Scaling in the massive antiferromagnetic XXZ spin-1/2 chain near the isotropic point

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The scaling limit of the Heisenberg XXZ spin chain at zero magnetic field is studied in the gapped antiferromagnetic phase. For a spin-chain ring having N_x sites, the universal Casimir scaling function, which characterizes the leading finite-size correction term in the large-N_x expansion of the ground-state energy, is calculated by numerical solution of the nonlinear integral equation of the convolution type. It is shown that the same scaling function describes the temperature dependence of the free energy of the infinite XXZ chain at low enough temperatures in the gapped scaling regime.

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I. INTRODUCTION

Integrable models of statistical mechanics and field theory [1,2] provide us with a very important source of information about the thermodynamic and dynamical properties of the magnetically ordered systems. Of particular importance is any progress in solutions of such models in the scaling region near the continuous phase transition points, since, due to the universality of critical fluctuations, it does not only yield the exact and detailed information about the model itself but also about the whole universality class it represents.

In this paper we address the universal finite-size and thermodynamic properties of the anisotropic spin-1/2 XXZ chain in the massive antiferromagnetic phase in the critical region close to the quantum phase transition at the isotropic point. The Hamiltonian of the model has the form

$$H = \frac{J}{2}\sum_{j=1}^{N_x}\big(\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta\,\sigma_j^z\sigma_{j+1}^z\big). \tag{1}$$

Here the index j enumerates the spin-chain sites, $\sigma_j^{\mathfrak{a}}$ are the Pauli matrices, $\mathfrak{a} = x, y, z$, $J > 0$ is the antiferromagnetic coupling constant, and Δ is the anisotropy parameter. The number of sites will be chosen even, $N_x = 2M$, and periodic boundary conditions will be implied, $\sigma_{j+N_x}^{\mathfrak{a}} \sim \sigma_j^{\mathfrak{a}}$. The massive antiferromagnetic phase is realized in this model at $\Delta > 1$. Following Lukyanov and Terras [3], we shall use the following convenient parametrization,

$$J = \frac{1}{a\pi}, \quad x = aj, \quad \Delta = \cosh\eta, \tag{2}$$

where $\eta > 0$, a denotes the lattice spacing, and x is the dimensionful spatial coordinate of the lattice site j. So, the length of the chain is $L_x = N_x a$. The Euclidean evolution in this model is described by the operator $U(y) = \exp(-yH)$.

In the thermodynamic limit $N_x \to \infty$, the antiferromagnetic ground state of model (1) is doubly degenerate at $\Delta > 1$. Its particle sector is represented by the kinklike topological excitations, which interpolate between two antiferromagnetic vacua [4]. Since these excitations carry spin 1/2, they are usually called "spinons."

For finite N_x, the ground-state energy $E_{N_x}(\eta, a)$ of the model (1) can be represented as

$$E_{N_x}(\eta, a) = N_x\,\mathcal{E}_b(\eta, a) + E_C(N_x, \eta, a), \tag{3}$$

where $N_x\,\mathcal{E}_b(\eta, a)$ is the bulk term calculated and studied for all Δ by Yang and Yang [5,6] by means of the coordinate Bethe ansatz. The *Casimir energy* term $E_C(N_x, \eta, a)$ exponentially vanishes in the thermodynamic limit $N_x \to \infty$ at fixed η and a. This term describing the finite-size correction to the bulk ground-state energy has been extensively studied by many authors [7–12] by means of the technique utilizing a certain nonlinear integral equation (NLIE) of the convolution type. Most attention in these studies has been concentrated on the $|\Delta| \leqslant 1$ gapless Luttinger liquid phase. For the massive antiferromagnetic phase that takes place at $\Delta > 1$, the NLIE was derived by de Vega and Woynarowich [11], and further studied by Dugave *et al.* [12].

Note that study of the Casimir energy finite-size correction term $E_C(N_x, \eta, a)$ does not have immediate experimental implications, though it is important for the theory and crucial for the interpretation of the results of the computer simulation, which are typically performed on finite-size systems. In contrast, calculations of the *per*-site free energy

$$f(J, \eta, T) = -T \lim_{N_x\to\infty} \frac{1}{N_x} \ln \operatorname{Tr} e^{-H/T} \tag{4}$$

of the infinite XXZ chain has a major importance for the experiments, since it yields the specific heat $c(J, \eta, T) = -T\,\partial_T^2 f(J, \eta, T)$ that can be directly measured in quantum quasi-one-dimensional antiferromagnets. The most systematic approach to the thermodynamics of the XXZ spin chain is based on the thermodynamic Bethe ansatz (TBA) method, the first version of which was invented in 1969 by Yang and Yang [13], who used it to study the one-dimensional gas of delta-interacting bosons. Application of the TBA for calculation of the thermodynamic quantities in the XXZ spin chain was started in 1971 by Takahashi [14] and Gaudin [15], and later continued by many other authors [10,16–19]. Thermodynamics of the more general XYZ spin-chain model was studied by means of the TBA in [16,20,21]. Further references on the TBA method and its applications in the theory of the integrable spin-chain models can be found in monographs [22,23].

The specific heat $c(J, \eta, T)$, apart from the trivial linear dependence on the coupling constant J, depends on temperature T and on the anisotropy parameter η. For a given $\eta > 0$, the temperature dependence of $c(J, \eta, T)$ can be found by means of the TBA method, see Fig. 4(a) in [21], where the plot of the specific heat $c(1, \text{arccosh}(3/2), T)$ obtained this way is shown.

At the isotropic point $\eta = 0$, the XXZ chain (1) undergoes a continuous quantum phase transition and the correlation length diverges. Close to the isotropic point for $0 < \eta \ll 1$, the correlation length becomes much larger than the lattice spacing and the spin chain arrives at the massive scaling regime. It will be shown later that one should expect in this regime the following scaling behavior of the specific heat at low enough temperatures $T \ll J$,

$$c(J, \eta, T) = \frac{T}{\pi J} X(t), \tag{5}$$

where $X(t)$ is the universal scaling function depending solely on the scaling parameter $t = T/m(J, \eta)$ and $m(J, \eta)$ is the spinon mass, which is equal to the half of the gap in the two-spinon excitation energy spectrum. The Casimir energy $E_C(N_x, \eta, a)$ should have the analogous universal scaling behavior at $\eta \ll 1$; see Eq. (9) below. Surprisingly, the scaling behavior of the specific heat and Casimir energy in the XXZ spin chain at $0 < \eta \ll 1$ has never been studied in literature, and the corresponding universal scaling functions $X(t)$ and $Y(u)$ remained unknown. The aim of the present paper is to fill this gap.

First, we modify the nonlinear integral equation derived by Dugave *et al.* [12] and proceed in it to the scaling limit in the massive antiferromagnetic phase in order to describe the scaling behavior of the Casimir energy $E_C(N_x, \eta, a)$. The scaling limit is understood in the usual way,

$$a \to 0, \quad \eta \to +0, \quad N_x \to \infty, \tag{6}$$
$$\xi(\eta, a) = \text{const}, \quad L_x \equiv aN_x = \text{const}.$$

Here $\xi(\eta, a)$ is the correlation length, which behaves [12] at small $\eta > 0$ as

$$\xi(\eta, a) = [2\, m(\eta, a)]^{-1}\, [1 + O(\exp[-\pi^2/\eta])], \tag{7}$$

and the spinon mass $m(\eta, a)$ has the following asymptotic behavior [24]:

$$m(\eta, a) = \frac{4\, \exp[-\pi^2/(2\eta)]}{a} \tag{8}$$

at $\eta \to +0$.

It follows from dimension arguments [25] that the Casimir energy takes the scaling form in the limit (6),

$$E_C(N_x, \eta, a) \simeq \frac{Y(u)}{L_x}, \tag{9}$$

where

$$u = L_x\, m(\eta, a) = 4N_x \exp[-\pi^2/(2\eta)] \tag{10}$$

is the scaling parameter and $Y(u)$ is the universal Casimir scaling function. We calculated this function numerically by iterative solution of the NLIE written in the scaling limit (6). The plot of the resulting Casimir scaling function is shown in Fig. 1.

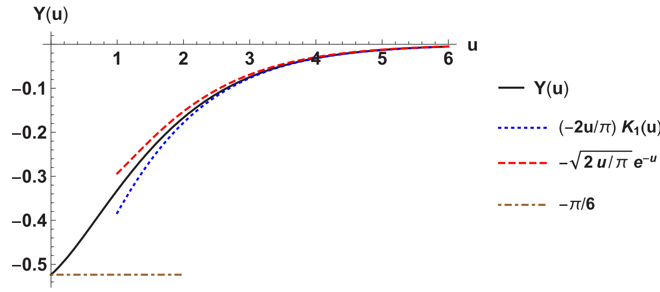


FIG. 1. Plot of the Casimir scaling function $Y(u)$ (black solid line). Its large-u asymptotics determined by Eqs. (48) and (49) are shown by the dotted blue and dashed red lines, respectively. The value at the critical point $Y(0) = -\pi/6$ agrees with the CFT prediction.

