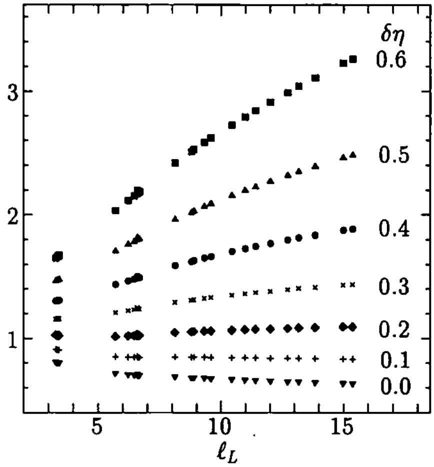

Fig. 16. Crossover function $Y(l_L)$ multiplied by $l_L^{\delta\eta}$ with $\delta\eta = 0.0$–0.6 in the spin-3/2 Heisenberg chain.

Affleck and Haldane[23] increase slowly with the increase of the effective scale l_L. If the crossover continues to larger distances than those we now observe, then the results in Fig. 16 do not contradict the Affleck–Haldane conjecture.

Although we have not been able to give a conclusive result, we have proposed consistent interpretations of the numerical results of the correlation by Moreo[39] and Lin[64] from the point of view of the Affleck–Haldane argument.

APPENDIX A. ZERO-TEMPERATURE MONTE CARLO METHOD

In this appendix, we review a Monte Carlo method which deals directly with a quantum system at zero temperature. We applied the method to the spin-1/2 Heisenberg chain in order to calculate the spin–spin correlation function, whose data are used in Section 3.3.

As is well known, techniques based on the path integral idea are effective for analyzing quantum systems at finite temperatures. In particular, the quantum Monte Carlo method[25–27,74] and the quantum transfer matrix method[75,35,17] have been widely used to study quantum many-body systems. However, to obtain information about a quantum system at zero temperature within the same formalism, one must extrapolate quantities at finite temperatures to those at zero temperature. The procedure sometimes yields enormous errors, which makes it difficult to arrive at conclusive results.

A Monte Carlo method which deals directly with a quantum system at zero temperature was first proposed by Kubo *et al.*[12] in order to study the logarithmic correction to the spin–spin correlation of the spin-1/2 Heisenberg antiferromagnetic chain. The system satisfies the so-called Sutherland relation[76] that the Hamiltonian commutes with the transfer matrix of the six-vertex model with certain Boltzmann weights.[17] The application of the Perron–Frobenius theorem (see, e.g., refs. 77 and 78) to the Hamiltonian and the transfer matrix yields immediately the result that the eigenvector with the maximum eigenvalue of the transfer matrix can be identified with the ground state of the quantum system, so that a correlation function of the six-vertex model is identical to a certain correlation function of the ground state of the Heisenberg chain.

Generalizing the idea proposed by Kubo *et al.*, we assume that the transfer matrix W_N of a classical system and the Hamiltonian $\mathscr{H}_N$ of a system with N sites are defined on the same Hilbert space, and that the eigenvector Φ_N satisfies

$$W_N \Phi_N = \Lambda_N^{\max} \Phi_N \tag{A.1}$$

and

$$\mathscr{H}_N \Phi_N = E_N^{(0)} \Phi_N \tag{A.2}$$

with nondegenerate eigenvalues $\Lambda_N^{\max}$ and $E_N^{(0)}$ which are the maximum eigenvalue of W_N and the ground-state energy of $\mathscr{H}_N$, respectively.

Under these assumptions, the correlation between two observables ϕ_i and ϕ_j defined as

$$\langle \phi_i \phi_j \rangle_{N \times M, \mathrm{P}} := \frac{\mathrm{Tr}[\phi_i \phi_j (W_N)^M]}{\mathrm{Tr}(W_N)^M} \tag{A.3}$$

for the classical system with the size $N \times M$ is related to the quantum mechanical correlation for the ground state Φ_N by

$$\langle \phi_i \phi_j \rangle_N := (\Phi_N, \phi_i \phi_j \Phi_N) = \lim_{M \uparrow \infty} \langle \phi_i \phi_j \rangle_{N \times M, \mathrm{P}} \tag{A.4}$$

where the subscript P indicates the use of the periodic boundary condition in the transfer direction of the transfer matrix. Thus, by combining (A.3) with a Monte Carlo method, one can directly calculate the ground-state correlation of a quantum system without an extrapolation with respect to temperature.

[17] More precisely, Sutherland showed that the Hamiltonian of the spin-1/2 XYZ Heisenberg chain commutes with the transfer matrix of the eight-vertex model with certain Boltzmann weights. Therefore the Kubo–Kaplan–Borysowicz method can be applied also to the XYZ chain.

However, there often arises the problem that usual updating procedures consisting of local spin flips do not necessarily satisfy the condition of the ergodicity of the Monte Carlo sequences. To guarantee the ergodicity of the Monte Carlo simulations of the six-vertex model, Kubo *et al.*[12] introduced updating procedures of global flips. But the acceptance ratio of global flips decreases very rapidly with increase of the system size.

In our earlier work[16,17] we avoided this difficulty by modifying the Kubo–Kaplan–Borysowicz method as follows. Instead of imposing periodic boundary conditions in the transfer direction of the transfer matrix, we used "free boundary" conditions. Thereby the ergodicity of the Monte Carlo sequences are guaranteed by using only local spin flips, without global flips.[79] As is well known, the periodic boundary conditions in the six-vertex model lead to global constrains related to the conservation of winding number.[12] In general, it is proved[79] that the use of "free boundary" conditions removes such constraints. Consequently, the modification is equivalent to choosing

$$\langle \phi_i \phi_j \rangle_{N \times M,\, \mathrm{F}} := \frac{(\Psi, (W_N)^{M/2}\, \phi_i \phi_j (W_N)^{M/2}\, \Psi)}{(\Psi, (W_N)^{M}\, \Psi)} \tag{A.5}$$

instead of (A.3) as the approximate correlation function. Here M is even and the subscript F denotes the "free boundary" condition, which is determined by the way we choose a trial vector Ψ. Clearly, there arises another problem, namely that one cannot measure the observable $\phi_i \phi_j$ near the free boundaries of the system. But this demerit can be outweighed by choosing the trial vector Ψ carefully. We chose Ψ so that the original six-vertex model feels the standard free boundary conditions.[16,17] It turns out that this choice leads to a more rapid convergence than the periodic boundary condition imposed in (A.3). In consequence, the modification enables us to treat much longer chains of the spin-1/2 isotropic Heisenberg antiferromagnetic model. (See Appendix B for details.)

We can make the following two remarks.

- This zero-temperature Monte Carlo method can be applied also to the Hubbard chain, which satisfies a similar Sutherland relation,[80] namely that the Hamiltonian commutes with the transfer matrix of the double-layer six-vertex model.
- It is not clear whether the present method applies effectively to a general quantum system. We must first find a "simple" classical system which satisfies the above requirements, but even this might not be easy in general.

APPENDIX B. ZERO-TEMPERATURE MONTE CARLO SIMULATION OF THE SPIN-1/2 ISOTROPIC HEISENBERG ANTIFERROMAGNETIC CHAIN

As mentioned in Appendix A, Kubo *et al.*[12] performed a Monte Carlo simulation for the six-vertex model by relying on the relation between the spin-1/2 Heisenberg chain and the six-vertex model. They calculated the spin–spin correlation at the isotropic antiferromagnetic point up to the length $L=40$ of the chain. Later we reperformed a Monte Carlo simulation up to[18] $L=80$, modifying the Kubo–Kaplan–Borysowicz method as in Appendix A. In this appendix, we will explain only crucial points for performing our modified Monte Carlo simulations. See ref. 12 for the details of the updating procedures in the simulations.

B.1. Statistical Error in Monte Carlo Simulations

Since the system which we treat is at criticality, the dynamics of a Monte Carlo simulation may become very slow. Therefore, we must carefully estimate the statistical error in the Monte Carlo simulations.

As usual we define the average $E[O]$ of the observable O with respect to the Monte Carlo sequence $\{\omega_i\}_{i=1}^{\mathcal{N}}$ as

$$E[O] := \frac{1}{\mathcal{N}} \sum_{i=1}^{\mathcal{N}} O(\omega_i) \tag{B.1}$$

In the limit $\mathcal{N} \uparrow \infty$, the average $E[O]$ converges to the exact value of the thermal average of O. But, for finite Monte Carlo steps $\mathcal{N}$, $E[O]$ deviates from the exact value. To estimate the deviation, we take the following strategy. We perform Monte Carlo simulations so that we have $\mathcal{K}$ Monte Carlo sequences $\{\omega_i^{(j)}\}_{i=1}^{\mathcal{N}}$ $(j=1, 2,..., \mathcal{K})$ which are independent of each other and have common Monte Carlo steps $\mathcal{N}$. We determine the standard deviation $\sigma[O]$ by

$$(\sigma[O])^2 := \frac{1}{\mathcal{K}} \sum_{j=1}^{\mathcal{K}} \{E^{(j)}[O]\}^2 - \left\{\frac{1}{\mathcal{K}} \sum_{j=1}^{\mathcal{K}} E^{(j)}[O]\right\}^2 \tag{B.2}$$

where $E^{(j)}[\cdots]$ denotes the average with respect to the jth Monte Carlo sequence $\{\omega_i^{(j)}\}_{i=1}^{\mathcal{N}}$. From this standard deviation $\sigma[O]$, the statistical

[18] Our computations were done on Fujitsu S-4/2, SONY NWS-3460, and HP Apollo 9000/720 and /730 workstations at Gakushuin University.

error $\delta[O]$ with respect to a Monte Carlo sequence $\{\omega_i\}_{i=1}^{\mathcal{N}_{\rm tot}}$ ($\mathcal{N}_{\rm tot}=\mathcal{N}\mathcal{K}$) can be estimated by

$$\delta[O]:=\left(\frac{\mathcal{N}}{\mathcal{N}_{\rm tot}}\right)^{1/2}\sigma[O] \tag{B.3}$$

In practical simulations for the spin-1/2 isotropic Heisenberg antiferromagnetic chain, we took $\mathcal{N}\sim 10^4$ Monte Carlo steps per spin, $\mathcal{K}\sim 10^4$, and $\mathcal{N}_{\rm tot}\sim 10^8$ Monte Carlo steps per spin, after equilibration runs of 10^5 Monte Carlo steps per spin.

