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 characterises 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.

**Introduction and main results** – 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

\[
H = \frac{J}{2} \sum_{j=1}^{N_x} (\sigma_j^x \sigma_{j+1}^x + \sigma_j^y \sigma_{j+1}^y + \Delta \sigma_j^x \sigma_{j+1}^x). \tag{1}
\]

Here the index \( j \) enumerates the spin-chain sites, \( \sigma_j^a \) are the Pauli matrices, \( a = x, y, z, J > 0 \) is the antiferromagnetic coupling constant, \( \Delta \) is the anisotropy parameter. The number of sites will be chosen even, \( N_x = 2M \), and the periodic boundary conditions will be implied, \( \sigma_{j+N_x} \approx \sigma_j^z \). 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 \( U(y) = \exp(-yH) \).

The ground state energy \( E_{N_x}(\eta, a) \) of the model [4] can be represented as,

\[
E_{N_x}(\eta, a) = N_x E_0(\eta, a) + E_C(N_x, \eta, a), \tag{3}
\]

where \( N_x E_0(\eta, a) \) is the bulk term calculated and studied for all \( \Delta \) by C. N. Yang and C. P. Yang [4, 5] 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 \( \eta \) and \( a \). This term describing the finite-size correction to the bulk ground-state energy has been extensively studied by many authors [6–11] by means the technique utilising a certain nonlinear integral equation (NLIE) of the convolution type. Most attention in these studies has been concentrated on the \( |\Delta| \leq 1 \) gapless Luttinger liquid phase. For the massive antiferromagnetic phase that takes place at \( \Delta > 1 \), the NLIE was derived by de Vega and Woynarowich [10], and further studied by Dugave et al. [11]. We modify this integral equation and proceed in it to the scaling limit in the massive antiferromagnetic phase in order to describe the scaling behaviour of the Casimir energy \( E_C(N_x, \eta, a) \).

The scaling limit is understood in the usual way,

\[
a \to 0, \quad \eta \to +0, \quad N_x \to \infty, \quad \xi(\eta, a) = \text{Const}, \quad L_x \equiv aN_x = \text{Const}. \tag{4}
\]

Here \( \xi(\eta, a) \) is the correlation length, which behaves [11] at small \( \eta > 0 \) as,

\[
\xi(\eta, a) = [2m(\eta, a)]^{-1} \left[ 1 + O(\exp[-\pi^2/\eta]) \right], \quad \tag{5}
\]

and \( m(\eta, a) \) denotes the mass of the elementary kink excitation [12],

\[
m(\eta, a) = \frac{4 \exp[-\pi^2/(2\eta)]}{a} \tag{6}
\]

at \( \eta \to +0 \).

It follows from the dimension arguments [13], that the Casimir energy takes the scaling form in the limit [4],

\[
E_C(N_x, \eta, a) \approx \frac{Y(u)}{L_x}, \tag{7}
\]

where

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

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 [4]. The plot of the resulting Casimir scaling function is shown in Figure 1.
The scaling limit [4] of model [1] can be described by the Euclidean quantum field theory (EQFT) that 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 low 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 \( (x,y) \)-plane. This allows one [13] to relate the ground state energy [9], [7] of the EQFT with the free energy of the chain having infinite length \( L_y \to \infty \) at a nonzero temperature \( T = 1/L_z \). As the result, one arrives to the following representation for the free energy per the chain site \( f(J, \eta, T) \) in the scaling regime [4],

\[
f(J, \eta, T) = \mathcal{E}_0(J, \eta) + \frac{T^2}{\pi J} Y(u),
\]

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

\[
m(J, \eta) = 4\pi J \exp\left(\frac{\pi^2}{2\eta}\right)
\]

is the kink mass. Note, that we have changed notations in equations [9], [10] using the coupling constant \( J \) instead of the lattice spacing \( a = (\pi J)^{-1} \) as the argument of the functions \( f, \mathcal{E}_0, m \). The free energy reduces to the form [9] in the scaling regime, which is realised at \( aT \ll 1 \) and \( a \eta \ll 1 \). In terms of the original parameters of the XXZ chain Hamiltonian, these two strong inequalities read,

\[
T \ll \pi J, \quad 4 \exp\left(-\frac{\pi^2}{2\eta}\right) \ll 1.
\]

