Low energy effective Hamiltonian for the XXZ spin chain

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Abstract
Coupling constants for the most relevant terms in the low energy effective Hamiltonian of the XXZ spin chain are derived. Using this result we study the low energy (low temperature, weak magnetic field) thermodynamics, finite size effects and subleading long distance asymptotics of correlation functions.
1. Introduction

An effective Hamiltonian approach is an important tool for a qualitative understanding of low energy effects in Quantum Field Theory and Statistical Mechanics \[1\]. The quantitative description involves some problems. First, it is not generally clear how to derive coupling constants of an effective Hamiltonian in terms of parameters of a microscopic Hamiltonian. (The latter is in common use for the study of a high energy behavior.) When it is not possible to relate the large scale physics to the microscopic parameters directly, one uses instead the coupling constants of the effective Hamiltonian as phenomenological parameters of the model under consideration. A related problem concerns a control over an accuracy of perturbative expansions. An effective Hamiltonian density is a series which involves an infinite set of local irrelevant fields and the corresponding perturbation theory is unrenormalizable. Thus, it is impossible to make a uniform (on the energy scale) estimate of an accuracy in a given order of the perturbation theory generated by the low energy effective Hamiltonian.

Two dimensional exactly solvable models provide unique opportunity to refine our understanding of the effective Hamiltonian approach. Recently a significant progress was made in this field of research. In the works \[2\], \[3\], \[4\] the method have been developed, which enables one to find an exact relation between short and long distance asymptotic behaviors of physically interesting quantities. As a result the coupling constants of the effective Hamiltonians are expressed explicitly in terms of the microscopic parameters for many interesting integrable models.

This work constitutes an attempt to apply the effective Hamiltonian approach to a quantitative study of low-energy effects in the XXZ Heisenberg spin chain \[5\], \[6\]. The model was chosen for several reasons. First of all, the method of the papers \[2\], \[3\], \[4\] is suitable for calculation of the XXZ effective Hamiltonian. Next, due to more than sixty years of study, a huge amount of numerical data is available. Finally, the XXZ Heisenberg spin chain still comes to the attention of Condensed Matter physicists \[7\], \[8\].

In Section 2, we fix our notations and present the coupling constants of the most relevant terms in the effective XXZ Hamiltonian. In Sections 3 and 4, relying on the effective Hamiltonian, we develop the perturbation theory to study the low energy thermodynamics and finite size corrections to vacuum energies. In Section 5, we discuss the subleading long distance asymptotics of the two-point correlation function of the XXZ spin chain.
2. Low energy effective Hamiltonian

In this work we consider the XXZ spin chain \([5], [6]\),

\[
H_{XXZ} = -\frac{J}{2} \sum_{k=1}^{N} \left( \sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta (\sigma_k^z \sigma_{k+1}^z - 1) \right),
\]

(2.1)

\(\sigma_k^x, \sigma_k^y\) and \(\sigma_k^z\) are the Pauli matrices associated with the site \(k\) of the chain. We assume that \(N\) is an even integer, and supplement (2.1) with the boundary conditions

\[
\sigma_1^\pm = e^{\pm 2\pi i \theta} \sigma_{N+1}^\pm, \\
\sigma_1^z = \sigma_{N+1}^z,
\]

(2.2)

with the real parameter \(0 < \theta < 1\). Let the parameter \(J\) be positive and

\[-1 < \Delta < 1.\]

(2.3)

The regime (2.3) is usually referred to as the “disorder regime”. Notice that the unitary transformation,

\[
U^+ \sigma_k^x U = (-1)^k \sigma_k^x, \quad U^+ \sigma_k^y U = (-1)^k \sigma_k^y, \quad U^+ \sigma_k^z U = \sigma_k^z,
\]

(2.4)

can be equivalently described by the substitution

\[
J \rightarrow -J, \quad \Delta \rightarrow -\Delta.
\]

(2.5)

In particular, the model (2.1) with \(\Delta = -1\) is unitary equivalent to the \(SU(2)\)-invariant antiferromagnetic XXX spin chain. It will be convenient for us to parameterize the constants in the following manner

\[
\Delta = \cos(\pi \beta^2), \\
J = \frac{1 - \beta^2}{\sin(\pi \beta^2)} a^{-1},
\]

(2.6)

with \(0 < \beta^2 \leq 1, \quad a > 0\).