B.2. Efficiency of the Modification

In order to examine the efficiency of the modification for the Kubo–Kaplan–Borysowicz method in Appendix A, we compare the speed of the convergence of the correlation $\langle S_j^x S_{j+r}^x\rangle_{L\times M,\mathrm{F}}$, (A.5), with that of $\langle S_j^x S_{j+r}^x\rangle_{L\times M,\mathrm{P}}$, (A.3), as M tends to ∞.

As demonstration, we calculate exactly $\langle S_j^x S_{j+r}^x\rangle_{L\times M,\mathrm{F}}$ and $\langle S_j^x S_{j+r}^x\rangle_{L\times M,\mathrm{P}}$ for $L=12$ and $r=6$ by multiplying numerically the transfer matrix of the six-vertex model by itself repeatedly. As shown in Fig. 17, we observe that the correlation $\langle S_j^x S_{j+r}^x\rangle_{L\times M,\mathrm{F}}$ converges to the exact numerical result $\langle S_j^x S_{j+r}^x\rangle_L$ of ref. 63 much more rapidly than $\langle S_j^x S_{j+r}^x\rangle_{L\times M,\mathrm{P}}$ as M tends to ∞.

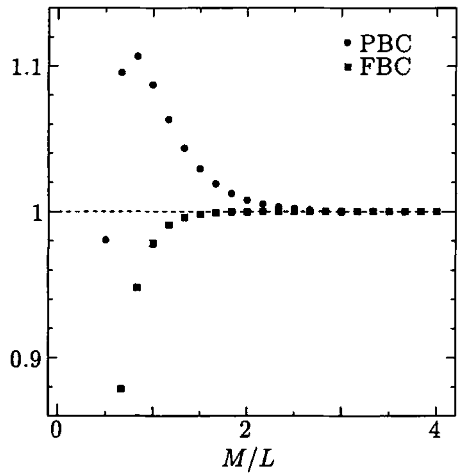

Fig. 17. For $L=12$ and $r=6$, $\langle S_j^x S_{j+r}^x\rangle_{L\times M,\mathrm{F}}/\langle S_j^x S_{j+r}^x\rangle_L$ and $\langle S_j^x S_{j+r}^x\rangle_{L\times M,\mathrm{P}}/\langle S_j^x S_{j+r}^x\rangle_L$ are plotted versus M/L, where we have used the exact numerical result of ref. 63 as $\langle S_j^x S_{j+r}^x\rangle_L$; FBC and PBC denote, respectively, free and periodic boundary conditions. Clearly, FBC exhibits more rapid convergence than PBC.

Next, we study the effect of free boundaries, which might affect the expectation value of the correlations. For this purpose, we consider the correlation

$$\langle S_j^x S_{j+r}^x \rangle_{L\times 2L,\,\mathrm{F}} := \frac{(\Psi, (W_L)^l S_j^x S_{j+r}^x (W_L)^{2L-l} \Psi)}{(\Psi, (W_L)^{2L} \Psi)} \tag{B.4}$$

which measures the observable $S_j^x S_{j+r}^x$ at the depth l $(1 \leqslant l \leqslant L)$ from one of the free boundaries. Here, for $l = L$, we have $\langle S_j^x S_{j+r}^x \rangle_{L\times 2L,\,\mathrm{F}}(l = L) = \langle S_j^x S_{j+r}^x \rangle_{L\times 2L,\,\mathrm{F}}$. Figure 18 shows $\langle S_j^x S_{j+r}^x \rangle_{L\times 2L,\,\mathrm{F}}(l)$ for $L = 40$ and $r = 1, 2, 10, 20$, and Fig. 19 for $L = 40$ and $r = 20$. In particular, as shown in Fig. 19, for large depth l, the errors due to the free boundaries are less than the statistical errors in the Monte Carlo simulations. From this observation, we conclude that

$$|\langle S_j^x S_{j+r}^x \rangle_{L\times M,\,\mathrm{F}} - \langle S_j^x S_{j+r}^x \rangle_L| \lesssim \delta[S_j^x S_{j+r}^x] \tag{B.5}$$

for a fixed r if $M \geqslant 2L$. Relying on (B.5), we identify $\langle S_j^x S_{j+r}^x \rangle_{L\times 2L,\,\mathrm{F}}$ as $\langle S_j^x S_{j+r}^x \rangle_L$. Then the deviation from the true $\langle S_j^x S_{j+r}^x \rangle_L$ is evaluated by $\delta[S_j^x S_{j+r}^x]$.

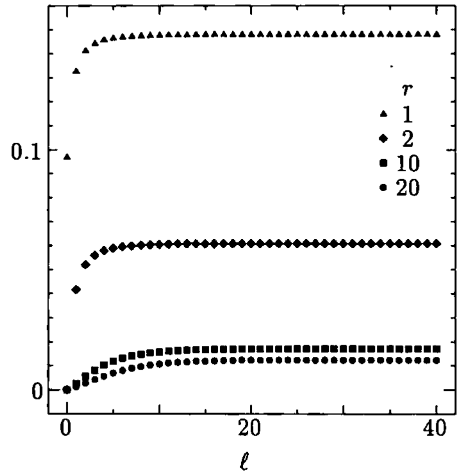

Fig. 18. Plot of $\langle S_j^x S_{j+r}^x \rangle_{L\times 2L,\,\mathrm{F}}(l)$ against the depth l from a free boundary for $L = 40$ and $r = 1, 2, 10, 20$.

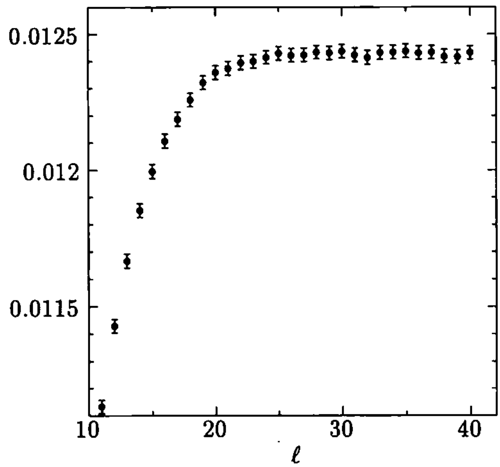

Fig. 19. Plot of $\langle S_j^x S_{j+r}^x \rangle_{L\times 2L,\,\mathrm{F}}(l)$ against the depth l from the free boundary for $L=40$ and $r=20$. The errors are due to the statistical uncertainty in the Monte Carlo simulations.

APPENDIX C. RENORMALIZATION GROUP METHOD

In this appendix, we briefly review the renormalization group method for a d-dimensional Euclidean scalar field theory (see, e.g., ref. 81). In particalur, the critical theory of antiferromagnetic quantum spin chains is believed to be described by two-dimensional massless field theories, among which the sine-Gordon theory for the spin-1/2 XXZ Heisenberg chain (see, e.g., ref. 82) is probably the most popular.

C.1. Renormalization Group Equations

This section is a review of the well-known results from renormalization group analysis, but it is necessary for the calculations in Sections C.2 and C.3.

We denote the bare two-point function by

$$G_0(r, \Lambda, \lambda) = \langle \phi(\mathbf{r})\, \phi(0) \rangle \tag{C.1}$$

where Λ and λ are a momentum cutoff and the bare coupling constant of the interaction in the Lagrangian, respectively. The corresponding renormalized two-point function for the massless theory is given by[19]

$$G_{\mathrm{R}}(r, \kappa, g) = Z^{-1}(\kappa, \Lambda, \lambda)\, G_0(r, \Lambda, \lambda) \tag{C.2}$$

[19] Of course, we assume the renormalizability of the theory.

where Z, κ, and g are the field renormalization constant, the renormalization momentum, and the dimensionless renormalized coupling constant, respectively. Since the bare two-point function G_0 with a fixed λ and a fixed Λ does not depend on the renormalization momentum κ, i.e.,

$$0 = \kappa \frac{\partial}{\partial \kappa}\bigg|_{\lambda, \Lambda} G_0(r, \Lambda, \lambda) \tag{C.3}$$

we have the renormalization group equation

$$\left(\kappa \frac{\partial}{\partial \kappa} + \beta \frac{\partial}{\partial g} + 2\gamma\right) G_{\mathrm{R}} = 0 \tag{C.4}$$

from (C.2), where

$$\beta = \kappa \frac{\partial}{\partial \kappa}\bigg|_{\lambda, \Lambda} g \tag{C.5}$$

and

$$\gamma = \frac{1}{2} \kappa \frac{\partial}{\partial \kappa}\bigg|_{\lambda, \Lambda} \log Z \tag{C.6}$$

In the limit $\Lambda \uparrow \infty$, a dimensional analysis shows that β and γ become functions of only a single variable g.