Accordingly, the specific heat per the chain site \( c(J, \eta, T) \) scales under conditions [11] to the form

\[
c(J, \eta, T) = \frac{T}{\pi J} X[T/m(J, \eta)],
\]

where

\[
X(t) = \left[-2Y(u) + 2uY'(u) - u^2Y''(u)\right]_{u=1/t}.
\]

The plot of the universal specific heat scaling function \( X(t) \) determined from equation [13] is shown in Figure 2.
The logarithmic derivative in $\lambda$ of equation (15) reads
\[
\phi'(\lambda) = \frac{p'_0(\lambda)}{2\pi} - \frac{1}{N_x} \sum_{l=1}^{M} \mathcal{K}(\lambda - \lambda_l),
\tag{22}
\]
where
\[
p'_0(\lambda) = \cot(\lambda - i\pi) - \cot(\lambda + i\pi),
\tag{23}
\]
\[
\mathcal{K}(\lambda) = \frac{\cot(\lambda - i\pi) - \cot(\lambda + i\pi)}{2\pi i}.
\tag{24}
\]

**Nonlinear integral equation.** Assuming that the counting function $\phi(\lambda)$ corresponding to the ground state strictly increases at real $\lambda$, and taking into account (20), (21), one concludes, that equation (14) 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 the Cauchy’s integral formula to the sums in the right-hand sides of (22) and (17) with subsequent integration by parts leads to the following integral representations of these equations (11),

\[
\phi'(\lambda) = \frac{p'_0(\lambda)}{2\pi} - \int_{-\pi}^{0} d\mu \mathcal{K}(\lambda - \mu)\phi'(\mu) + \frac{1}{\pi N_x} \int_{-\pi}^{0} d\mu \mathcal{K}(\lambda - \mu) \text{Im} \partial_\mu \log[1 + f(\mu + i0)],
\tag{25}
\]

\[
E_{N_x} = N_x \int_{-\pi}^{0} d\lambda \varepsilon_0(\lambda)\phi'(\lambda) - \frac{1}{\pi} \int_{-\pi}^{0} d\lambda \varepsilon_0(\lambda) \text{Im} \partial_\lambda \log[1 + f(\lambda + i0)].
\tag{26}
\]

Let us define the linear integral operator $K$ that acts on a $\pi$-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 the both sides of equation (25), and subsequent integration in $\lambda$, one modifies it to the form

\[
-\int_{-\pi}^{0} d\mu \mathcal{Q}(\lambda - \mu|\eta) \text{Im} \log[1 + f(\mu + i0|\eta, N_x)],
\tag{27}
\]

where

\[
\mathcal{Q}(\lambda|\eta) \equiv (1 + K)^{-1}[\mathcal{K}](\lambda) = \sum_{n=-\infty}^{\infty} \frac{e^{2i\eta\lambda}}{\pi(1 + e^{-2|\eta|n})},
\tag{28}
\]

\[
\phi'_0(\lambda|\eta) \equiv \frac{1}{2\pi} (1 + K)^{-1}[p'_0](\lambda) = \sum_{n=-\infty}^{\infty} \frac{e^{2i\lambda}}{2\pi \cosh(\eta n)},
\tag{29}
\]

\[
\log f(-\pi/2|\eta, N_x) = 0, \quad \phi_0(-\pi/2|\eta) = 0.
\tag{30}
\]

Similarly, the ground state energy (26) can be represented in the form (3), where

\[
E_0(\eta, a) = \int_{-\pi}^{0} d\lambda \varepsilon_0(\lambda)\phi'_0(\lambda),
\tag{31}
\]

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

\[
E_C(N_x, \eta, a) = -J \sinh \eta \int_{-\pi}^{0} d\lambda \phi'_0(\lambda) \text{Im} \log[1 + f(\lambda)].
\tag{32}
\]