In the thermodynamic limit

\[
N \rightarrow \infty, \quad a \rightarrow 0, \quad L = Na - \text{fixed} \quad (N - \text{even})
\]

(2.7)

the XXZ spin chain in the disorder regime (2.3) renormalizes to the continuous quantum field theory – the Gaussian model \([9], [10], [11]\),

\[
\lim_{a \rightarrow 0} \left( H_{XXZ} - a^{-1} L \mathcal{E}_0 \right) = H_{Gauss}.
\]

(2.8)
Here \( E_0 = -\frac{2}{\pi a} (1 - \beta^2) \int_0^\infty dt \frac{\sinh(\beta^2 t)}{\sinh(t) \cosh((1 - \beta^2)t)} \). \hfill (2.9)

To define the Hamiltonian of the Gaussian model let us introduce the set of operators satisfying the commutation relations

\[
[a_n, a_m] = 2n \delta_{n+m,0}, \quad [Q, P] = i, \\
[\bar{a}_n, \bar{a}_m] = 2n \delta_{n+m,0}, \quad [\bar{Q}, \bar{P}] = i.
\] \hfill (2.10)

The Heisenberg algebra admits representation in the Fock spaces, i.e. the spaces generated by the action of \( a_n, \bar{a}_k \) with \( n, k < 0 \) on the “vacuum states” \(|p, \bar{p}\rangle\) which obey the equations

\[
a_n|p, \bar{p}\rangle = \bar{a}_n|p, \bar{p}\rangle = 0 \quad \text{for} \quad n > 0, \\
P|p, \bar{p}\rangle = p|p, \bar{p}\rangle, \quad \bar{P}|p, \bar{p}\rangle = \bar{p}|p, \bar{p}\rangle.
\] \hfill (2.11)

Then

\[
H_{Gauss} = \frac{2\pi}{L} \left\{ P^2 + \bar{P}^2 - \frac{1}{12} + \frac{1}{2} \sum_{n>0} (a_{-n}a_n + \bar{a}_{-n}\bar{a}_n) \right\}.
\] \hfill (2.12)

This operator acts in the Hilbert space

\[
\mathcal{H} = \oplus_{p, \bar{p}} \mathcal{F}_{p, \bar{p}},
\] \hfill (2.13)

with

\[
p - \bar{p} = s \beta, \\
p + \bar{p} = (\theta + m) \beta^{-1},
\] \hfill (2.14)

here \( m \) and \( s \) are arbitrary integers. It is convenient to introduce the fields

\[
\phi(x) = Q + \frac{4\pi x}{L} P - \frac{1}{2} \sum_{n \neq 0} \frac{a_n}{n} e^{\frac{2\pi i}{L} x n}, \\
\bar{\phi}(x) = \bar{Q} - \frac{4\pi x}{L} \bar{P} - \frac{1}{2} \sum_{n \neq 0} \frac{\bar{a}_n}{n} e^{-\frac{2\pi i}{L} x n}.
\] \hfill (2.15)

The Hamiltonian (2.12) can be written in the form

\[
H_{Gauss} = \int_0^L \frac{dx}{2\pi} \left\{ T + \bar{T} \right\},
\] \hfill (2.16)

where

\[
T(x) = \frac{1}{4} : (\partial_x \phi)^2 : -\frac{\pi^2}{6L^2}, \\
\bar{T}(x) = \frac{1}{4} : (\partial_x \bar{\phi})^2 : -\frac{\pi^2}{6L^2}.
\] \hfill (2.17)
To describe the bosonization of the matrix $\sigma^a_k$, we define the fields

$$\varphi(x) = \phi - \bar{\phi}$$
$$\bar{\varphi}(x) = \phi + \bar{\phi} .$$

(2.18)

In the leading order in $a$ \[9\],

$$\sigma^\pm_k \simeq a^{\beta^2} \frac{\sqrt{F}}{2} e^{\pm i \beta \varphi}(x) ,$$
$$\sigma^z_k \simeq \frac{a}{2\pi \beta} \partial_x \bar{\varphi}(x) ,$$

(2.19)

with $x = ka$. To give a precise meaning to the constant $F$ one needs to specify the normalization of the exponential fields. We will normalize exponential operators in accordance with the short distance expansion

$$e^{i\alpha \varphi(x)} e^{-i\alpha \varphi(x')} \rightarrow |x - x'|^{-4\alpha^2} \quad \text{as} \quad |x - x'| \rightarrow 0 ,$$