To find a solution $G_{\mathrm{R}} = G_{\mathrm{R}}(r, \kappa, g)$ of (C.4), we introduce three-dimensional Cartesian coordinates $(\kappa, g, G_{\mathrm{R}})$. Then Eq. (C.4) is equivalent to the condition that the vector $(\kappa, \beta, -2\gamma G_{\mathrm{R}})$ is orthogonal to the normal vector

$$\left(\frac{\partial G_{\mathrm{R}}}{\partial \kappa}, \frac{\partial G_{\mathrm{R}}}{\partial g}, -1\right) \tag{C.7}$$

of the surface $G_{\mathrm{R}} = G_{\mathrm{R}}(r, \kappa, g)$ with a fixed r. In other words, $(\kappa, \beta, -2\gamma G_{\mathrm{R}})$ is a tangent vector of the surface.

Consider the characteristic curve $(\kappa, g, G_{\mathrm{R}}) = (\kappa(s), g(s), G_{\mathrm{R}}(s))$ with a parameter s, which is defined by the solution of the system of ordinary differential equations

$$\frac{d}{ds} \kappa = \kappa \tag{C.8}$$

$$\frac{d}{ds} g = \beta(g) \tag{C.9}$$

$$\frac{d}{ds} G_{\mathrm{R}} = -2\gamma(g)\, G_{\mathrm{R}} \tag{C.10}$$

That is, the derivative of the vector $(\kappa(s), g(s), G_{\mathrm{R}}(s))$ is equal to the tangent vector $(\kappa, \beta, -2\gamma G_{\mathrm{R}})$ of the surface. Then the solution $G_{\mathrm{R}}(s) = G_{\mathrm{R}}(r, \kappa(s), g(s))$ to the ordinary differential equations satisfies the renormalization group equation (C.4).

The solution of (C.8) is given by

$$\kappa(s) = \kappa_0 e^s = \kappa_0 \rho \tag{C.11}$$

where κ_0 is the initial value of the renormalization momentum κ, and we have introduced the new scale parameter ρ. Using the scale parameter ρ, we can rewrite Eq. (C.9) as

$$\rho \frac{d}{d\rho} g(\rho) = \beta(g(\rho)) \tag{C.12}$$

Further, from (C.10), we have

$$G_{\mathrm{R}}(r, \kappa_0\rho, g(\rho)) = \exp\left[-2\int_1^\rho \frac{d\rho'}{\rho'}\gamma(g(\rho'))\right] G_{\mathrm{R}}(r, \kappa_0, g(1)) \tag{C.13}$$

From dimensional analysis, the left-hand side of (C.13) can be rewritten as

$$G_{\mathrm{R}}(r, \kappa_0\rho, g(\rho)) = (\kappa_0\rho)^{d-2} \times F(\kappa_0\rho r, g(\rho)) \tag{C.14}$$

with a function F of two dimensionless variables $\kappa_0\rho r$ and $g(\rho)$. Using (C.14), we can rewrite Eq. (C.13) as

$$G_{\mathrm{R}}\left(\frac{r}{\rho}, \kappa_0, g(1)\right) = (\kappa_0\rho)^{d-2} \times \exp\left[2\int_1^\rho \frac{d\rho'}{\rho'}\gamma(g(\rho'))\right] \times F(\kappa_0 r, g(\rho)) \tag{C.15}$$

where we have replaced r by r/ρ. In particular, when the coupling constant g is given by a fixed point g^* of the function β, i.e., $g = g^*$ is given by $\beta(g^*) = 0$, we have

$$G_{\mathrm{R}}(r/\rho, \kappa_0, g^*) = (\kappa_0\rho)^{d-2} \times \rho^{2\gamma(g^*)} \times F(\kappa_0 r, g^*) \tag{C.16}$$

This implies that the critical exponent is given by $\eta = 2\gamma(g^*)$. In the case with $g \neq g^*$, we assume that the function F with a fixed $\kappa_0 r$ is almost constant for small ρ. Under this assumption, we have

$$G_R\left(\frac{r}{\rho}, \kappa_0, g(1)\right) \sim \text{const} \times (\kappa_0 \rho)^{d-2} \times \exp\left[2\int_1^\rho \frac{d\rho'}{\rho'} \gamma(g(\rho'))\right] \quad \text{(C.17)}$$

for a fixed r as $\rho \sim 0$. Thus we get $\eta = 2\gamma(g^*)$ again.

Similarly, for the Fourier transform $\hat{G}_R(k, \kappa_0, g(1))$ of $G_R(r, \kappa_0, g(1))$, we have

$$\hat{G}_R(\rho\kappa, \kappa_0, g(1)) \sim \text{const} \times (\kappa_0 \rho)^{-2} \times \exp\left[2\int_1^\rho \frac{d\rho'}{\rho'} \gamma(g(\rho'))\right] \quad \text{(C.18)}$$

for a fixed momentum k as $\rho \sim 0$.

C.2. Logarithmic Correction to Correlations

In this section we review the case where there is a marginally irrelevant perturbation in a Lagrangian whose unperturbed Lagrangian corresponds to a fixed point in a parameter space of coupling constants. As is well known, a marginally irrelevant perturbation leads to a logarithmic correction to power-law decay of correlations,[81] as in the correlation (3.14) of the spin-1/2 Heisenberg chain. Although results in this section are well known, they are useful for the analysis of correlations of the spin-1/2 Heisenberg chain in Section 3.3, and are necessary for the calculation in Section C.3.

For a small coupling constant of a perturbation, we can expand formally the function β as

$$\beta(g) = -(d-x)\,g + b_2 g^2 + \cdots \quad \text{(C.19)}$$

in powers of the renormalized couping g of the perturbation, where x is the scaling dimension of an operator of the perturbation. In particular, when $x = d$, we say that the operator is marginal. Then the approximation up to order g^2 gives

$$g(\rho) \cong -\frac{1}{b_2 \log(\rho/\rho_0)} \quad \text{(C.20)}$$

with

$$g(1) = \frac{1}{b_2 \log \rho_0} \quad \text{(C.21)}$$

from (C.12). Here, if $b_2 g(1) > 0$, then the operator is irrelevant. In fact, since we have $\rho_0 > 1$ from (C.21), $g(\rho)$ varies from $g(1)$ to 0 when ρ varies from 1 to 0. Thus the effective coupling g goes to 0 as $\rho \downarrow 0$. In the following, we concentrate on the case that the operator of the perturbation is marginal and irrelevant.

For a small coupling g, we can write the function γ in (C.17) as

$$\gamma(g) = \gamma^* + d_1 g + d_2 g^2 + \cdots \tag{C.22}$$

in powers of g, where $\gamma^* = \gamma(g^*)$ for a fixed point $g^* = 0$ corresponding to the unperturbed system. Substituting (C.20) into (C.22), we have

$$\gamma(g(\rho)) \cong \gamma^* - \frac{d_1}{b_2 \log(\rho/\rho_0)} \tag{C.23}$$

where we have dropped higher orders than g^2 in (C.22). This combined with (C.17) gives

$$G_{\mathrm{R}}(r/\rho, \kappa_0, g(1)) \sim \mathrm{const} \times \rho^{d-2+\eta} \times |\log(\rho/\rho_0)|^{\sigma} \tag{C.24}$$

with $\sigma = -2d_1/b_2$. This implies

$$G_{\mathrm{R}}(r, \kappa_0, g(1)) \sim \mathrm{const} \times \frac{1}{r^{d-2+\eta}} \times \left[\log\left(\frac{r}{r_0}\right)\right]^{\sigma} \tag{C.25}$$

for large distance r, where r_0 is a constant.

Similarly, from (C.18), we have

$$\hat{G}_{\mathrm{R}}(k, \kappa_0, g(1)) \sim \mathrm{const} \times k^{-2+\eta} \times [\log(k_0/k)]^{\sigma} \tag{C.26}$$

for small momentum k, where k_0 is a constant.

We remark the following. Clearly the higher order terms in the functions β of (C.19) and γ of (C.22) give additive corrections. But these are suppressed by additional powers of $1/\log(r/r_0)$.[19,22]

The results (C.23) can be interpreted as follows. The effective critical exponent is given by

$$\eta_{\mathrm{eff}}(\rho) \cong \eta + \frac{\sigma}{\log(\rho/\rho_0)} \tag{C.27}$$

for the scale ρ. In particular, we expect that, for a finite system of linear dimension L, the effective exponent is given by

$$\eta_{\mathrm{eff}}(L) \cong \eta - \frac{\sigma}{\log(L/L_0)} \tag{C.28}$$

where L_0 is a nonuniversal constant. This result (C.28) should be well known, but has not been written down explicitly as far as we know.