The scaling limit (6) of model (1) can be described by the sine-Gordon quantum field theory [3,26], in which the coupling constant β_s^2 approaches its upper boundary value $\beta_s^2 \to 8\pi$. This Euclidean quantum field theory (EQFT) lives on the torus having the periods L_x, L_y, in the limit $L_y \to \infty$. Under the choice (2) of the coupling constant J, the dispersion law of the elementary excitations in this continuous EQFT takes the relativistic form $\omega(p) = \sqrt{p^2 + m(\eta, a)^2}$, indicating the rotational symmetry of the theory in the $\langle x, y\rangle$ plane. As it was explained by Al. B. Zamolodchikov [25], this allows one to relate the ground-state energy of the EQFT [determined in our case by Eqs. (3) and (9)] with the free energy of the chain having the infinite length $L_y \to \infty$ at a nonzero temperature $T = 1/L_x$; see Eq. (2.8) in [25]. As a result, one arrives at the following representation for the per-site free energy (4) in the scaling regime (6):

$$f(J, \eta, T) = \mathcal{E}_b(J, \eta) + \frac{T^2}{\pi J} Y(u), \tag{11}$$

where $u = m(J, \eta)/T$ is the scaling parameter and

$$m(J, \eta) = 4\pi J\, \exp\left(-\frac{\pi^2}{2\eta}\right) \tag{12}$$

is the spinon mass. Note that we have changed notations in Eqs. (11) and (12) using the coupling constant J instead of the lattice spacing $a = (\pi J)^{-1}$ as the argument of the functions $f, \mathcal{E}_b, m$. The free energy reduces to the form (11) in the scaling regime, which is realized at $aT \ll 1$ and $a\, m \ll 1$. In terms of the original parameters of the XXZ chain Hamiltonian, these two strong inequalities read

$$T \ll J, \quad \exp\left(-\frac{\pi^2}{2\eta}\right) \ll 1. \tag{13}$$

Accordingly, the specific heat per chain site $c(J, \eta, T)$ must scale under conditions (13) to the form (5), where

$$X(t) = [-2Y(u) + 2uY'(u) - u^2 Y''(u)]|_{u=1/t}. \tag{14}$$

The plot of the universal specific heat scaling function $X(t)$ determined from Eq. (14) is shown in Fig. 2.

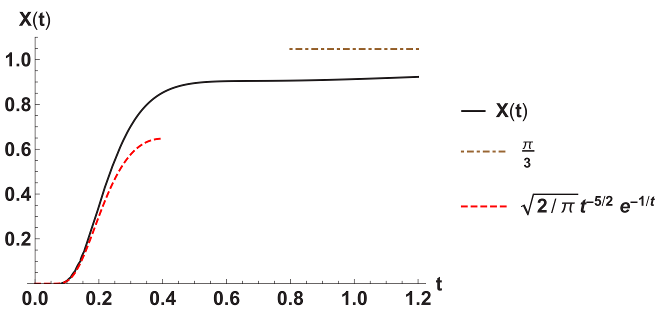


FIG. 2. Plot of the specific heat scaling function $X(t)$ versus the scaled temperature parameter $t = T/m(J,\eta)$ (black sold line). The small-t asymptotics (55) of $X(t)$ is shown by the red dashed line. At large t, $X(t)$ approaches very slowly to its CFT value $\pi/3$.

In what follows, we will describe how these results were obtained and present them in more details. In particular, in Sec. II we recall briefly a few basic results on the Bethe ansatz calculation of the ground-state energy of the finite XXZ spin chain in the gapped antiferromagnetic phase. The well-known representation of this ground-state energy in terms of the solution of a nonlinear integral equation is described in Sec. III. New results are presented in Sec. IV. First, we proceed in it to the scaling limit in the nonlinear integral equation, and then describe the numerical and analytical results for the universal scaling functions characterizing the Casimir energy, the free energy, and specific heat of the XXZ spin chain in the antiferromagnetic gapped near-critical regime. Section V contains concluding remarks. Finally, in the two Appendixes we describe two alternative analytical calculations of the Casimir scaling function $Y(u)$ in the limit $u \ll 1$. In Appendix A we exploit to this end the small-u asymptotical analysis of the nonlinear TBA equations, while in Appendix B we use the renormalization group perturbation-theory technique.

II. BETHE-ANSATZ SOLUTION FOR THE GROUND STATE AT Δ > 1

The ground state $|\Phi\rangle$ of the $2M$-site chain is characterized by the set of M real Bethe roots $\{\lambda_n\}_{n=1}^{M}$, $-\pi/2 < \lambda_1 < \lambda_2 \cdots < \lambda_M < \pi/2$, which solve the equations

$$\mathcal{F}(\lambda_n) + 1 = 0, \tag{15}$$

where $n = 1, \dots, M$, and

$$\mathcal{F}(\lambda) = \left[\frac{\sin\left(\lambda - \frac{i\eta}{2}\right)}{\sin\left(\lambda + \frac{i\eta}{2}\right)}\right]^{N_x} \prod_{j=1}^{M} \frac{\sin(\lambda - \lambda_j + i\eta)}{\sin(\lambda - \lambda_j - i\eta)}. \tag{16}$$

Note that $\lambda_n = -\lambda_{M-n+1}$ for the Bethe roots describing the ground state and

$$\mathcal{F}(\lambda + \pi) = \mathcal{F}(\lambda), \quad \mathcal{F}(\pi/2) = 1,$$
$$\mathcal{F}(\pi - \lambda) = \frac{1}{\mathcal{F}(\lambda)} = \overline{\mathcal{F}(\bar{\lambda})}. \tag{17}$$

The ground-state energy of the N_x-site chain reads

$$E_{N_x} = \sum_{n=1}^{M} \varepsilon_0(\lambda_n), \tag{18}$$

where

$$\varepsilon_0(\lambda) = 2J[-\Delta + \cos p_0(\lambda)] \tag{19}$$

and

$$\exp[i p_0(\lambda)] = \frac{\sin\left(\lambda - \frac{i\eta}{2}\right)}{\sin\left(\lambda + \frac{i\eta}{2}\right)}. \tag{20}$$

Note that $\varepsilon_0(\lambda) = -J\, p_0'(\lambda) \sinh\eta$.

The counting function $\phi(\lambda)$ can be defined near the real axis by the relations

$$\mathcal{F}(\lambda) = \exp[2\pi i N_x \phi(\lambda)], \quad \phi(-\pi/2) = 0. \tag{21}$$

The counting function $\phi(\lambda)$ is analytic in the strip $-\eta/2 < \mathrm{Im}\,\lambda < \eta/2$ and quasiperiodic there,

$$\phi(\lambda + \pi) = \phi(\lambda) + \tfrac{1}{2}. \tag{22}$$

The logarithmic derivative in λ of Eq. (16) reads

$$\phi'(\lambda) = \frac{p_0'(\lambda)}{2\pi} - \frac{1}{N_x}\sum_{j=1}^{M} \mathcal{K}(\lambda - \lambda_j), \tag{23}$$

where

$$p_0'(\lambda) = \frac{\cot\left(\lambda - \frac{i\eta}{2}\right) - \cot\left(\lambda + \frac{i\eta}{2}\right)}{i}, \tag{24}$$

$$\mathcal{K}(\lambda) = \frac{\cot(\lambda - i\eta) - \cot(\lambda + i\eta)}{2\pi i}. \tag{25}$$

III. NONLINEAR INTEGRAL EQUATION

Assuming that the counting function $\phi(\lambda)$ corresponding to the ground state strictly increases at real λ, and taking into account (21) and (22), one concludes that Eq. (15) has exactly M real solutions in the interval $-\pi/2 < \lambda < \pi/2$, and these solutions coincide with the Bethe roots $\{\lambda_n\}_{n=1}^{M}$. Application of Cauchy's integral formula to the sums in the right-hand sides of (23) and (18) leads to the following integral representations of these equations [12]:

$$\phi'(\lambda) = \frac{p_0'(\lambda)}{2\pi} - \int_{-\pi}^{0} d\mu\, \mathcal{K}(\lambda - \mu)\phi'(\mu) + \frac{1}{\pi N_x}\int_{-\pi}^{0} d\mu\, \mathcal{K}(\lambda - \mu)\, \mathrm{Im}\, \partial_\mu \ln[1 + \mathcal{F}(\mu + i0)], \tag{26}$$

$$E_{N_x} = N_x \int_{-\pi}^{0} d\lambda\, \varepsilon_0(\lambda)\phi'(\lambda) - \frac{1}{\pi}\int_{-\pi}^{0} d\lambda\, \varepsilon_0(\lambda)\, \mathrm{Im}\, \partial_\lambda \ln[1 + \mathcal{F}(\lambda + i0)]. \tag{27}$$

Let us define the linear integral operator K that acts on a π-periodical function $\psi(\lambda)$ of $\lambda \in \mathbb{R}$ as follows:

$$K[\psi](\lambda) = \int_{-\pi}^{0} d\mu\, \mathcal{K}(\lambda - \mu)\psi(\mu).$$