(2.20)

for an arbitrary $\alpha$. In this normalization the constant $F = F(\beta^2)$ was found in Ref. \[13\]

$$F = \frac{1}{2} \frac{1 - \beta^2}{2(1 - \beta^2)^2} \left[ \frac{\Gamma\left(\frac{\beta^2}{1 - 2\beta^2}\right)}{2\sqrt{\pi} \Gamma\left(\frac{1}{2 - 2\beta^2}\right)} \right]^{\beta^2} \times$$

$$\exp\left\{ - \int_0^\infty \frac{dt}{t} \left( \frac{\sinh(t)}{\sinh(t) \cosh\left(1 - \beta^2\right) t} - \beta^2 e^{-2t} \right) \right\} .$$

(2.21)

The Hamiltonians (2.1) and (2.16) coincide in the lowest nontrivial order of the lattice parameter $a$ (2.8). In the next orders irrelevant fields contribute to the density of $H_{XXZ}$. These irrelevant fields should be local with respect to the spin fields (2.19) and commute with the operator

$$S^z = \frac{1}{2} \sum_{s=1}^N \sigma^z_s = (P - \bar{P}) \beta^{-1} .$$

(2.22)

A simple analysis shows that the most important corrections have the form \[11\]

$$H_{XXZ} = a^{-1} L \mathcal{E}_0 + \int_0^L \frac{dx}{2\pi} \left\{ T + \bar{T} - a^2 \left( \lambda_+ T \bar{T} + \lambda_- (T^2 + \bar{T}^2) \right) + \right.$$

$$\left. \frac{a^{\beta^2 - 2}}{2\pi} \lambda \cos\left(\bar{\varphi}/\beta\right) + \ldots \right\} .$$

(2.23)

\footnote{In the case of $\sigma^\pm_k$, Eq.(2.19) gives the leading order in $a$ for $0 < \beta^2 < \frac{1}{2}$.}
Here, the field $T^2$ ($\bar{T}^2$) is defined as a regular part of the operator product expansion of two operators $T$ ($\bar{T}$). The dots in (2.23) and below mean a contribution of higher dimensional local counterterms. In the Appendix we describe the calculation of the coupling constants in the low energy effective Hamiltonian (2.23),

$$
\lambda = \frac{4 \Gamma(\beta^{-2})}{\Gamma(1 - \beta^{-2})} \left[ \frac{\Gamma(1 + \frac{\beta^2}{2-2\beta^2})}{2\sqrt{\pi} \Gamma(1 + \frac{1}{2-2\beta^2})} \right]^{\frac{1}{\beta^2}-2},$
$$
\lambda_+ = \frac{1}{2\pi} \tan \left( \frac{\pi}{2 - 2\beta^2} \right),
$$
\lambda_- = \frac{\beta^2}{12\pi} \frac{\Gamma \left( \frac{3}{2-2\beta^2} \right) \Gamma^3 \left( \frac{\beta^2}{2-2\beta^2} \right)}{\Gamma \left( \frac{3\beta^2}{2-2\beta^2} \right) \Gamma^3 \left( \frac{1}{2-2\beta^2} \right)}.
$$

For the XXX spin chain ($\Delta = -1$),

$$
\lambda_+ = 0, \\
\lambda_- = \frac{\sqrt{3}}{4\pi}.
$$

We discuss how to treat “$\lambda$-term” from (2.23) at the limit $\beta^2 \to 1$ in the next section.

It is important to note that except for the “$\lambda_-$-term”, the Hamiltonian (2.23) coincides with low energy effective Hamiltonian for the sausage model with the value of the $\theta$-angle equals to $\pi$ [3]. The fields $T^2$ and $\bar{T}^2$ have Lorenz spins 4 and $-4$ respectively. Therefore, the “$\lambda_-$-term” destroys the rotational symmetry of the Gaussian model in the infinite volume and appears because of the lattice nature of the Hamiltonian (2.1).

3. Temperature and magnetic field corrections to specific free energy

The effective Hamiltonian (2.23) can be applied to the study of infrared corrections of physically interesting quantities in the XXZ spin chain. Here we deal with the low temperature thermodynamics. Let us consider the model (2.1) at the low temperature $T$ ($T/J \ll 1$) and in the weak magnetic field $h$ ($|h/J| \ll 1$). With the result (2.23) one can use the notation $\lambda$ and $M$ which are related with the parameters $\beta^2$ and $a$ as following,

$$
\lambda = 1 - \beta^2, \quad M = 4a^{-1}.
$$

\[2\] V.A. Fateev et al. use the notation $\lambda$ and $M$ which are related with the parameters $\beta^2$ and $a$ as following,
can develop the perturbation expansion in the small parameter $a$ of the specific free energy $f_{XXZ}$,

\[ e^{-\frac{\lambda}{T}} f_{XXZ} = \text{Tr}_{\mathcal{H}} \left[ e^{-\frac{1}{T} H_{XXZ} + \frac{\lambda}{2T} S^z} \right]. \quad (3.1) \]