C.3. Crossover in Correlations Decaying by Power Law

In order to treat the crossover phenomenon in the spin-3/2 isotropic Heisenberg antiferromagnetic chain in Section 4, in this section we review a critical theory with a marginally irrelevant perturbation and a relevant perturbation.

For simplicity, we assume that the unperturbed system is described by a critical theory for a fixed point in the parameter space of coupling constants. Then the original critical theory of the unperturbed system changes into another critical theory owing to the relevant perturbation. Namely a crossover occurs in the system.

In a similar way as in Appendix C.1, we can write down the renormalization group equation as

$$\left(\rho\frac{\partial}{\partial\rho}+\beta_1\frac{\partial}{\partial g_1}+\beta_2\frac{\partial}{\partial g_2}+2\gamma\right)G_R=0 \tag{C.29}$$

with

$$\rho\frac{d}{d\rho}g_1=\beta_1(g_1) \tag{C.30}$$

and

$$\rho\frac{d}{d\rho}g_2=\beta_2(g_2) \tag{C.31}$$

with the scale parameter $\rho=\kappa/\kappa_0$, where we have assumed that there is no mixing between two renormalized coupling constants g_1 (irrelevant) and g_2 (relevant) in the functions β_1 and β_2. In the same way as in Section C.1, we have

$$G_R\left(\frac{r}{\rho},\kappa_0,g(1),g_2(1)\right)=(\kappa_0\rho)^{d-2}\exp\left[2\int_1^\rho\frac{d\rho'}{\rho'}\gamma(g_1(\rho'),g_2(\rho'))\right]$$
$$\times F(\kappa_0 r,g_1(\rho),g_2(\rho)) \tag{C.32}$$

for the renormalized two-point function G_R. We further assume that there is no mixing between two renormalized coupling constants g_1 and g_2 also in the function γ. Namely, the function γ can be written as

$$\gamma(g_1,g_2)=\gamma^*+\gamma_1(g_1)+\gamma_2(g_2) \tag{C.33}$$

where γ^* is the value of γ at the fixed point corresponding to the unperturbed system. Then we have

$$G_R\left(\frac{r}{\rho}, \kappa_0, g(1), g_2(1)\right) \sim \text{const} \times \rho^{d-2+\eta} \left|\log\left(\frac{\rho}{\rho_0}\right)\right|^{\sigma} \times \exp\left[2\int_1^{\rho} \frac{d\rho'}{\rho'} \gamma_2(g_2(\rho'))\right] \tag{C.34}$$

in the same way as in Section C.2.

Since the coupling constant $g_2(\rho)$ approaches the fixed point $g_2^* \neq 0$ as $\rho \to 0$ from the assumption, we can approximate the function β_2 as

$$\beta_2(g_2) \cong b_{21}(g_2 - g_2^*) \tag{C.35}$$

near the fixed point g_2^*. Here we assume that the constant b_{21} is positive, i.e., the corresponding operator is not marginal.[20] Using the approximation (C.35), we obtain the solution of (C.31)

$$g_2(\rho) - g_2^* = \left(\frac{\rho}{\rho_1}\right)^{b_{21}} [g_2(\rho_1) - g_2^*] \tag{C.36}$$

for small ρ and small ρ_1 ($>\rho$). Similarly, near the fixed point, we have

$$\begin{aligned} &\int_1^{\rho} \frac{d\rho'}{\rho'} \gamma_2(g_2(\rho')) \\ &\quad \cong \text{const} + \int_{\rho_1}^{\rho} \frac{d\rho'}{\rho'} \{\gamma_2(g_2^*) + d_{21}[g_2(\rho') - g_2^*]\} \\ &\quad = \text{const} + \gamma_2(g_2^*) \log\left(\frac{\rho}{\rho_1}\right) + \frac{d_{21}}{b_{21}} \left(\frac{\rho}{\rho_1}\right)^{b_{21}} [g_2(\rho_1 - g_2^*] \end{aligned} \tag{C.37}$$

for small ρ and small ρ_1 ($>\rho$), where we have used (C.36). Substituting this into (C.34), we get

$$G_R(r/\rho, \kappa_0, g_1(1), g_2(1)) \sim \text{const} \times \rho^{d-2+\eta+\delta\eta} |\log(\rho/\rho_0)|^{\sigma} \tag{C.38}$$

for small ρ, where $\delta\eta = 2\gamma_2(g_2^*)$.

[20] When the constant b_{21} is vanishing, the operator is marginal at the fixed point g_2^*. This contradicts the following. In the $k=1$ Wess–Zumino–Witten model corresponding to the spin-3/2 isotropic Heisenberg antiferromagnetic chain, it is known that there appears only one marginal operator,[19] which is already taken into account as the coupling g_1.

We summarize the results in this section as follows. The two-point correlation function behaves as

$$G_{\mathrm{R}}(r, \kappa_0, g_1(1), g_2(1)) \sim \mathrm{const} \times \frac{1}{r^{d-2+\eta}} \left[\log\left(\frac{r}{r_0}\right)\right]^{\sigma} \times Y\left(\frac{r}{r_0}\right) \tag{C.39}$$

where Y is a crossover function whose asymptotic forms are given by

$$Y(l) \sim \begin{cases} \mathrm{const} & \text{for small } l \\ \mathrm{const} \times 1/l^{\delta\eta} & \text{for large } l \end{cases} \tag{C.40}$$

Similarly, we have

$$\hat{G}_{\mathrm{R}}(k, \kappa_0, g_1(1), g_2(1)) \sim \mathrm{const} \times k^{-2+\eta}[\log(k_0/k)]^{\sigma} \times Y(k_0/k) \tag{C.41}$$

in momentum space for small momentum k, where k_0 is a positive constant. The results (C.39) and (C.41) should be well known, but have not been written explicitly as far as we know.

Thus the critical exponent exhibits crossover from η to $(\eta + \delta\eta)$.

APPENDIX D. CONFORMAL TOWERS IN ENERGY SPECTRA

In this appendix, we briefly review Cardy's argument[30] for a two-dimensional conformally invariant system of an infinitely long strip with finite width L, in order to proceed to an analysis for a more complicated system such as the spin-1/2 Heisenberg chain. The argument in this appendix is useful in the succeeding Appendices E–G.

We start from (2.13). By using the identity

$$\frac{1}{\sinh(\pi z/L)} = \frac{2e^{-\pi z/L}}{1 - e^{-2\pi z/L}} \tag{D.1}$$

for $z \in \mathbf{C}$, we can rewrite the two-point correlation (2.13) as

$$\langle \phi(w')\, \phi(w) \rangle_L = \left(\frac{2\pi}{L}\right)^{\eta} e^{-2\pi x u/L} \times e^{-2\pi i s v/L} \times \left(\frac{1}{1 - e^{-2\pi z/L}}\right)^{2h} \left(\frac{1}{1 - e^{-2\pi \bar{z}/L}}\right)^{2\bar{h}} \tag{D.2}$$

with the scaling dimension $x = (h + \bar{h})$ and the "spin" $s = (h - \bar{h})$, where we have put $w' - w = z = u + iv$ ($u, v \in \mathbf{R}$). For a positive u, the right-hand side of (D.2) can be expanded as

$$\langle \phi(w')\,\phi(w)\rangle_L = \left(\frac{2\pi}{L}\right)^{\eta} \sum_{m,\bar{m}=0}^{\infty} a_m a_{\bar{m}} \times \exp\left[\frac{-2\pi(x+m+\bar{m})u}{L} - \frac{2\pi i(s+m-\bar{m})v}{L}\right] \quad \text{(D.3)}$$

On the other hand, the correlation can be written as

$$\langle \phi(w')\,\phi(w)\rangle_L = \lim_{M\uparrow\infty} \frac{\operatorname{Tr}[\hat{\phi}(0)\,(W_L)^u\,\hat{\phi}(v)(W_L)^{M-u}]}{\operatorname{Tr}(W_L)^M} \quad \text{(D.4)}$$

in terms of a transfer matrix W_L and an operator $\hat{\phi}$. We assume that the matrix W_L is positive, i.e., the Hamiltonian $\mathscr{H}_L$ defined by $W_L = \exp[-\mathscr{H}_L]$ is Hermitian. We further assume that the maximum eigenvalue of W_L is nondegenerate.

We note that

$$\frac{\operatorname{Tr}[\hat{\phi}(0)\,(W_L)^u\,\hat{\phi}(v)(W_L)^{M-u}]}{\operatorname{Tr}(W_L)^M} = \frac{1}{\sum_l e^{-E_l M}} \sum_{l,n} (\Phi^{(l)}, \hat{\phi}(0)\,\Phi^{(n)})\, e^{-E_n u - ik_n v} \times (\Phi^{(n)}, \hat{\phi}(0)\,\Phi^{(l)})\, e^{-E_l(M-u)} \quad \text{(D.5)}$$

where $\Phi^{(n)}$ is the eigenvector of the Hamiltonian $\mathscr{H}_L$ with energy eigenvalue E_n and with momentum k_n ($n = 0, 1, 2,...$). The collection of $\Phi^{(n)}$ forms an orthonormal complete system. In the limit $M \uparrow \infty$, we have

$$\langle \phi(w')\,\phi(w)\rangle_L = \sum_{n\neq 0} |(\Phi^{(0)}, \hat{\phi}(0)\,\Phi^{(n)}|^2 \times e^{-(E_n - E_0)u} \times e^{-ik_n v} \quad \text{(D.6)}$$

where E_0 indicates the ground-state energy.