By action with the operator $(1 + K)^{-1}$ on both sides of Eq. (26), and subsequent integration in λ, one modifies it to the form

$$-i\,\ln\mathcal{F}(\lambda|\eta,N_x) = 2\pi N_x\phi_0(\lambda|\eta) + 2\int_{-\pi}^{0} d\mu\, Q(\lambda-\mu|\eta) \times \text{Im}\,\ln[1+\mathcal{F}(\mu+i0|\eta,N_x)], \quad (28)$$

where

$$Q(\lambda|\eta) \equiv (1+K)^{-1}[\mathcal{K}](\lambda) = \sum_{n=-\infty}^{\infty} e^{2in\lambda}\frac{e^{-2\eta|n|}}{\pi(1+e^{-2\eta|n|})}, \quad (29)$$

$$\phi_0'(\lambda|\eta) \equiv \frac{1}{2\pi}(1+K)^{-1}[p_0'](\lambda) = \sum_{n=-\infty}^{\infty}\frac{e^{2in\lambda}}{2\pi\,\cosh(\eta\, n)} = \sum_{l=-\infty}^{\infty}\frac{1}{2\eta\,\cosh[\pi(\lambda-\pi l)/\eta]}, \quad (30)$$

$$\ln\mathcal{F}(-\pi/2|\eta,N_x) = 0, \quad \phi_0(-\pi/2|\eta) = 0. \quad (31)$$

Similarly, the ground-state energy (27) can be represented in the form (3), where

$$\mathcal{E}_b(\eta,a) = \int_{-\pi}^{0} d\lambda\,\varepsilon_0(\lambda)\phi_0'(\lambda) \quad (32)$$

is the ground-state energy per site in the infinite chain and the finite-size correction (Casimir energy) reads

$$E_C(N_x,\eta,a) = -2J\,\sinh\eta\int_{-\pi}^{0} d\lambda\,\phi_0''(\lambda) \times \text{Im}\,\ln[1+f(\lambda+i0)]. \quad (33)$$

IV. SCALING LIMIT

In the scaling limit (6), the solution $\mathcal{F}(\lambda|\eta,N_x)$ of Eq. (28) approaches very fast to its bulk limit $\exp[2\pi i N_x\,\phi_0(\lambda|\eta)]$ everywhere in the real λ axis, apart from the small vicinities of the points $\lambda^{(n)} = -\pi/2+\pi n$. To describe the scaling limit of Eq. (28) near one of such points $\lambda^{(0)} = -\pi/2$, let us make in it the linear change of the rapidity variables λ, μ,

$$\lambda = -\frac{\pi}{2}-\frac{\eta\,\alpha}{\pi}, \quad \mu = -\frac{\pi}{2}-\frac{\eta\,\alpha'}{\pi}, \quad (34)$$

where α,α' are the rescaled rapidities.

The function $\mathcal{F}(\lambda|\eta,N_x)$ reduces in the vicinity of the point $\lambda^{(0)}$ in the scaling limit (6) to the form

$$\mathcal{F}(\lambda|\eta,N_x)_{\lambda=-\pi/2-\eta\alpha/\pi} = \frac{1}{\mathfrak{f}(\alpha|u)} + (\text{corrections to scaling}). \quad (35)$$

The scaling limit of the first term on the right-hand side of the integral equation (28) reads

$$2\pi N_x\,\phi_0(\lambda|\eta)_{\lambda=-\pi/2-\eta\alpha/\pi} = -u\,\sinh\alpha\,[1+O(ma)^2]. \quad (36)$$

To prove this, let us note that the leading contribution to the sum in the second line of (30) comes at $\eta\to+0$ and $\lambda\approx-\pi/2$ from the two terms with $l=-1,0$. Then simple calculations yield

$$\phi_0'(\lambda|\eta)_{\lambda=-\pi/2-\eta\alpha/\pi} = \frac{ma}{2\eta}\cosh\alpha\;[1+O(am)^2]. \quad (37)$$

Integration of this equality with respect to λ with (31) taken into account leads to (36).

In order to find the scaling limit of the kernel $Q(\lambda-\mu|\eta)$ in Eq. (28), we replace the sum on the right-hand side of (29) by the integral

$$Q(\lambda-\mu|\eta) = \frac{\pi}{\eta}\,\mathcal{Q}(\alpha-\alpha') + O(\eta),$$

where λ, μ according to (34) are related to α,α', and

$$\mathcal{Q}(\Lambda) = \frac{1}{\pi}\int_0^{\infty} dy\,\cos(2y\Lambda)\frac{e^{-\pi y}}{\cosh(\pi y)}. \quad (38)$$

The integral on the right-hand side can be explicitly calculated,

$$\mathcal{Q}(\Lambda) = \lim_{\gamma_s\to\infty}\frac{1}{2\pi i}\frac{\partial\,\ln S(\Lambda,\gamma_s)}{\partial\Lambda}, \quad (39)$$

where $S(\Lambda,\gamma_s)$ is the soliton-soliton scattering amplitude in the sine-Gordon model [27,28],

$$S(\Lambda,\gamma_s) = -\exp\left[-i\int_0^{\infty}\frac{dy}{y}\frac{\sin(2\Lambda y)\sinh[(\pi-\frac{\gamma_s}{8})y]}{\cosh(\pi y)\sinh(\gamma_s y/8)}\right], \quad (40)$$

$$\lim_{\gamma_s\to\infty} S(\Lambda,\gamma_s) = -\frac{\Gamma\left(1+\frac{i\Lambda}{2\pi}\right)\Gamma\left(\frac{1}{2}-\frac{i\Lambda}{2\pi}\right)}{\Gamma\left(1-\frac{i\Lambda}{2\pi}\right)\Gamma\left(\frac{1}{2}+\frac{i\Lambda}{2\pi}\right)}. \quad (41)$$

Here the parameter γ_s is simply related to the coupling constant β_s^2 in the sine-Gordon model $\gamma_s = \beta_s^2/(1-\frac{\beta_s^2}{8\pi})$. It is well known [29,30] that Eq. (40) describes also the amplitude of the spinon-spinon scattering in the XXZ model (1) in the gapless phase $|\Delta|<1$, if the parameter $\gamma=\arccos\Delta$ is chosen so that

$$\gamma = \frac{8\pi^2}{8\pi+\gamma_s} = \pi\left(1-\frac{\beta_s^2}{8\pi}\right). \quad (42)$$

The limit $\gamma_s=\infty$ corresponds to the isotropic antiferromagnetic point of the XXZ spin chain, in which $\gamma=0$ and $\Delta=1$. The spinon-spinon scattering phase factor (41) at this point of model (1) was first obtained by Faddeev and Takhtajan [31].

The nonlinear integral equation (28) reduces in the scaling limit to the form

$$-i\,\ln\mathfrak{f}(\alpha|u) = u\,\sinh\alpha + 2\int_{-\infty}^{\infty} d\alpha'\,\mathcal{Q}(\alpha-\alpha') \times \text{Im}\,\ln[1+\mathfrak{f}(\alpha'+i0|u)], \quad (43)$$

with real $\alpha,\alpha'\in\mathbb{R}$, and the scaling limit of the Casimir energy (33) reads

$$E_C(N_x,\eta,a) = -\frac{m}{\pi}\int_{-\infty}^{\infty} d\alpha\,\sinh\alpha \times \text{Im}\,\ln[1+\mathfrak{f}(\alpha+i0|u)]. \quad (44)$$

Equations (43) and (44) coincide with the $\gamma\to0$ limit of Eqs. (5.9) and (5.8) obtained by Destri and de Vega [10] for the massive Thirring (sine-Gordon) model. However, concentrating in their article on the massive Thirring model with a finite $\gamma>0$ and on the gapless case of the XXZ spin chain, the authors of [10] did not apply their results to describe the massive scaling regime of the XXZ chain, which we address here. Perhaps, for this reason, Destri and de Vega did not study in [10] the nontrivial $\gamma \to 0$ limit of their integral equation (5.9), which is relevant to the XXZ model in the massive scaling regime.

Let us analytically continue the function $\mathfrak{f}(\alpha|u)$ into the strip $|\mathrm{Im}\,\alpha| \leqslant \pi/2$ and introduce two auxiliary complex functions (the pseudoenergies) $\varepsilon(\beta|u)$, $\bar{\varepsilon}(\beta|u)$,

$$\varepsilon(\beta|u) = -\ln \mathfrak{f}(\beta + i\pi/2|u),$$
$$\bar{\varepsilon}(\beta|u) = \ln \mathfrak{f}(\beta - i\pi/2|u). \quad (45)$$

At real β, these functions are complex conjugate to one another. They must satisfy the system of two nonlinear integral TBA equations [compare with Eqs. (3.3) and (3.4) in [25]], which follow from (43),

$$\varepsilon(\beta|u) = u \cosh\beta - \int_{-\infty}^{\infty} d\beta'\, \mathcal{Q}(\beta-\beta') \ln[1+e^{-\varepsilon(\beta'|u)}] + \int_{-\infty}^{\infty} d\beta'\, \mathcal{Q}(\beta-\beta'+i\pi-i0) \ln[1+e^{-\bar{\varepsilon}(\beta'|u)}], \quad (46a)$$

$$\bar{\varepsilon}(\beta|u) = u \cosh\beta - \int_{-\infty}^{\infty} d\beta'\, \mathcal{Q}(\beta-\beta') \ln[1+e^{-\bar{\varepsilon}(\beta'|u)}] + \int_{-\infty}^{\infty} d\beta'\, \mathcal{Q}(\beta-\beta'-i\pi+i0) \ln[1+e^{-\varepsilon(\beta'|u)}]. \quad (46b)$$

In turn, the Casimir energy (44) takes the form (9), with the scaling function

$$Y(u) = -\frac{u}{\pi} \int_{-\infty}^{\infty} d\beta\, \cosh\beta\, \mathrm{Re}\, \ln[1+e^{-\varepsilon(\beta|u)}]. \quad (47)$$

The nonlinear integral equations (46) with a different first term in the right-hand sides, however, were studied by Klümper [18,21], who used them to calculate the temperature dependence of the specific heat and magnetic susceptibility in the isotropic antiferromagnetic XXX spin-1/2 chain.