**Scaling limit.** In the scaling limit (4), the solution $f(\lambda|\eta, N_x)$ of equation (27) approaches very fast to its bulk limit $\exp[2\pi i N_x \phi_0(\lambda|\eta)]$ everywhere in the real $\lambda$-axis, apart of the small vicinities of the points $\lambda^{(n)} = -\pi/2 + \pi n$. To describe the scaling limit of equation (27) near one of such points $\lambda^{(0)} = -\pi/2$, let us make in it the linear change of the rapidity variables $\lambda, \mu$,

\[
\lambda = -\frac{\pi}{2} - \frac{\eta}{\pi} \alpha, \quad \mu = -\frac{\pi}{2} - \frac{\eta}{\pi} \alpha',
\tag{33}
\]

where $\alpha, \alpha'$ are the rescaled rapidities.

The function $f(\lambda|\eta, N)$ reduces in the vicinity of the point $\lambda^{(0)}$ in the scaling limit (4) to the form

\[
f(\lambda|\eta, N)_{\lambda=-\pi/2-\eta/\pi} = \frac{1}{f(\alpha|u)} + \text{corrections to scaling}.
\tag{34}
\]

The function $f(\alpha|u)$ must satisfy the nonlinear integral equation

\[
-\int_{-\infty}^{\infty} d\alpha' \mathcal{Q}(\alpha - \alpha') \text{Im} \log[1 + f(\alpha' + i0|u)],
\tag{35}
\]

with real $\alpha, \alpha' \in \mathbb{R}$, and the integral kernel

\[
\mathcal{Q}(\lambda) = \frac{1}{\pi} \int_{0}^{\infty} dy \cos(2\gamma \lambda) \frac{e^{-\pi y}}{\cosh(\pi y)} = \frac{1}{2\pi i} \partial_\lambda \log \left[ \frac{\Gamma \left( 1 + \frac{\lambda}{2\pi} \right) \Gamma \left( 1 - \frac{\lambda}{2\pi} \right)}{\Gamma \left( 1 - \frac{\lambda}{2\pi} \right) \Gamma \left( 1 + \frac{\lambda}{2\pi} \right)} \right].
\tag{36}
\]

The scaling limit of the Casimir energy (32) reads

\[
E_C(N_x, \eta, a) = -\frac{m}{\pi} \int_{-\infty}^{\infty} da' \left( \sinh \alpha \cdot \text{Im} \log[1 + f(\alpha + i0|u)] \right).
\tag{37}
\]

Equations (35), (37) coincide with the $\gamma \to +0$ limit of equations (5.9), (5.8) obtained by Destri and de Vega [9] for the massive Thirring (sine-Gordon) model. However, concentrating in their article on the massive Thirring model and on the gapless case of the XXZ spin chain, the authors of [9] did not apply their results to describe the massive scaling regime of the XXZ chain, which we
the scaling function

In turn, the Casimir energy (37) takes the form (7), with another. They must satisfy the system of two nonlinear\[β \bar{β} + i \pi/2 | u \rangle, \varepsilon(\bar{β}| u \rangle = \log \varepsilon(\bar{β} - i \pi/2 | u \rangle).\] (38)

At real β, these functions are complex conjugate to one another. They must satisfy the system of two nonlinear integral Thermodynamic Bethe-Ansatz Equations [13], which follow from [35],

\[
\varepsilon(β| u \rangle = u \cosh β - \int_{−∞}^{∞} dβ' \mathcal{Q}(β - β') \log[1 + e^{-ε(β'| u \rangle}]
\]

\[
+ \int_{−∞}^{∞} dβ' \mathcal{Q}(β - β' + i \pi - i0) \log[1 + e^{-ε(β'| u \rangle}], \quad (39)
\]

\[
\varepsilon(\bar{β}| u \rangle = u \cosh β - \int_{−∞}^{∞} dβ' \mathcal{Q}(β - β') \log[1 + e^{-ε(β'| u \rangle}]
\]

\[
+ \int_{−∞}^{∞} dβ' \mathcal{Q}(β - β' - i \pi + i0) \log[1 + e^{-ε(β'| u \rangle}]. \quad (40)
\]