Comparing (D.6) with (D.3), Cardy[30] obtained the relations

$$E_n - E_0 = \frac{2\pi}{L}(x + m + \bar{m}) \quad \text{(D.7)}$$

and

$$k_n = \frac{2\pi}{L}(s + m - \bar{m}) \quad \text{(D.8)}$$

In particular, from the former, the critical exponent is derived as[29]

$$\eta = 2x = \frac{L}{\pi}\,\Delta E \tag{D.9}$$

by measuring the energy gap ΔE.[21] The latter, (D.8), implies that the "spin" s must be equal to an integer because of the translation invariance of the system which respects periodic boundary conditions.

APPENDIX E. LOGARITHMIC CORRECTIONS TO ENERGY GAP AND TO POWER-LAW DECAY OF CORRELATIONS

When there are logarithmic corrections to a power-law decay of correlations, then there often appear logarithmic corrections also in the energy gap ΔE.[58,51–53,19,36,22] In fact, such logarithmic corrections are observed in many systems.[51–53,22]

In this appendix, we will show the following. Under a certain scaling assumption for two-point correlations, the energy gap ΔE has the form[58,19,22]

$$\Delta E \cong \frac{\pi}{L}\left\{\eta - \frac{\sigma}{\log[L/(2r_0)]}\right\} \tag{E.1}$$

for a system of an infinitely long strip with finite width L, provided the two-point correlation in infinite volume behaves as

$$\langle \phi(0,0)\,\phi(r,0)\rangle_\infty = \langle \phi(0,0)\,\phi(0,r)\rangle_\infty \sim \frac{A}{r^\eta}\left[\log\left(\frac{r}{r_0}\right)\right]^\sigma \tag{E.2}$$

for large distance r. Here η, σ are critical exponents and A, r_0 are real constants. The result (E.1) is essentially Cardy's result,[58] but our derivation is different from his.

We write the correlation of an infinitely long strip with finite width L in the form

$$\langle \phi(0,0)\,\phi(y_1,y_2)\rangle_L = \left(\frac{2\pi}{L}\right)^\eta \sum_{m,\bar{m}=0}^{\infty} a_m a_{\bar{m}} \exp\left[\frac{-2\pi(\tilde{x}(L)+m+\bar{m})\,y_2}{L}\right] \times \exp\left[\frac{-2\pi i(s+m-\bar{m})\,y_1}{L}\right] \tag{E.3}$$

[21] The formula (D.9) was conjectured from model calculations before Cardy explained the formula from the point of view of conformal field theory.[29] See, for example, ref. 7 and references cited therein.

in the same way as in the preceding section. Here $\tilde{x}(L)$ is related to the energy gap ΔE by

$$\Delta E = \frac{2\pi\tilde{x}(L)}{L} \tag{E.4}$$

Following the argument in Section 2.4, we assume that the scaling law in the y_1 directions is

$$\begin{aligned} Q\left(\frac{r}{L}, L\right) &:= \left[\frac{\pi r}{L\sin(\pi r/L)}\right]^{\eta_{\rm eff}(L)} \\ &\cong \frac{\langle\phi(0,0)\,\phi(r,0)\rangle_L}{\langle\phi(0,0)\,\phi(r,0)\rangle_\infty} \end{aligned} \tag{E.5}$$

with an effective critical exponent $\eta_{\rm eff}(L)$. Similarly, by combining the same argument with the expression (2.13), we assume that the scaling law in the y_2 direction is given by

$$\begin{aligned} \tilde{Q}\left(\frac{r}{L}, L\right) &:= \left[\frac{\pi r}{L\sinh(\pi r/L)}\right]^{\eta_{\rm eff}(L)} \\ &\cong \frac{\langle\phi(0,0)\,\phi(0,r)\rangle_L}{\langle\phi(0,0)\,\phi(0,r)\rangle_\infty} \end{aligned} \tag{E.6}$$

To determine $\tilde{x}(L)$ from the asymptotic form (E.2) of the correlation, we consider an "analytic continuation" along the pure imaginary axis with respect to y_2.[22] For the correlations (E.2) and (E.3), we have formally

$$\begin{aligned} &\langle\phi(0,0)\,\phi(0,iL/2)\rangle_\infty \\ &\quad\cong \langle\phi(0,0)\,\phi(L/2,0)\rangle_\infty \times e^{-\pi i\eta/2} \times \left\{1 + \frac{i\pi/2}{\log[L/(2r_0)]}\right\}^\sigma \end{aligned} \tag{E.7}$$

and

$$\langle\phi(0,0)\,\phi(0,iL/2)\rangle_L = \langle\phi(0,0)\,\phi(L/2,0)\rangle_L \times e^{-\pi i\tilde{x}(L)} \tag{E.8}$$

where we have used that the "spin" s in (E.3) is an integer because of the translation invariance of the system. Similarly, for the scaling functions (E.5) and (E.6), we have

$$Q(1/2, L) = \tilde{Q}(i/2, L) = \left(\frac{\pi}{2}\right)^{\eta_{\rm eff}(L)} \tag{E.9}$$

[22] Of course, the analyticities of the correlation function (E.2) and of the scaling functions have not yet been established. Therefore we use "analytic continuation" in a formal sense.

Combining this with (E.5)–(E.8), we have

$$1 \cong \exp\left[\frac{-\pi i\tilde{x}(L) + \pi i\eta}{2}\right] \times \left\{1 + \frac{i\pi/2}{\log[L/(2r_0)]}\right\}^{-\sigma} \tag{E.10}$$

This implies

$$2\tilde{x}(L) \cong \eta - \frac{\sigma}{\log[L/(2r_0)]} \tag{E.11}$$

for a large linear dimension L of system. Thus, combining this with (E.4), we have (E.1).

If we define the effective critical exponent by

$$\eta_{\mathrm{eff}}(L) = \frac{L}{\pi}\Delta E \tag{E.12}$$

as an extension of the formula (D.9), then we get

$$\eta_{\mathrm{eff}}(L) \cong \eta - \frac{\sigma}{\log[L/(2r_0)]} \tag{E.13}$$

from (E.11) and (E.4). This is identical to (C.28). In conclusion, we can expect that an effective critical exponent η_{eff} is derived from energy gap ΔE, following from the formula (E.12).

APPENDIX F. EFFECTIVE CRITICAL EXPONENT η_{eff} OF THE SPIN–SPIN CORRELATION OF THE SPIN-1/2 ISOTROPIC HEISENBERG ANTIFERROMAGNETIC CHAIN

In this appendix, we calculate the effective critical exponent $\eta_{\mathrm{eff}}(L)$ of the spin–spin correlation of the spin-1/2 isotropic Heisenberg antiferromagnetic chain of a finite length L by using a similar formula to (E.12).[23] For this purpose, we introduce the six-vertex model, which is the two-dimensional classical system corresponding to the spin-1/2 isotropic Heisenberg antiferromagnetic chain.

[23] However, it is known that the formula (E.12) does not necessarily give a correct exponent η for several models under certain conditions.[83–85] Fortunately, we do not encounter such situations.

F.1. Transfer Matrices in the Six-Vertex Model

In this section we study properties of transfer matrices of the six-vertex model.

Consider the correlation

$$\langle S_1^+ S_{1+r}^- \rangle_{M\times L,\mathrm{T}} := \frac{\mathrm{Tr}[S_1^+ S_{1+r}^- (W_M)^L (T_M)^L]}{\mathrm{Tr}[(W_M)^L (T_M)^L]} \tag{F.1}$$

of the six-vertex model with $M\times L$ vertices, where $S_j^\pm := S_j^x \pm iS_j^y$, W_M is the row-to-row transfer matrix of the six-vertex model,[76,86] and the matrix T_M shifts any periodic array of the spin states by one lattice unit forward. (See Fig. 20.) Here we have introduced the twisted boundary condition for convenience of the following calculations. In the limit $L\uparrow\infty$, as we showed in (A.4), we have the spin–spin correlation function

$$\langle S_1^+ S_{1+r}^- \rangle_M = (\Phi_M^{(0)}, S_1^+ S_{1+r}^- \Phi_M^{(0)}) \tag{F.2}$$

with respect to the ground state $\Phi_M^{(0)}$ of the spin-1/2 isotropic Heisenberg antiferromagnetic chain of length M, because the transfer matrix W_M commutes with the translation operator T_M.[76]

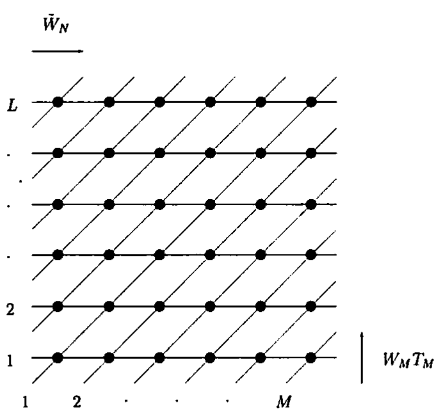

Fig. 20. Lattice for the six-vertex model, and the transfer matrices $W_M T_M$ and $\tilde{W}_N$ in the vertical and the horizontal directions, respectively. The arrows (Ising spins) of the vertex model are placed on each bond (solid line) connecting neighbor sites (solid circles).