Note that the nonlinear integral equations (46) can be derived in a completely different way exploiting Klümper's results [21] for the general XYZ spin chain. If one starts from the TBA equations (3.19) derived in [21] for the XYZ chain, proceeds to the limit corresponding to the XXZ chain in the gapped antiferromagnetic phase $\Delta > 1$, and afterwards proceeds to the scaling limit $\eta \to +0$, one arrives at Eqs. (46). In turn, formula (3.21) in [21] representing the free energy of the XYZ chain reduces after these two limiting procedures to the scaling form (11) with the scaling function $Y(u)$ given by (47).

The system of nonlinear integral equations (46) can be solved numerically by iterations. The convergence of iterations is perfect at large and intermediate values of the scaling parameter u, but retards at very small u. The plot of the resulting Casimir scaling function $Y(u)$ is shown in Fig. 1.

The scaling function $Y(u)$ exponentially decays at large $u \to +\infty$,

$$Y(u) = -\frac{2u}{\pi} K_1(u) + O(e^{-2u}) \quad (48)$$
$$= -\sqrt{\frac{2u}{\pi}}\, e^{-u}\, [1 + O(1/u)], \quad (49)$$

where $K_1(u)$ is the Macdonald function. As in the case of the massive Thirring model at a finite $\gamma > 0$ [see Eqs. (6.9)–(6.11) in [10]], the large-u asymptotics (48) can be easily obtained by replacing the function $\varepsilon(\beta|u)$ in (47) by its "zeros iteration" $u \cosh\beta$ and then expanding the resulting logarithm in the integrand to the first order, $\ln[1+\exp(-u\cosh\beta)] \to \exp(-u\cosh\beta)$.

At the isotropic point $u = 0$, the scaling function takes the value

$$Y(0) = -\pi/6, \quad (50)$$

in agreement with the CFT prediction [10,25] for the Gaussian field theory with the central charge $c = 1$. A rather involved perturbative calculation of three further terms in the small-u expansion of $Y(u)$ is described in Appendix A. The final results read

$$Y(u) = -\frac{\pi}{6} + \frac{\pi}{16\, R(u)^3} + \frac{3\pi\, \ln[2R(u)]}{32\, R(u)^4} + \frac{a_4}{R(u)^4} + \cdots, \quad (51)$$

where $a_4 \approx -0.193$ and $R(u) = \ln(2/u)$.

The logarithmic singularity of the Casimir scaling function at $u = 0$ predicted by Eq. (51) is too weak to be resolved in Fig. 1. However, this singularity is clearly seen in Fig. 3(a), which displays at small $u < 0.005$ the deviation of $Y(u)$ from its CFT limit (50), $\Delta Y(u) = Y(u) + \pi/6$. The numerical data shown by dots slowly approach with decreasing u the solid curve representing the asymptotical formula (51). The same tendency remains at very small u, as one can see in Fig. 3(b). The dots in this figure display the numerical data for the function $R(u)^3\, \Delta Y(u)$ in the interval $10^{-11} \leqslant u \leqslant 10^{-4}$ plotted against $R(u)^{-1}$. The solid curve represents the small-u asymptotics for this function,

$$R(u)^3\, \Delta Y(u) \approx \frac{\pi}{16} + \frac{3\pi}{32} R(u)^{-1} \ln[2R(u)] - 0.193\, R(u)^{-1}, \quad (52)$$

corresponding to (51). The asymptotic low- and high-temperature behavior of the free energy $\Delta f(T) = f(T) - f(0)$ per site can be read from (11), (48), and (51),

$$\Delta f(T) = -\frac{T^2}{6J}\left[1 - \frac{3}{8\,\ln^3(2T/m)} - \frac{9\,\ln[2\,\ln(2T/m)]}{16\,\ln^4(2T/m)} - \frac{6\,a_4}{\pi\,\ln^4(2T/m)} + \cdots\right], \quad (53)$$

at $m \ll T \ll J$, and

$$\Delta f(T) = -\frac{1}{\pi J}\sqrt{\frac{2m}{\pi}}\, T^{3/2}\, e^{-m/T}\, [1 + O(T/m)], \quad (54)$$

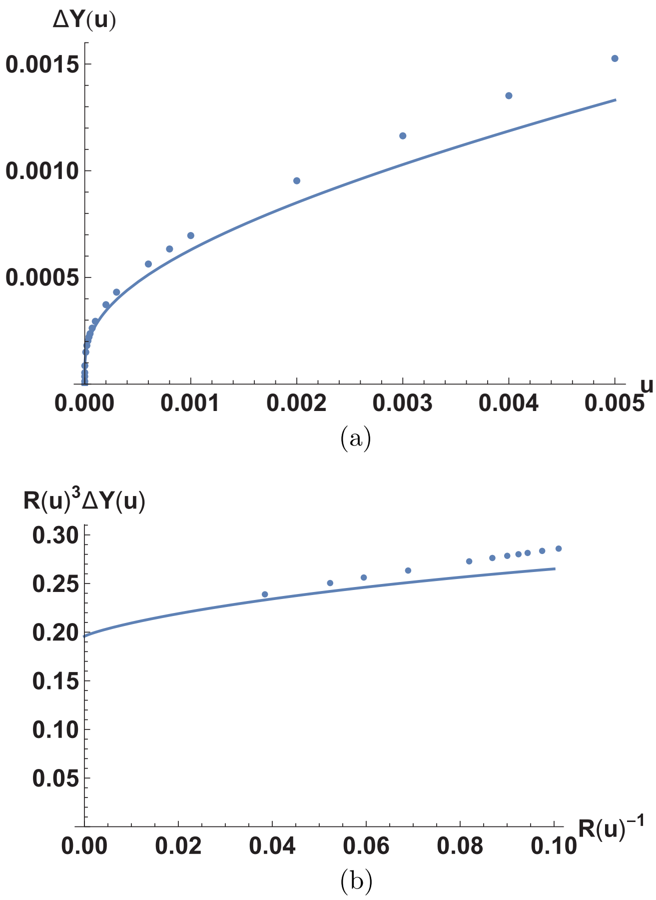


FIG. 3. Comparison of analytical and numerical results for the scaling function $\Delta Y(u) = Y(u) + \pi/6$ at small u. (a) Numerical data (dots) for the function $\Delta Y(u)$ and its asymptotical behavior (51) (solid curve) at $u < 0.005$. (b) Numerical data (dots) for the function $R(u)^3\,\Delta Y(u)$ plotted against $R(u)^{-1}$ at $10^{-11} \leqslant u \leqslant 10^{-4}$. The solid curve displays the small-u asymptotic formula (52) for this function.

at $T \ll m \ll J$, where m is given by (12). The corresponding small-t asymptotics of the scaling function $X(t)$ takes the form

$$X(t) = -\sqrt{\frac{2}{\pi}}\, t^{-5/2} e^{-1/t}[1 + O(t)] \quad \text{at } t \to 0, \tag{55}$$

and $X(t)$ slowly approaches the CFT value $\pi/3$ at very large $t \to \infty$.

For the total free energy $F(T, L_y) = N_y\,\Delta f(T)$ of the spin chain of the length $L_y \to \infty$, which has $N_y = \pi J L_y$ sites, the low-temperature asymptotics following from (54) reads

$$F(T, L_y) = -2L_y\sqrt{\frac{m}{2\pi}}\, T^{3/2}\, e^{-m/T}\, [1 + O(T/m)]. \tag{56}$$

This result has a transparent physical interpretation. One can easily see that the right-hand side of Eq. (56) is just the grand canonical potential $\Omega(T, L_y)$ of the classical ideal gas of two kinds of nonrelativistic particles (spinons with spins oriented up and down) having the same mass m and the chemical potential $\mu = m$, which move in one dimension in the line of the length L_y.

It is interesting to compare two asymptotical formulas for the ground-state energy of the XXZ spin chain of finite length L_x supplemented with periodic boundary conditions.

The first one

$$E_{N_x}(0, a) = N_x\,\mathcal{E}_b(0, a) - \frac{\pi}{6L_x} - \frac{\pi}{16L_x\,\ln^3\frac{L_x}{a}} + \cdots \tag{57}$$

contains three initial terms in the large-L_x expansion of the XXZ spin-chain ground-state energy at the isotropic point $\eta = 0$. The third term on the right-hand side was first obtained by Affleck *et al.* [32] in the conformal perturbation theory approach, and later confirmed (for the analogous low-temperature expansion of the free energy) by Klümper [18] in the discrete-lattice TBA calculations.

The second formula

$$E_{N_x}(\eta, a) = N_x\,\mathcal{E}_b(\eta, a) - \frac{\pi}{6L_x} - \frac{\pi}{16L_x\,\ln^3\frac{L_x}{\xi(\eta)}} + \cdots \tag{58}$$

holds in the gapped antiferromagnetic phase in the scaling regime $0 < \eta \ll 1$ at $L_x \ll \xi(\eta)$. Equation (58) results from the substitution of two initial terms of the small-u expansion (51) into (3) and (9).

Though formulas (57) and (58) look remarkably similar, there are two important differences between them.