In turn, the Casimir energy [37] takes the form [7], with the scaling function

\[
Y(u) = \frac{−u}{π} \int_{−∞}^{∞} dβ \cosh β \Re \log[1 + e^{-ε(β| u \rangle}]. \quad (41)
\]

The nonlinear integral equations [39], [40] with a different first term in the right-hand sides, however, were studied by Klümper [14], who used them to calculate the temperature dependence of the specific heat and magnetic susceptibility in the isotropic antiferromagnetic XXX spin-1/2 chain.

The system of nonlinear integral equations [39], [40] 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 Figure [1].

The scaling function Y(u) exponentially decays at large u → +∞,

\[
Y(u) = \frac{-2u}{π} K_1(u) + O(e^{-2u}) = \frac{-2u}{π} e^{-u} [1 + O(1/u)], \quad (42)
\]

where K_1(u) is the MacDonald function. As in the case of the massive Thirring model at a finite γ > 0 (see equations (6.9)-(6.11) in [9]), the large-u asymptotics [42] can be easily obtained by replacing the function ε(β| u \rangle in (41) by its the ”zeroes iteration” u cosh β and then expanding the resulting logarithm in the integrand to the first order, log[1 + exp(−u cosh β)] → exp(−u cosh β).

At the isotropic point u = 0, the scaling function takes the value Y(0) = −π/6 in agreement with the CFT prediction [9, 13] for the Gaussian field theory with the central charge c = 1. The perturbative calculation of further terms in the small-u expansion of Y(u) is rather difficult, and will be published elsewhere. Here we present only the final result,

\[
Y(u) = −\frac{π}{6} + \frac{π}{16 \log^3(2/ u)} + \frac{3π \log[2 \log(2/ u)]}{32 \log^2(2/ u)} + \frac{a_4}{\log^2(2/ u)} + \ldots,
\]

where a_4 ≈ −0.193.

The asymptotic high- and low-temperature behaviour of the free energy ∆f(T) = f(T) − f(0) per site can be read from [9, 42],

\[
\Delta f(T) = −\frac{T^2}{6J} \left[1 - \frac{3}{8 \log(2T/m)} - \frac{9 \log(2 \log(2T/m))}{16 \log^2(2T/m)} - \frac{6 a_4}{\pi \log^2(2T/m)} + \ldots, \right.
\]

at m ≪ T ≪ J, and

\[
\Delta f(T) = −\frac{1}{π J} \sqrt{\frac{2m}{π}} T^{3/2} e^{-m/T} [1 + O(T/m)], \quad (46)
\]

to at m ≪ J, where m is given by [14].

For the total free energy F(T, L_y) = N_y ∆f(T) of the spin chain of the length L_y → ∞, which has N_y = πJL_y sites, the low-temperature asymptotics following from [46] reads,

\[
F(T, L_y) = −2L_y \sqrt{\frac{m}{2π}} T^{3/2} e^{-m/T} [1 + O(T/m)]. \quad (47)
\]

This result has a transparent physical interpretation. One can easily see, that the right-hand side of equation [47] is just the grand canonical potential Ω(T, L_y) of the classical ideal gas of two kinds of non-relativistic particles (kinks with spins oriented up and down) having the same mass m and the chemical potential µ = m, which move in one dimension in the line of the length L_y.

Conclusions – Considering the Heisenberg XXZ spin-chain ring in the gapped antiferromagnetic phase Δ > 1 close to the quantum phase transition point Δ = 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 the 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 \([9, 14–18]\) of the specific heat in the XXZ spin chain, our results are universal, since we have limited analysis to the scaling regime. It would be interesting to experimentally observe in quasi-one-dimensional antiferromagnetic compounds the universal specific-heat scaling temperature dependence \([12]\). It would be also interesting and important for the experimental applications to study corrections in small \( \eta \) to the scaling dependences \([7\) and \(12]\).

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