On the other hand, the correlation $\langle S_1^+ S_{1+r}^- \rangle_{M\times L,\mathrm{T}}$ can be written as

$$\langle S_1^+ S_{1+r}^- \rangle_{M\times L,\mathrm{T}} = \frac{\mathrm{Tr}[\tilde{\sigma}_1^+ (\tilde{W}_N)^r \tilde{\sigma}_1^- (\tilde{W}_N)^{M-r}]}{\mathrm{Tr}(\tilde{W}_N)^M} \tag{F.3}$$

in terms of the diagonal-to-diagonal transfer matrix

$$\tilde{W}_N := \tilde{T}_N \times \tilde{R}_N \tag{F.4}$$

in the horizontal direction in Fig. 20, where $N = 2L$,[24] and the matrix $\tilde{T}_N$ shifts any periodic array of the spin states by one lattice unit backward. The matrix $\tilde{R}_N$ is given by[87]

$$\tilde{R}_N := \prod_{l=1}^{L} \tilde{Q}_{2l-1,2l} \tag{F.5}$$

and

$$\tilde{Q}_{i,j} := \tfrac{1}{2}(\tilde{\sigma}_i^x \tilde{\sigma}_j^x + \tilde{\sigma}_i^y \tilde{\sigma}_j^y - \tilde{\sigma}_i^z \tilde{\sigma}_j^z + 3) \tag{F.6}$$

Here $(\tilde{\sigma}_j^x, \tilde{\sigma}_j^y, \tilde{\sigma}_j^z)$ is the Pauli matrix at the "site" j $(=1, 2,..., 2L)$,[25] and

$$\tilde{\sigma}_j^{\pm} := \tfrac{1}{2}(\tilde{\sigma}_j^x \pm i\tilde{\sigma}_j^y) \tag{F.7}$$

We note that

$$[\tilde{W}_N, \tilde{S}_N^{\mathrm{tot}}] = 0 \tag{F.8}$$

where

$$\tilde{S}_N^{\mathrm{tot}} := \tfrac{1}{2} \sum_{j=1}^{N} \tilde{\sigma}_j^z \tag{F.9}$$

This implies that the transfer matrix $\tilde{W}_N$ can be rewritten in a block-diagonal form with the direct sum of matrices as

$$\tilde{W}_N = \bigoplus_{k=0}^{N} \tilde{W}_{N;k} \tag{F.10}$$

where the subscript k denotes the restriction to the k-down-spin subspace. It is known that the maximum eigenvalue $\Lambda_{N;k}^{\max}$ for each block is non-degenerate and positive, and that the maximum eigenvalue $\Lambda_N^{\max}$ of the transfer matrix $\tilde{W}_N$ is given by the maximum eigenvalue $\Lambda_{N;L}^{\max}$ of the matrix $\tilde{W}_{N;L}$.[87]

[24] N spins on the bonds are arranged on a straight line in the vertical direction, as in Fig. 20.
[25] These "sites" correspond to bonds on a straight line in the vertical direction in Fig. 20.

In the limit $M \uparrow \infty$, we have

$$\langle S_1^+ S_{1+r}^- \rangle_{L,\mathrm{T}} := \lim_{M \uparrow \infty} \langle S_1^+ S_{1+r}^- \rangle_{M \times L,\mathrm{T}}$$

$$= (\tilde{\Phi}_N^{\max}, \tilde{\sigma}_1^+ (\tilde{W}_N)^r \tilde{\sigma}_1^- \tilde{\Phi}_N^{\max}) \times (\Lambda_N^{\max})^{-r} \quad \text{(F.11)}$$

where $\tilde{\Phi}_N^{\max}$ is the eigenvector with the maximum eigenvalue $\Lambda_N^{\max}$ of the transfer matrix $\tilde{W}_N$. Further, for a sufficiently large r, we have

$$\langle S_1^+ S_{1+r}^- \rangle_{L,\mathrm{T}} \sim \text{const} \times e^{-\Delta E_N r} \quad \text{(F.12)}$$

with the energy gap

$$\Delta E_N := \log \Lambda_{N;L}^{\max} - \log \Lambda_{N;L-1}^{\max} \quad \text{(F.13)}$$

for a fixed $N = 2L$.

Since the transfer matrix $\tilde{W}_N$ is not positive, i.e., the corresponding Hamiltonian is not Hermitian, we cannot simply use the scheme of Appendix E to calculate the effective exponent η_{eff}. But, fortunately, we can obtain the spectrum of the transfer matrix $(\tilde{W}_N)^2$ from that of another *positive* transfer matrix $\tilde{V}_N$, (F.17) below.

To show this, let us introduce the transfer matrix

$$\tilde{U}_N := \tilde{R}'_N \tilde{R}_N \quad \text{(F.14)}$$

with

$$\tilde{R}'_N := \tilde{T}_N \tilde{R}_N \tilde{T}_N^{-1} \quad \text{(F.15)}$$

Then we have

$$(\tilde{W}_N)^2 = \tilde{U}_N \times (\tilde{T}_N)^2 \quad \text{(F.16)}$$

from the definition (F.4) of the transfer matrix $\tilde{W}_N$, because the matrix $\tilde{R}_N$ commutes with the matrix $(\tilde{T}_N)^2$. Further, the matrix $\tilde{U}_N$ also commutes with $(\tilde{T}_N)^2$. In consequence, the spectrum of the matrix $(\tilde{W}_N)^2$ is given by that of $\tilde{U}_N$ except for momentum shifts which come from the translation operator $\tilde{T}_N$. .

Next we shall show that the matrix $\tilde{U}_N$ has exactly the same spectrum as the positive matrix $\tilde{V}$, (F.17) below. Since the matrix $\tilde{R}_N$ is strictly positive from the definition (F.5), we can define the matrices $(\tilde{R}_N)^{1/2}$ and $(\tilde{R}_N)^{-1/2}$ to be positive. By using these positive matrices, we define the transfer matrix $\tilde{V}_N$ by

$$\tilde{V}_N := (\tilde{R}_N)^{1/2} \tilde{U}_N (\tilde{R}_N)^{-1/2} \quad \text{(F.17)}$$

This implies that the spectrum of the matrix $\tilde{U}_N$ is completely equivalent to that of $\tilde{V}_N$. Further, from the definition (F.14) of the matrix $\tilde{U}_N$, we have

$$\tilde{V}_N = (\tilde{R}_N)^{1/2} \tilde{R}'_N (\tilde{R}_N)^{1/2} \tag{F.18}$$

This implies that the matrix $\tilde{V}_N$ is positive.

F.2. Calculation of Sound Velocity

The aim of this section is to calculate a sound velocity v_s which appears as a nonuniversal constant in the correlations.

For a general correlation function, the two unit lengths in the two directions are not necessarily equal to each other. This implies that (E.3) must be replaced with

$$\begin{aligned}\langle \phi(0,0)\,\phi(y_1,y_2)\rangle_L &= \left(\frac{2\pi}{L}\right)^{\eta} \sum_{m,\bar{m}=0}^{\infty} a_m a_{\bar{m}} \exp\left[\frac{-2\pi v_s(\tilde{x}(L)+m+\bar{m})\,y_2}{L}\right] \\ &\quad \times \exp\left[\frac{-2\pi i(s+m-\bar{m})\,y_1}{L}\right]\end{aligned} \tag{F.19}$$

in such a general situation. Here there appears an unknown positive constant v_s called the sound velocity. Similarly, (E.12) must be replaced with

$$\eta_{\text{eff}}(L) = \frac{L}{\pi} \times \frac{\Delta E}{v_s} \tag{F.20}$$

Since the sound velocity v_s is nonuniversal, we must calculate v_s, in order to obtain the effective critical exponent η_{eff} by using (F.20).

To calculate the sound velocity v_s for the transfer matrix $\tilde{W}_N$, we consider the system[26] defined by the transfer matrix $\tilde{U}_N$ and calculate the sound velocity u_s for $\tilde{U}_N$. Then the sound velocity v_s for the transfer matrix $\tilde{W}_N$ is obtained from u_s. In fact, from (F.16), we have

$$\left\{\exp\left[-\frac{2\pi}{L} v_s \frac{\eta_{\text{eff}}}{2}\right]\right\}^2 = \exp\left[-\frac{2\pi}{L} u_s \frac{\eta_{\text{eff}}}{2} \times 2\right] \tag{F.21}$$

This implies $v_s = u_s$.

[26] A similar system appears as the path integral form of the partition function of the spin-1/2 Heisenberg chain when one uses the "Trotter decomposition" for the density matrix.[88,87] The decomposition is often called the "checkerbord (CB) decomposition."[27]

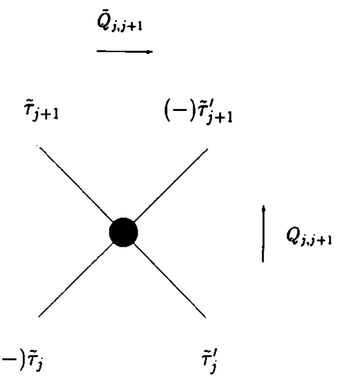

Fig. 21. Local transfer matrices $\tilde{Q}_{j,j+1}$ and $Q_{j,j+1}$ in the horizontal and vertical directions, respectively.