(1) The third term on the right-hand side of (57) explicitly depending on the lattice spacing a describes the discrete-lattice correction to scaling in the ground-state energy. In contrast, the third term on the right-hand side of (58) does not depend on a and describes the universal scaling behavior of the ground-state energy at $0 < \eta \ll 1$.

(2) The ratio L/a is the large parameter in Eq. (57) and the third term on its right-hand side is, therefore, negative. In contrast, the ratio $L/\xi(\eta)$ is the small parameter in the asymptotic expansion (58) and the analogous correction term in the latter is positive.

It turns out that expansion (58) can be also obtained by means of the perturbative CFT technique applied in [32] for the derivation of (57). The difference is that the log-correction term in (57) was caused by the marginally irrelevant perturbation of the Gaussian CFT Hamiltonian, whereas in the case of (58) the perturbing field is marginally relevant. The field-theoretical derivation of formula (58) is described in Appendix B.

V. CONCLUSIONS

Considering the Heisenberg XXZ spin-chain ring in the gapped antiferromagnetic phase $\Delta > 1$ close to the quantum phase transition point $\Delta = 1$, we expressed its ground-state energy universal Casimir scaling function in terms of the solution of the nonlinear integral equation. We calculated this Casimir scaling function numerically by iterative solution of the nonlinear integral equation, and also analytically determined its asymptotical form at large and small values of the scaling parameter. Then, using the correspondence in the scaling regime between the ground-state energy of the finite ring of length L_x with the free energy of the infinite chain at temperature $T = 1/L_x$, we calculated the universal scaling function $X(t)$ describing the temperature dependence of the specific heat of the infinite chain at low temperatures $T \ll J$ and $0 < \Delta - 1 \ll 1$.

In contrast to many previous studies [10,14–16,18,21] of the specific heat in the XXZ spin chain, our results are universal, since we have limited analysis to the scaling regime. Due to its universality, the obtained scaling function $X(t)$ should describe exactly the specific heat temperature dependences in those quasi-one-dimensional magnetic compounds in the scaling regime close to the isotropic point, whose magnetic Hamiltonian falls into the universality class of the XXZ spin-1/2 chain model.

In presenting the results, we followed the important recommendation of Tracy and McCoy in [33]: "We strongly recommend that all data be presented in scale-variable and scale-function language."

It would be interesting to experimentally observe in quasi-one-dimensional antiferromagnetic compounds the universal specific-heat scaling temperature dependence (5). It would be also interesting and important for the experimental applications to study corrections in small η to the scaling dependences (9) and (5).

ACKNOWLEDGMENTS

I am thankful to H. W. Diehl for interesting discussions and to A. Klümper for numerous suggestions leading to improvement of the text.

APPENDIX A: PERTURBATIVE DERIVATION OF (51)

In this Appendix we perform the asymptotic analysis of the nonlinear TBA integral equations (46) at a small $u \to 0$, and describe briefly the derivation of formula (51) for the Casimir scaling function (47). Our calculations are based to some extent on the techniques developed by Destri and de Vega [10] and by Klümper [18] for different TBA integral equations. We will comment on these works later.

Let us rewrite the integral equations (46) in the equivalent form,

$$\varepsilon(\beta|u) = u \cosh\beta - 2\int_{-\infty}^{\infty} d\beta'\, \mathcal{Q}(\beta-\beta')\,\mathrm{Re}\,\chi(\beta'|u) - \int_{-\infty}^{\infty} d\beta'\, g(\beta-\beta'-i0)\,\overline{\chi(\beta'|u)}, \tag{A1a}$$

$$\bar\varepsilon(\beta|u) = u \cosh\beta - 2\int_{-\infty}^{\infty} d\beta'\, \mathcal{Q}(\beta-\beta')\,\mathrm{Re}\,\chi(\beta'|u) - \int_{-\infty}^{\infty} d\beta'\, \overline{g(\beta-\beta'-i0)}\,\chi(\beta'|u), \tag{A1b}$$

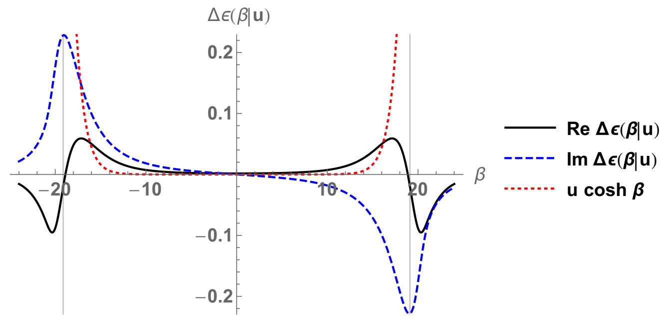
where

$$g(\Lambda) = -\frac{1}{2\Lambda(\Lambda+i\pi)}, \tag{A2}$$

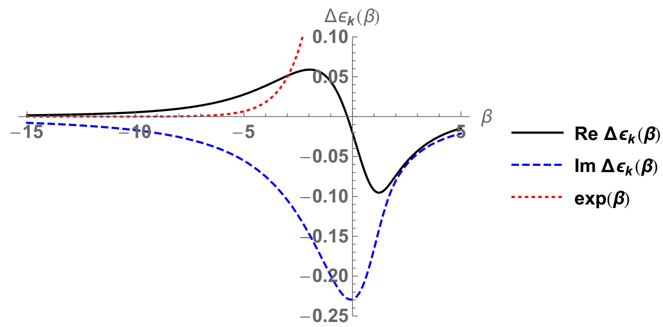
$$\chi(\beta|u) = \ln[1+e^{-\varepsilon(\beta|u)}]. \tag{A3}$$

The integral kernel $\mathcal{Q}(\Lambda)$ determined by Eqs. (39) and (41) is real at real Λ, and behaves at large $|\Lambda|$ as

$$\mathcal{Q}(\Lambda) = \frac{1}{4\Lambda^2} + \frac{\pi^2}{8\Lambda^4} + O(\Lambda^{-6}). \tag{A4}$$



(a)



(b)

FIG. 4. Real and imaginary parts of the pseudoenergy versus rapidity β (a) at $u = 10^{-8}$ and (b) at $u = 0$. (a) Real (solid) and imaginary (dashed) parts of the function $\Delta\varepsilon(\beta|u)$ defined by (A7) at $u = 10^{-8}$. Vertical lines are located at $\pm\ln(2/u)$. (b) Real (solid) and imaginary (dashed) parts of the function $\Delta\varepsilon_k(\beta) = \varepsilon_k(\beta) - \exp(\beta)$.

The reflection symmetry of the integral kernels in (A1)

$$\mathcal{Q}(\Lambda) = \mathcal{Q}(-\Lambda), \quad g(\Lambda - i0) = \overline{g(-\Lambda - i0)} \tag{A5}$$

ensures the reflection symmetry of the pseudoenergy

$$\varepsilon(\beta|u) = \bar\varepsilon(-\beta|u) \tag{A6}$$

at real β.

Besides the solution $\varepsilon(\beta|u)$ of Eqs. (A1), it is also useful to consider the difference

$$\Delta\varepsilon(\beta|u) = \varepsilon(\beta|u) - u\cosh\beta. \tag{A7}$$

Figure 4(a) displays its real and imaginary parts plotted against β at the small value of the scaling parameter, $u = 10^{-8}$. As one can see from this figure, the function $\Delta\varepsilon(\beta|u)$ vanishes outside two regions located near the points $\beta \approx \pm R(u)$, where $R(u) = \ln(2/u)$. These two regions become well separated from one another at very small u. By this reason, it is useful to shift the argument in the solutions of (A1) by $R(u)$, and to introduce new functions

$$\varepsilon_R(\beta|u) = \varepsilon(\beta + R(u)|u), \quad \bar\varepsilon_R(\beta|u) = \bar\varepsilon(\beta + R(u)|u). \tag{A8}$$

These two functions solve the integral equations, which are obtained from (A1) by replacement of the driving term

$$u\cosh\beta \to e^{\beta} + \frac{u^2}{4}e^{-\beta} \tag{A9}$$

in their right-hand sides.

Proceeding in (A8) and (A9) to the limit $u \to 0$, one obtains the pseudoenergies

$$\varepsilon_k(\beta) = \lim_{u\to 0} \varepsilon(\beta + R(u)|u), \quad \bar{\varepsilon}_k(\beta) = \lim_{u\to 0} \bar{\varepsilon}(\beta + R(u)|u), \tag{A10}$$

which correspond to the isotropic point of the XXZ spin chain and solve the TBA integral equations,

$$\varepsilon_k(\beta) = e^\beta - 2\int_{-\infty}^{\infty} d\beta'\, \mathcal{Q}(\beta-\beta')\,\mathrm{Re}\,\chi_k(\beta') - \int_{-\infty}^{\infty} d\beta'\, g(\beta-\beta'-i0)\overline{\chi_k(\beta')}, \tag{A11a}$$

$$\bar{\varepsilon}_k(\beta) = e^\beta - 2\int_{-\infty}^{\infty} d\beta'\, \mathcal{Q}(\beta-\beta')\,\mathrm{Re}\,\chi_k(\beta') - \int_{-\infty}^{\infty} d\beta'\, \overline{g(\beta-\beta'+i0)}\chi_k(\beta'), \tag{A11b}$$

where $\chi_k(\beta) = \ln[1+e^{-\varepsilon_k(\beta)}]$. After subtraction of e^β from $\varepsilon_k(\beta)$, the resulting difference

$$\Delta\varepsilon_k(\beta) = \varepsilon(\beta) - e^\beta \tag{A12}$$

decays at $\beta \to \pm\infty$. The real and imaginary parts of this function are plotted in Fig. 4(b). Since the kernels $\mathcal{Q}(\Lambda), g(\Lambda)$ decay $\sim\Lambda^{-2}$ at $|\Lambda| \to \infty$, the difference (A12) also vanishes as $\Delta\varepsilon_k(\beta) \sim \beta^{-2}$ at large $|\beta|$. Of course, the function $\varepsilon_k(\beta)$ decays $\sim\beta^{-2}$ as well at $\beta \to -\infty$, due to (A12).