The advantage of the use of the transfer matrix $\tilde{U}_N$ is that the corresponding system has an invariance under the $\pi/2$ rotation of the lattice.[89]

To show this invariance, we first define the local transfer matrix $Q_{j,j+1}$ in the vertical direction in Fig. 20 by

$$(\tilde{\tau}_j, \tilde{\tau}'_j |\, Q_{j,j+1} \,| \tilde{\tau}_{j+1}, \tilde{\tau}'_{j+1}) = (-\tilde{\tau}_j, \tilde{\tau}_{j+1} |\, \tilde{Q}_{j,j+1} \,| \tilde{\tau}'_j, \tilde{\tau}'_{j+1}) \tag{F.22}$$

with the matrix $\tilde{Q}_{j,j+1}$, (F.6), where $|\tilde{\tau}_j)$ is the system of orthonormal basis of the eigenvectors of the matrix $\tilde{\sigma}_j^z$ with the eigenvalues $\tilde{\tau}_j = \pm 1$ at the site j. (See Fig. 21.) Then one can take the matrix $Q_{i,j}$ to have the same expression as $\tilde{Q}_{i,j}$, (F.6), in terms of the Pauli matrix. This implies that, from (F.14), (F.15), and (F.5), the system defined by the transfer matrix $\tilde{U}_N$ in (F.14) is invariant under the $\pi/2$ rotation of the lattice. (See Fig. 22.) This property leads also to the invariance of correlations under the $\pi/2$ rotation. In fact, the correlation

$$\langle \tilde{\sigma}_1^+ \tilde{\sigma}_{1+r}^- \rangle_{L\times L}^{\mathrm{CB}} := \frac{\mathrm{Tr}[\tilde{\sigma}_1^+ \tilde{\sigma}_{2r+1}^- (\tilde{U}_N)^L]}{\mathrm{Tr}(\tilde{U}_N)^L} \tag{F.23}$$

can be expressed also as

$$\langle \tilde{\sigma}_1^+ \tilde{\sigma}_{1+r}^- \rangle_{L\times L}^{\mathrm{CB}} = \frac{\mathrm{Tr}[\tilde{\sigma}_1^+ (\tilde{U}_N)^r \tilde{\sigma}_1^- (\tilde{U}_N)^{L-r}]}{\mathrm{Tr}(\tilde{U}_N)^L} \tag{F.24}$$

This implies that the unit lengths of the scales in two directions are equal to each other. In other words, the sound velocity satisfies $u_s = 1$. Consequently, we get $v_s = u_s = 1$.

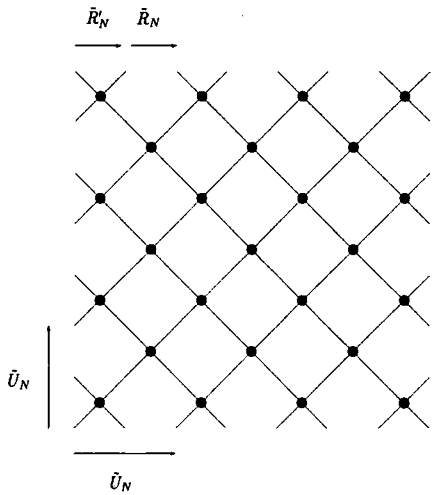

Fig. 22. The system is invariant under the $\pi/2$ rotation.

F.3. Bethe Ansatz for Transfer Matrix $\tilde{W}_N$

In order to obtain the eigenvalues $\Lambda_{N;L}^{\max}$ and $\Lambda_{N;L-1}^{\max}$ of the transfer matrix $\tilde{W}_N$, we use the Bethe ansatz method.[90] As is well known, the six-vertex model is "solvable"[91,92] in the sense that one can reduce an eigenvalue problem of a transfer matrix to solving a system of algebraic equations which are called Bethe ansatz equations. By combining the results of $\Lambda_{N;L}^{\max}$ and $\Lambda_{N;L-1}^{\max}$ in this section with the formulas (F.13) and (F.20) and with the result $v_s = 1$ for the sound velocity in the preceding section, we get the desired effective critical exponent $\eta_{\text{eff}}(L)$ of the spin–spin correlation for the spin-1/2 isotropic Heisenberg antiferromagnetic chain.

Following the Bethe's original idea,[90] we assume that the eigenvectors of $\tilde{W}_{N;k}$ have the Bethe ansatz form[93,87]

$$\Phi_k := \sum_{1 \leqslant y_1 < \cdots < y_k \leqslant N} \sum_P A_P F(z_{P1}, y_1) \cdots F(z_{Pk}, y_k)\, \Phi(y_1, \ldots, y_k) \quad \text{(F.25)}$$

with

$$F(z, y) := \begin{cases} a_j z_j^{(y+1)/2} & (y = \text{odd}) \\ z_j^{y/2} & (y = \text{even}) \end{cases} \quad \text{(F.26)}$$

($j=1, 2,..., k$; $k=0, 1, 2,..., 2L$), where $\Phi(y_1,..., y_k)$ is the state with all the spins up except those k spins at the sites $y_1,..., y_k$; the summations run over all the possible distributions of k down spins and all the permutations P of $(1, 2,..., k)$. The numbers z_j, a_j, and A_P are determined by

$$z_j=\frac{\zeta_j+3}{\zeta_j(\zeta_j-1)} \tag{F.27}$$

$$a_j=\frac{1}{2}(\zeta_j-1) \tag{F.28}$$

and

$$\frac{A_{(P1,...,P(j+1),Pj,...,Pk)}}{A_{(P1,...,Pj,P(j+1),...,Pk)}}=-\frac{\zeta_{Pj}\zeta_{P(j+1)}+2\zeta_{Pj}+1}{\zeta_{Pj}\zeta_{P(j+1)}+2\zeta_{P(j+1)}+1} \tag{F.29}$$

where Pl is the number which replaces l under this permutation P. The complex numbers $\zeta_1,..., \zeta_k$ are determined by the system of the Bethe ansatz equations

$$\left[\frac{\zeta_j+3}{\zeta_j(\zeta_j-1)}\right]^L=(-1)^{k-1}\prod_{l=1}^{k}\frac{\zeta_j\zeta_l+2\zeta_l+1}{\zeta_j\zeta_l+2\zeta_j+1} \tag{F.30}$$

with $j=1, 2,..., k$. The eigenvalues of the transfer matrix $\tilde{W}_{N;k}$ are given by

$$\Lambda_{N;k}=\zeta_1\zeta_2\cdots\zeta_k \tag{F.31}$$

A clear presentation of the physics underlying the Bethe ansatz method can be found in Sutherland's lecture notes.[94] The basis of the above Bethe ansatz calculation is summarized in the following theorem, which is proved in ref. 87.

Theorem 1.[87] The maximum eigenvalue $\Lambda_{N;k}^{\max}$ of the transfer matrix $\tilde{W}_{N;k}$ can be obtained from $\Lambda_{N;k}$ in (F.31) with a solution $(\zeta_1,..., \zeta_k)$ to the Bethe ansatz equations (F.30).

In order to solve the system of the Bethe ansatz equations (F.30), we have to resort to numerical calculations. For this purpose, it is convenient to introduce variables p_j ($j=1, 2,..., k$) which are defined by

$$\zeta_j=\frac{3i/4-p_j}{i/4+p_j} \tag{F.32}$$

We note that

$$\frac{\zeta_j+3}{\zeta_j(\zeta_j-1)}=\exp\left[-2i\tan^{-1}(4p_j)-2i\tan^{-1}\left(\frac{4p_j}{3}\right)\right] \tag{F.33}$$

and

$$\frac{\zeta_j\zeta_l+2\zeta_l+1}{\zeta_j\zeta_l+2\zeta_j+1}=\exp[-2i\tan^{-1}(p_j-p_l)] \tag{F.34}$$

In terms of p_j, the Bethe ansatz equations (F.30) and the eigenvalues $\Lambda_{N;k}$ in (F.31) can be rewritten as

$$\tan^{-1}(4p_j)+\tan^{-1}\left(\frac{4p_j}{3}\right)=\frac{\pi}{L}I_j+\frac{1}{L}\sum_{l=1}^{k}\tan^{-1}(p_j-p_l) \tag{F.35}$$

and

$$\log\Lambda_{N;k}=\frac{1}{2}\sum_{l=1}^{k}\log\left[\frac{(3/4)^2+p_l^2}{(1/4)^2+p_l^2}\right]+i\sum_{l=1}^{k}\left[\tan^{-1}\left(\frac{4p_l}{3}\right)+\tan^{-1}(4p_l)\right] \tag{F.36}$$

where

$$I_j=\begin{cases}\text{half-odd integer,} & k=\text{even}\\ \text{integer,} & k=\text{odd}\end{cases} \tag{F.37}$$

Here, in particular, it is known[87] that the solution for

$$I_j=-\frac{k+1}{2}+j \tag{F.38}$$

($j=1, 2,..., k$) leads to the maximum eigenvalue $\Lambda_{N;k}^{\max}$. Then we have

$$\log\Lambda_{N;k}^{\max}=\frac{1}{2}\sum_{l=1}^{k}\log\left[\frac{(3/4)^2+p_l^2}{(1/4)^2+p_l^2}\right] \tag{F.39}$$

by using the Bethe ansatz equations (F.35).