As it was mentioned above, the value $Y(0) = -\pi/6$ of the Casimir scaling function at the isotropic point is determined by the CFT. It is well known [9,10,25], that the CFT predicted value of finite-size correction to the ground-state energy can be alternatively obtained in the TBA approach without explicit solution of the integral TBA equations. Let us describe such an alternative derivation of the CFT result (50).

The integral representation (47) of the Casimir scaling function reduces at $u = 0$ to the form

$$Y(0) = \frac{2}{\pi}\,\mathrm{Re}\int_{-\infty}^{\infty} d\beta\, e^\beta\, \chi_k'(\beta). \tag{A13}$$

Let us now rewrite Eq. (A11a) as

$$e^\beta = \varepsilon_k(\beta) + 2\int_{-\infty}^{\infty} d\beta'\, \mathcal{Q}(\beta-\beta')\,\mathrm{Re}\,\chi_k(\beta') + \int_{-\infty}^{\infty} d\beta'\, g(\beta-\beta'-i0)\overline{\chi_k(\beta')}. \tag{A14}$$

The key step of this calculation is the counterintuitive substitution of the right-hand side of (A14) instead of e^β into the integrand in (A13). As the result, one obtains

$$Y(0) = -\frac{2}{\pi}\,\mathrm{Re}\int_{-\infty}^{\infty} d\beta\, \varepsilon_k(\beta)\, \frac{\varepsilon_k'(\beta)}{1+e^{\varepsilon_k(\beta)}} + \frac{4}{\pi}\iint_{-\infty}^{\infty} d\beta\, d\beta'\, \mathrm{Re}\,[\chi_k'(\beta)]\mathcal{Q}(\beta-\beta')\,\mathrm{Re}\,[\chi_k(\beta')] + \frac{2}{\pi}\,\mathrm{Re}\iint_{-\infty}^{\infty} d\beta\, d\beta'\, \chi_k'(\beta)\, g(\beta-\beta'-i0)\,\overline{\chi_k(\beta')}.$$

Both double integrals in the right-hand side vanish due to the kernel symmetry (A5). After the change of the integration variable $x = \varepsilon_k(\beta)$ in the first integral, we arrive at the desired CFT result (50),

$$Y(0) = -\frac{2}{\pi}\int_0^\infty dx\, \frac{x}{1+e^x} = -\frac{\pi}{6}.$$

For the subsequent analysis, we need the explicit form of the asymptotic expansion of the function $\varepsilon_k(\beta)$ at $\beta \to -\infty$. We obtained three terms in this expansion by the straightforward perturbative solution of the integral equations (A11) at large negative β. The result reads

$$\varepsilon_k(\beta) = \frac{b_2}{\beta^2} + \frac{b_3}{\beta^3} - \frac{b_2\ln(-\beta)}{\beta^3} + O(\beta^{-4}\ln(-\beta)), \tag{A15}$$

where

$$b_2 = -\left(\frac{\pi\,\ln 2}{2} + \mathrm{Im}\,A_1\right)i, \tag{A16a}$$

$$b_3 = \pi\,\mathrm{Im}\,b_2 + i\left(-\pi\,\mathrm{Re}\,A_1 + \frac{\mathrm{Im}\,b_2}{2} - \mathrm{Im}\,A_2\right). \tag{A16b}$$

Here A_1, A_2 denote the following converging integrals:

$$A_1 = \int_{-\infty}^{\infty} d\beta[\ln(1+e^{-\varepsilon_k(\beta)}) - \theta(-\beta)\,\ln 2], \tag{A17}$$

$$A_2 = \int_{-\infty}^{\infty} d\beta\left[2\beta\,\ln(1+e^{-\varepsilon_k(\beta)}) - 2\beta\,\theta(-\beta)\,\ln 2 + \frac{b_2}{\beta}\theta(-\beta-1)\right], \tag{A18}$$

and $\theta(x)$ is the unit-step function.

By numerical calculation of the integrals (A17) and (A18) we obtained the following values:

$$\mathrm{Re}\,A_1 = -0.38806\ldots, \tag{A19}$$

$$\mathrm{Im}\,A_1 = 0.48200\ldots, \tag{A20}$$

$$\mathrm{Im}\,A_2 = 1.026\ldots. \tag{A21}$$

It turns out that the numerical value of $\mathrm{Im}\,A_1$ is very close to $(\pi/2)(1-\ln 2) = 0.482003\ldots$ [34]. In fact, there are strong arguments [18] that the latter number is the exact value of the imaginary part of the integral (A17),

$$\mathrm{Im}\,A_1 = \frac{\pi}{2}(1-\ln 2) = 0.4820032816\ldots. \tag{A22}$$

Under this assumption, one finds from (A23), (A19), and (A21)

$$b_2 = -\frac{\pi i}{2}, \quad b_3 = -\frac{\pi^2}{2} - i\,0.592\ldots. \tag{A23}$$

We are now ready to return to the perturbative calculation of the Casimir scaling functions $Y(u)$ at a small $u > 0$. First, we write the solution of Eqs. (A1) in the form

$$\varepsilon(\beta|u) = \varepsilon^{(0)}(\beta|u) + v(\beta|u), \tag{A24}$$

where

$$\varepsilon^{(0)}(\beta|u) = \varepsilon_k(\beta - R(u)) + \overline{\varepsilon_k(-\beta - R(u))} \tag{A25}$$

is the zero-order term and $v(\beta|u)$ is the small correction. The latter could be in principal determined by means of the perturbative solution of the nonlinear integral equations (A1), with the small parameter $\delta = [R(u)]^{-1}$. Next, one could substitute (A24) into (47) and try to extract several initial terms in the small-u asymptotic expansion for $Y(u)$ from the resulting integrals. It turns out, however, that such direct perturbative calculations are extremely difficult and not suitable for evaluation of the higher terms in (51). Really, in order to calculate the smallest term $a_4\delta^4$ in expansion (51) in this approach, one has to solve perturbatively the nonlinear integral equations (A1) to the fourth order in the small parameter δ.

To avoid this problem, we have applied following [10,18] the improved technique, which allowed us to obtain (51) without solving perturbatively the integral equations (A1). First, we rewrite the integral representation (47) of the scaling function in the equivalent form,

$$Y(u) = -\frac{2}{\pi}\,\mathrm{Re}\int_{-\infty}^{\infty} d\beta\, e^{\beta}\,\chi_R(\beta|u), \tag{A26}$$

where $\chi_R(\beta|u) = \ln[1+e^{-\varepsilon_R(\beta|u)}]$. Then we split the integral $\int_{-\infty}^{\infty} d\beta$ on the right-hand side into two parts, $\int_{-\infty}^{\infty} d\beta = \int_{-\infty}^{-R(u)} d\beta + \int_{-R(u)}^{\infty} d\beta$. The first term is small $\sim u$ due to the [small at $\beta < -R(u)$] factor e^{β} in the integrand in (A26). After integration by parts in the second term, one obtains at $u \to 0$,

$$Y(u) = \frac{2}{\pi}\,\mathrm{Re}\int_{-R(u)}^{\infty} d\beta\, e^{\beta}\,\partial_\beta[\chi_R(\beta|u)] + O(u). \tag{A27}$$

This formula extends (A13) to the case of a small positive u. Recall next that the function $\varepsilon_R(\beta|u)$ defined by (A8) solves the integral equation (A1a) modified according to (A9). Let us rewrite this equation in the form similar to (A14),

$$\begin{aligned} e^{\beta} &= \varepsilon_R(\beta|u) - \frac{u^2}{4}e^{-\beta} + \int_{-\infty}^{\infty} d\beta'\,[2\mathcal{Q}(\beta-\beta')\,\mathrm{Re}\,\chi_R(\beta'|u) \\ &\quad + g(\beta-\beta'-i0)\,\overline{\chi_R(\beta'|u)}]. \end{aligned}\tag{A28}$$

After substitution of the right-hand side instead of e^{β} in the integrand in (A27) and straightforward calculations, one finds

$$Y(u) = -\frac{\pi}{6} + \Delta Y(u) + O([R(u)]^{-5}), \tag{A29}$$

where

$$\begin{aligned} \Delta Y(u) = \frac{2}{\pi}\mathrm{Re}\int_0^{\infty} d\beta \int_{-\infty}^{\infty} d\beta'\{&2\mathcal{Q}(\beta-\beta')\partial_\beta\chi(\beta|u) \\ &\times \mathrm{Re}\,[\chi(\beta'|u)] + g(\beta-\beta'-i0) \\ &\times \partial_\beta[\chi(\beta|u)]\overline{\chi(\beta'|u)}\}, \end{aligned}\tag{A30}$$

and $\chi(\beta|u)$ is given by (A3). In contrast to the $u = 0$ case, the double integral in the right-hand side of (A30) is nonzero at $u > 0$ due to the finite limits of integration. However, this integral decreases with decreasing u and vanishes at $u = 0$.