To obtain the maximum eigenvalues $\Lambda_{N;L}^{\max}$ and $\Lambda_{N;L-1}^{\max}$ in the formula (F.13), we solved (F.35) with (F.38) for $k=L, L-1$ by using numerical iteration method.[87]

Using the formulas (F.13) and (F.20) with these numerical results $\Lambda_{N;L}^{\max}$, $\Lambda_{N;L-1}^{\max}$, and the result $v_s=1$ in the preceding section, we obtain numerically the effective critical exponent $\eta_{\text{eff}}(L)$ of the spin–spin correlation for the spin-1/2 isotropic Heisenberg antiferromagnetic chain.

APPENDIX G. CORRELATION FUNCTIONS OF ONE-DIMENSIONAL QUANTUM SYSTEMS AT FINITE TEMPERATURES

In this appendix, we treat a conformally invariant one-dimensional quantum system at low temperatures. The results in this appendix should be well known, but have not been written down explicitly as far as we know.

Consider a two-point correlation of the system

$$\langle \hat{\phi}(0,0)\,\hat{\phi}(y_1,y_2)\rangle_L(\beta)=\frac{\mathrm{Tr}[\hat{\phi}(0)\,e^{-y_2\mathscr{H}}\hat{\phi}(y_1)\,e^{y_2\mathscr{H}}e^{-\beta\mathscr{H}}]}{\mathrm{Tr}\,e^{-\beta\mathscr{H}}} \tag{G.1}$$

where β is the inverse temperature. Using the path integral idea, we transform this correlation function into that of a two-dimensional classical system. For example, the spin–spin correlation of the spin-1/2 Heisenberg chain is mapped into a correlation function of the six-vertex model.[88] Then, as Affleck pointed out,[95] the inverse temperature β can be interpreted as a finite side of a rectangle in the two-dimensional classical system. Therefore Cardy's method can be applied also to correlations of the two-dimensional classical system. Actually, in the same way as in Section 2.2, we have[95]

$$\begin{aligned}\langle \hat{\phi}(0,0)\,\hat{\phi}(y_1,y_2)\rangle_\infty(\beta)=A\left(\frac{\pi}{v'\beta}\right)^{\eta}&\left\{\frac{1}{\sinh[\pi(y_1+iy_2)/(v'\beta)]}\right\}^{2h}\\&\times\left\{\frac{1}{\sinh[\pi(y_1-iy_2)/(v'\beta)]}\right\}^{2\bar{h}}\end{aligned} \tag{G.2}$$

in the thermodynamic limit $L\uparrow\infty$, where v' is a positive constant and A is a constant. To get the expression of the correlation with real time t, we replace y_2 by $-iv_st$ as

$$\begin{aligned}\langle \phi(0,0)\,\phi(y,t)\rangle_\infty(\beta)=A\left(\frac{\pi}{v'\beta}\right)^{\eta}&\left\{\frac{1}{\sinh[\pi(y+v_st)/(v'\beta)]}\right\}^{2h}\\&\times\left\{\frac{1}{\sinh[\pi(y-v_st)/(v'\beta)]}\right\}^{2\bar{h}}\end{aligned} \tag{G.3}$$

where $\phi(y,t):=\hat{\phi}(y,\ -iv_st)$, and v_s is the sound velocity. In the zero-temperature limit, we have

$$\langle \phi(0,0)\,\phi(y,t)\rangle_\infty(\infty)=A\left(\frac{1}{y+v_st}\right)^{2h}\times\left(\frac{1}{y-v_st}\right)^{2\bar{h}} \tag{G.4}$$

For $t=0$ and large y, we have

$$\langle \phi(0,0)\,\phi(y,0)\rangle_\infty(\beta) = A\left(\frac{2\pi}{v'\beta}\right)\times e^{-y/\xi(\beta)} \tag{G.5}$$

with the correlation length

$$\xi(\beta) := \frac{v'\beta}{\pi\eta} \tag{G.6}$$

Immediately, from (G.3) and (G.4), we have the scaling law as

$$\frac{\langle \phi(0,0)\,\phi(y,t)\rangle_\infty(\beta)}{\langle \phi(0,0)\,\phi(y,t)\rangle_\infty(\infty)} = \left\{\frac{\pi(y+v_s t)/(v'\beta)}{\sinh[\pi(y+v_s t)/(v'\beta)]}\right\}^{2h} \times\left\{\frac{\pi(y-v_s t)/(v'\beta)}{\sinh[\pi(y-v_s t)/(v'\beta)]}\right\}^{2\bar{h}} \tag{G.7}$$

Consider the Fourier transform of the correlation (G.3) as

$$\hat{G}(q,\omega) := \int_{-\infty}^{\infty} dy \int_{-\infty}^{\infty} dt\, e^{iqy+i\omega t}\langle \phi(0,0)\,\phi(y,t)\rangle_\infty(\beta) \tag{G.8}$$

The quantity $\hat{G}(q,\omega)$ is related directly to neutron scattering experiments. We assume $2h$, $2\bar{h}<1$. Then we have

$$\hat{G}(0,0) \sim \text{const}\times\beta^{2-\eta} \tag{G.9}$$

for $q=\omega=0$ and low temperatures.

Next we consider the case that there appear logarithmic corrections to the power decay of a correlation. For simplicity, in the rest of this appendix, we assume that the correlation behaves as

$$\langle \phi(0,0)\,\phi(y,0)\rangle_\infty(\infty) \sim A\,\frac{[\log(y/r_0)]^\sigma}{y^\eta} \tag{G.10}$$

for a large distance y and at $t=0$, where r_0 is a positive constant.

Using the thermal Bethe ansatz method,[87, 17] Nomura and Yamada[56] calculated numerically the correlation length $\xi(\beta)$ of the spin–spin correlation of the spin-1/2 isotropic Heisenberg antiferromagnetic chain at low temperatures. Their result is

$$\frac{1}{\xi(\beta)} = \frac{\pi}{v_s\beta}\,\eta_{\text{eff}}(\beta) \tag{G.11}$$

with the effective critical exponent

$$\eta_{\mathrm{eff}}(\beta) = \eta - \frac{\sigma}{\log(\beta/\beta_0)} + \cdots \tag{G.12}$$

for large β, where $\eta = 1$, $\sigma = 1/2$, and β_0 is a positive constant. Clearly, their result (G.11) corresponds to (G.6). Further, their result (G.12) can be obtained by formally replacing $L/(2r_0)$ by β/β_0 in (E.13). This implies that the interpretation of β as a finite width of the system is consistent with the result (G.12). A similar result to (G.11) for the Hubbard chain at half-filling was obtained by Tsunetsugu.[57]

Instead of the scaling law (G.7), we expect the scaling law

$$\begin{aligned} &\langle \phi(0,0)\,\phi(y,t)\rangle_\infty(\beta) \\ &\cong \left\{\frac{\pi(y+v_s t)/(v'\beta)}{\sinh[\pi(y+v_s t)/(v'\beta)]}\right\}^{2h_{\mathrm{eff}}(\beta)} \\ &\quad\times \left\{\frac{\pi(y-v_s t)/(v'\beta)}{\sinh[\pi(y-v_s t)/(v'\beta)]}\right\}^{2\bar{h}_{\mathrm{eff}}(\beta)} \\ &\quad\times \langle \phi(0,0)\,\phi(y,t)\rangle_\infty(\infty) \end{aligned} \tag{G.13}$$

which is obtained by replacing the scaling dimensions h and $\bar{h}$ in (G.7) by effective ones $h_{\mathrm{eff}}(\beta)$ and $\bar{h}_{\mathrm{eff}}(\beta)$.

Further, we expect that there appear logarithmic corrections to the power in (G.9) as[27]

$$\hat{G}(0,0) \sim \mathrm{const} \times \beta^{2-\eta} \times [\log(v'\beta/r_0)]^\sigma \tag{G.14}$$

We shall show (G.14) in the following.

Unlike the correlation (G.4), the correlation at zero temperature would have logarithmic corrections as

$$\begin{aligned} &\langle \phi(0,0)\,\phi(y,t)\rangle_\infty(\infty) \\ &= A\left(\frac{1}{y+v_s t}\right)^{2h} \times \left(\frac{1}{y-v_s t}\right)^{2\bar{h}} \times C(y+v_s t,\, y-v_s t) \end{aligned} \tag{G.15}$$

because the correlation (G.10) has a logarithmic correction. Here the function C is a logarithmic correction which satisfies

$$C(y,y) \sim [\log(y/r_0)]^\sigma \tag{G.16}$$

for large y.

[27] A similar anomaly was observed in the uniform susceptibilities of the Bethe-ansatz solvable Heisenberg antiferromagnetic chains.[96]

Combining (G.15) with (G.13), we obtain the desired result (G.14) under the assumption that

$$C[(y+v_s t)/\rho, (y-v_s t)/\rho] \sim \{\log[1/(r_0\rho)]\}^{\sigma} \qquad \text{(G.17)}$$

for a small, positive ρ, a fixed y, and a fixed t. The assumption (G.17) holds if C does not behave pathologically.

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