Using integration by parts and the symmetry properties (A5) and (A6), the double integral in (A30) can be conveniently represented as the sum of three terms,

$$\Delta Y(u) = A + B + C, \tag{A31}$$

where

$$A = \frac{2}{\pi}[\chi(0|u)]^2\,\mathrm{Re}\int_{2R(u)}^{\infty} d\beta\, U(\beta), \tag{A32a}$$

$$B = -\frac{2}{\pi}\chi(0|u)\,\mathrm{Re}\int_0^{\infty} d\beta\, U(\beta+R(u))\Psi(\beta|u), \tag{A32b}$$

$$\begin{aligned} C = \frac{4}{\pi}\iint_0^{\infty} d\beta\, d\beta'\,\mathcal{Q}(\beta+\beta')\mathrm{Re}\,[\partial_\beta\chi(\beta|u)]\mathrm{Re}\,[\Psi(\beta'|u)] \\ + \frac{2}{\pi}\mathrm{Re}\iint_0^{\infty} d\beta\, d\beta' g(\beta+\beta'-i0)\partial_\beta\chi(\beta|u)\Psi(\beta'|u), \end{aligned}\tag{A32c}$$

and

$$U(\beta) = 2\mathcal{Q}(\beta) + g(\beta), \tag{A33}$$

$$\Psi(\beta|u) = \chi(\beta|u) - \theta(R(u)-\beta)\chi(0|u). \tag{A34}$$

We substituted the function $\varepsilon(\beta|u)$ in the form (A24) into the integrals in (A32) and expanded the results in the small parameter $\delta = [R(u)]^{-1}$ to the fourth order. It turns out that, up to this order, (i) the correction term $v(\beta|u)$ in (A24) does not contribute to these integrals and (ii) these integrals can be expressed solely in terms of two numbers $\mathrm{Im}\, b_2$ and $\mathrm{Im}\, b_3$, which characterize the asymptotical behavior of the function $\varepsilon_k(\beta)$ at $\beta \to -\infty$; see (A15) and (A23). As the result, we obtained

$$A = \frac{\pi(\ln 2)^2\,\delta^3}{16} + O(\delta^5), \tag{A35}$$

$$B = \ln 2\left\{-\frac{(2\,\mathrm{Im}\, b_2 + \pi\,\ln 2)\,\delta^3}{16} + \frac{[-12\,\mathrm{Im}\, b_2\ln(2/\delta) + 3\,\mathrm{Im}\, b_2 + 12\,\mathrm{Im}\, b_3]\,\delta^4}{128}\right\} + o(\delta^4), \tag{A36}$$

$$\begin{aligned} C = \frac{\delta^3\,\mathrm{Im}\, b_2\,[2\,\mathrm{Im}\, b_2 + \pi\ln 2]}{8\pi} - \frac{\delta^4}{8\pi}\bigg\{ &-3\,\mathrm{Im}\, b_2\,\ln(2/\delta)\left(\mathrm{Im}\, b_2 + \frac{\pi\,\ln 2}{4}\right) \\ &+ \frac{\pi\ln 2}{16}(5\,\mathrm{Im}\, b_2 + 12\,\mathrm{Im}\, b_3) + \mathrm{Im}\, b_2(\mathrm{Im}\, b_2 + 3\,\mathrm{Im}\, b_3)\bigg\} + o(\delta^4). \end{aligned}\tag{A37}$$

This yields for (A31)

$$\Delta Y(u) = \frac{(\mathrm{Im}\, b_2)^2\delta^3}{4\pi} + \frac{3\,(\mathrm{Im}\, b_2)^2\,\delta^4\ln(2/\delta)}{8\pi} - \frac{\delta^4\,\mathrm{Im}\, b_2}{64\pi}\,(8\,\mathrm{Im}\, b_2 + 24\,\mathrm{Im}\, b_3 + \pi\ln 2) + o(\delta^4). \tag{A38}$$

After substitution of the obtained earlier values (A23) of the constants $\mathrm{Im}\, b_2$, $\mathrm{Im}\, b_3$ into this result, we arrive finally at (51).

To conclude this section, we comment on the perturbative analysis around the CFT critical point of two similar TBA equations, which were previously performed by Klümper [18] and by Destri and de Vega [10].

The nonlinear integral TBA equation (3) in [18] studied by Klümper describes the thermodynamic properties of the infinite antiferromagnetic isotropic spin-1/2 Heisenberg chain in the presence of a uniform magnetic field. In the case of zero magnetic field, this equation differs from Eq. (46b) only by one term. Namely, the driving term $u \cosh\beta$ in the right side of (46b) replaces [35] the term $\frac{\pi J/T}{\cosh\beta}$ in Eq. (3) in [18]. Despite this difference, the low-temperature asymptotical analysis of the nonlinear TBA equation (3) presented in Sec. 2 of [18] has some similarities with our small-u perturbative calculations described in this section. In particular, the small parameters $\frac{T}{\pi J}$ and $\mathfrak{L}^{-1} = 1/\ln(\pi J/T)$ used in Sec. 2 of [18] are analogous to the small parameters u and $\delta = 1/\ln(2/u)$, which we have exploited in the calculations described above. Note, finally, that we have calculated four temperature-dependent terms in the asymptotic expansion (53) for the free energy, while only two such terms were obtained in the analogous expansion (26) in [18].

The nonlinear integral TBA equation for the sine-Gordon (massive Thiring) model was obtained by Destri and de Vega; see Eq. (5.12) in [10]. Its asymptotical analysis close to the conformal regime was performed by these authors in Sec. 7.3. While the driving term in this equation is the same as in our Eqs. (46), the kernels $G_0(\Lambda,\gamma)$, $G_1(\Lambda,\gamma)$ [see Eq. (5.13) in [10] and the non-numbered foregoing equation there [36]] in the integral terms are different. Namely,

$$G_0(\Lambda,\gamma) = \frac{1}{2\pi i}\frac{\partial \ln S(\Lambda,\gamma_s(\gamma))}{\partial\Lambda} = \int_{-\infty}^{\infty}\frac{dk}{4\pi}\,\frac{\sinh\left[\left(\frac{\pi^2}{2\gamma}-\pi\right)k\right]}{\sinh\left[\left(\frac{\pi^2}{2\gamma}-\frac{\pi}{2}\right)k\right]\cosh(\pi k/2)}\,e^{ik\Lambda}, \tag{A39}$$

$$G_1(\Lambda,\gamma) = G_0(\Lambda+i\pi,\gamma), \tag{A40}$$

where $S(\Lambda,\gamma_s)$ is the soliton-soliton scattering amplitude (40) in the sine-Gordon model and parameters γ and γ_s are related according to (42). In the limit $\gamma\to 0$, the integral kernel (A39) degenerates to the form (38),

$$\lim_{\gamma\to 0} G_0(\Lambda,\gamma) = \mathcal{Q}(\Lambda).$$

So, the integral nonlinear TBA equations (46) describing the scaling behavior of the gapped XXZ spin chain represent the degenerate $\gamma\to 0$ limiting case of the TBA equations for the sine-Gordon model derived by Destri and de Vega. However, our small-u asymptotical analysis described in this section is to a large extent different from that developed by Destri and de Vega in Sec. 7.3 in [10]. The reason is that in our case the integral kernel $\mathcal{Q}(\Lambda) = G_0(\Lambda,0)$ decays slowly $\sim\Lambda^{-2}$ at large rapidities $|\Lambda|$, whereas in the nondegenerate case $\gamma>0$ studied in [10], the kernel (A39) exponentially vanishes at $|\Lambda|\to\infty$; see the non-numbered equations between (7.24) and (7.25) in [10].

APPENDIX B: FIELD-THEORETICAL DERIVATION OF (58)

The continuous limit of the XXZ spin chain (1) near the isotropic point $\Delta = 1$ can be described by the marginal perturbation of the Gaussian CFT [37,38],

$$H = H_{\mathrm{WZW}} - \frac{8\pi^2}{\sqrt{3}}\int_0^{L_x} dx\,[g_x(J^x\bar{J}^x + J^y\bar{J}^y) + g_z J^z\bar{J}^z]. \tag{B1}$$

Here H_{WZW} is the Hamiltonian of free bosons compactificated at the radius $\mathcal{R} = 1/\sqrt{2\pi}$ or, equivalently, the SU(2) Wess-Zumino-Witten (WZW) Hamiltonian of level $k=1$. Operators $J^{\mathfrak{a}}$ and $\bar{J}^{\mathfrak{a}}$, with $\mathfrak{a} = x,y,z$, represent the components of the holomorphic and antiholomorphic currents, respectively. Their normalization can be fixed by the operator product expansions (OPE),

$$J^{\mathfrak{a}}(z)J^{\mathfrak{b}}(z') = \frac{\delta^{\mathfrak{ab}}}{8\pi^2(z-z')^2} + \frac{i\epsilon^{\mathfrak{abc}}}{2\pi(z-z')}J^{\mathfrak{c}}(z)+\cdots,$$
$$\bar{J}^{\mathfrak{a}}(\bar{z})\bar{J}^{\mathfrak{b}}(\bar{z}') = \frac{\delta^{\mathfrak{ab}}}{8\pi^2(\bar{z}-\bar{z}')^2} + \frac{i\epsilon^{\mathfrak{abc}}}{2\pi(\bar{z}-\bar{z}')}\bar{J}^{\mathfrak{c}}(\bar{z})+\cdots. \tag{B2}$$

Following [32,37], the normalization in Eq. (B1) has been chosen to ensure that the operators multiplying g in the isotropic case [see Eq. (B7) below] have a correlation function with unit amplitude. The renormalization group (RG) flow of the scaling parameters in (B1) in the one-loop approximation is described by the Kosterlitz-Thouless RG equations [37],

$$\beta_x \equiv d\,g_x/dr = -\frac{4\pi}{\sqrt{3}}\,g_x\,g_z,$$
$$\beta_z \equiv d\,g_z/dr = -\frac{4\pi}{\sqrt{3}}\,g_x^2, \tag{B3}$$

where $r = \ln L$ and L is the length scale.

Two RG trajectories are shown in Fig. 5. The dashed bisector of the first quadrant $g_x = g_z \equiv g > 0$ corresponds to the isotropic point $\Delta = 1$ of the spin-chain Hamiltonian (1). The RG equations (B3) reduce in the isotropic case to the

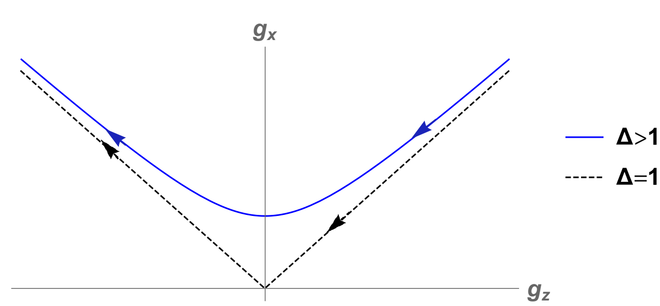


FIG. 5. Kosterlitz-Thouless RG flow corresponding to Eqs. (B3) at $\Delta > 1$ and $\Delta = 1$.

simple equation

$$\frac{dg(r)}{dr} = -\pi b\, g^2(r), \tag{B4}$$

with $b = 4/\sqrt{3}$. Its solution taking the value $g(r_0)$ at the initial point $r_0 \simeq \ln a$ reads as

$$g(r) = \frac{g(r_0)}{1 + \pi\, b\, g(r_0)(r - r_0)}. \tag{B5}$$

The leading asymptotics of this solution at $r \to \infty$ does not depend on $g(r_0)$,

$$g(r) = \frac{1}{\pi b\,(r - r_0)} + O(r^{-2}). \tag{B6}$$

Along the critical line, the effective Hamiltonian (B1) reduces to the form

$$H_{\rm XXX} = H_{\rm WZW} - g\int_0^{L_x} dx\, \varphi(x), \tag{B7}$$

where $\varphi(x)$ is the marginally irrelevant operator,

$$\varphi(x) = \frac{8\pi^2}{\sqrt{3}}\, \mathbf{J}(x)\cdot\bar{\mathbf{J}}(x). \tag{B8}$$

In the Euclidean plane, its two- and three-point correlation functions are fixed due to (B2),

$$\langle\varphi(\mathbf{r}_1)\varphi(\mathbf{r}_2)\rangle = \frac{1}{|\mathbf{r}_{1,2}|^4}, \tag{B9}$$

$$\langle\varphi(\mathbf{r}_1)\varphi(\mathbf{r}_2)\varphi(\mathbf{r}_3)\rangle = -\frac{b}{|\mathbf{r}_{1,2}|^2|\mathbf{r}_{1,3}|^2|\mathbf{r}_{2,3}|^2}, \tag{B10}$$

where $\mathbf{r}_{i,j} = \mathbf{r}_i - \mathbf{r}_j$.

Affleck *et al.* [32] considered the generalization of the effective Hamiltonian (B7) to the case of the WZW model with arbitrary positive integer k, and performed for it the perturbative calculation of the ground-state energy E_0 to the third order in g. In the case $k = 1$, their result [see the non-numbered equation between Eqs. (8) and (9) in [32]] reads

$$E_0(g) = e_0 L_x - \frac{\pi}{6L_x} - \frac{\pi^4}{3L_x} b g^3 + \cdots, \tag{B11}$$

where e_0 denotes the nonuniversal bulk energy density in the infinite system. Note that Affleck *et al.* [32] did not present the details of their calculation of $E_0(g)$. However, similar perturbative calculations were described earlier by Cardy [39,40], and in the most detailed form by Ludwig and Cardy [41]. After replacement of g in (B11) by its renormalization group improved value $g \to 1/[\pi b \ln(L/a)]$ with $L \sim L_x$ in accordance with (B6), the authors of [32] arrived finally at (57). This result was later confirmed by Lukyanov [38].

Let us turn now to the anisotropic case $0 < \eta \ll 1$, and show how the asymptotic formula (58) can be derived following the strategy outline above. To this end, consider the RG flow in the massive antiferromagnetic phase $\Delta > 1$, which is illustrated by the upper trajectory in Fig. 5. The first integral $A_x = g_x^2 - g_z^2$ of the Kosterlitz-Thouless RG equations (B3) remains positive along it. The solution of the RG equations (B3), which corresponds to this trajectory reads

$$g_z(r) = -\sqrt{A_x}\,\tan\left(4\pi r\sqrt{\frac{A_x}{3}}\right),$$
$$g_x(r) = \sqrt{A_x + g_z^2(r)}, \tag{B12}$$

with r varying in the interval $r_{\rm min} < r < r_{\rm max}$, where

$$r_{\rm max} = -r_{\rm min} = \frac{1}{8}\sqrt{\frac{3}{A_x}}.$$

The well-known arguments (see p. 124 in [42]) lead to the requirement $r_{\rm max} - r_{\rm min} \simeq \ln[\xi(\eta)/a]$, which allows one together with (7) and (8) to relate parameters A_x and η,

$$A_x = \frac{3\eta^2}{4\pi^4}. \tag{B13}$$

Note also that

$$r - r_{\rm min} \simeq \ln[L/a], \quad r_{\rm max} - r \simeq \ln[\xi(\eta)/L]. \tag{B14}$$

Let us choose now the running point $\{g_z(r), g_x(r)\}$ in the upper RG trajectory in such a way that

$$g_z(r) < 0, \quad g_x(r) > 0, \tag{B15}$$

$$\sqrt{A_x} \ll g_x(r) \ll 1. \tag{B16}$$

Under these conditions, the RG trajectory approaches its asymptote $g_x = -g_z$ in the second quadrant, the argument of the tangent in Eq. (B12) lies slightly below its pole at $\pi/2$, and one finds from (B12)–(B14)

$$g_z(r) \cong -\frac{\sqrt{3}}{4\pi(r_{\rm max} - r)} \cong -\frac{\sqrt{3}}{4\pi\,\ln[\xi(\eta)/L]}, \tag{B17}$$

$$g_x(r) \cong -g_z(r) \cong \frac{\sqrt{3}}{4\pi\,\ln[\xi(\eta)/L]}, \tag{B18}$$

where $\xi(\eta)/L \gg 1$. For such a choice of the scaling variables g_x, g_z, we can approximately represent the effective Hamiltonian (B1) in the form

$$H = H_{\rm WZW} - g_x\int_0^{L_x} dx\, \Phi(x), \tag{B19}$$

where $g_x > 0$, and $\Phi(x)$ is the following marginally relevant operator

$$\Phi(x) = \frac{8\pi^2}{\sqrt{3}}[J^x(x)\bar{J}^x(x) + J^y(x)\bar{J}^y(x) - J^z(x)\bar{J}^z(x)]. \tag{B20}$$

Its two- and three-point correlation functions in the plane can be easily found from (B2),

$$\langle\Phi(\mathbf{r}_1)\Phi(\mathbf{r}_2)\rangle = \frac{1}{3|\mathbf{r}_{1,2}|^4}, \tag{B21}$$

$$\langle\Phi(\mathbf{r}_1)\Phi(\mathbf{r}_2)\Phi(\mathbf{r}_3)\rangle = -\frac{b_\Phi}{|\mathbf{r}_{1,2}|^2|\mathbf{r}_{1,3}|^2|\mathbf{r}_{2,3}|^2}, \tag{B22}$$

where $b_\Phi = -4/\sqrt{3}$. Note that Eq. (B18) can be rewritten as

$$g_x(r) \cong \frac{1}{\pi\, b_\Phi \ln[L/\xi(\eta)]}. \tag{B23}$$

The ground-state energy of the Hamiltonian (B19) can be calculated perturbatively in the small parameter g_x. This calculation literally reproduces the derivation of Eq. (B11) outlined above, in which one should replace $\varphi(x) \to \Phi(x)$, $g \to g_x$, and $b \to b_\Phi$. Accordingly, one obtains instead of (B11)

$$E_0^{(af)}(L_x, g_x) = e_0\, L_x - \frac{\pi}{6L_x} - \frac{\pi^4}{3L_x}\, b_\Phi\, g_x^3 + \cdots. \tag{B24}$$

After further replacement of the scaling variable g_x by its RG improved value (B23) and setting $L \sim L_x$, one arrives at the final result (58).

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