Notice that “$\lambda_{\pm}$-terms” in (2.23) contribute to the first order of the perturbation series and lead to $a^3$-corrections. The term with $\lambda$ does not have diagonal matrix elements and its contribution appears only in the second order. This implies a correction which is proportional to $a^3$. Therefore the leading corrections to the specific free energy differ significantly in the domains $0 < \beta^2 < \frac{2}{3}$ and $\frac{2}{3} < \beta^2 < 1$ and have the form

\[ f_{XXZ} = \mathcal{E}_0 + a f_{\text{Gauss}} - \frac{a^3}{2\pi} \left( \lambda_+ \langle \langle T \rangle \rangle^2 + 2\lambda_- \langle \langle T^2 \rangle \rangle \right) + \ldots \quad \text{for} \quad 0 < \beta^2 < \frac{2}{3}, \]

\[ f_{XXZ} = \mathcal{E}_0 + a f_{\text{Gauss}} - \frac{\lambda^2 a^3}{16\pi^2} \int_0^L dx \int_0^{\frac{1}{T}} d\tau \langle \langle e^{i\tilde{\phi}/\beta} (x,\tau) e^{-i\tilde{\phi}/\beta} (0,0) \rangle \rangle + \ldots \quad \text{for} \quad \frac{2}{3} < \beta^2 < 1. \quad (3.2) \]

Here we use the notation

\[ e^{-\frac{\lambda}{T}} f_{\text{Gauss}} = \text{Tr}_{\mathcal{H}} \left[ e^{-\frac{1}{T} H_{\text{Gauss}} + \frac{\lambda}{2T} (P^z - \bar{P}^z)} \right], \]

\[ \langle \langle O \rangle \rangle = \text{Tr}_{\mathcal{H}} \left[ e^{-\frac{1}{T} H_{\text{Gauss}} + \frac{\lambda}{2T} (P^z - \bar{P}^z)} O \right]/\text{Tr}_{\mathcal{H}} \left[ e^{-\frac{1}{T} H_{\text{Gauss}} + \frac{\lambda}{2T} (P^z - \bar{P}^z)} \right], \]

and

\[ \tilde{\phi}(x,\tau) = \phi(x + iT) + \bar{\phi}(x - iT). \]

The calculation of (3.2) is straightforward. We will not discuss here the most general expressions but restrict our attention to the case $T \gg L^{-1}$. Under this condition the system develops an effective correlation length and all finite size effects are suppressed by the exponentially small factor $e^{-\pi LT}$. Omitting the finite size terms, one obtains

\[ f_{XXZ} = \mathcal{E}_0 + 4\pi a T^2 I_1 \left( \frac{i\hbar}{8\pi\beta T} \right) - (2\pi a)^3 T^4 \left\{ \lambda_+ I_1 \left( \frac{i\hbar}{8\pi\beta T} \right) + 2\lambda_- I_3 \left( \frac{i\hbar}{8\pi\beta T} \right) \right\} + \ldots. \quad (3.3) \]

for $0 < \beta^2 < \frac{2}{3}$. If $\frac{2}{3} < \beta^2 < 1$, the leading correction comes from the second order perturbation theory term

\[ f_{XXZ} = \mathcal{E}_0 + 4\pi a T^2 I_1 \left( \frac{i\hbar}{8\pi\beta T} \right) - 4a T^2 \beta^8 \sin^2 \left( \frac{2\pi}{\beta^2} \right) \left| \frac{\sqrt{\Gamma(1 + \frac{\beta^2}{2-2\beta^2})}}{\Gamma(1 + \frac{1}{2-2\beta^2})} \right| \frac{a}{\beta^4} \left| \tilde{H}_1 \left( \frac{i\hbar}{8\pi\beta T} \right) \right|^2 + \ldots. \quad (3.4) \]
The auxiliary functions in (3.3), (3.4) read explicitly
\[
I_1(p) = p^2 - \frac{1}{24},
I_3(p) = p^4 - \frac{p^2}{4} - \frac{4\beta^4 - 17\beta^2 + 4}{960\beta^2},
\]
\[
\tilde{H}_1(p) = \frac{\Gamma(-2)\Gamma(1-2\beta^2)}{\beta^4\Gamma(1-\beta^2)} \frac{\Gamma(\beta^2+2p\beta^{-1})}{\Gamma(1-\beta^2+2p\beta^{-1})},
\tag{3.5}
\]
and \(\lambda_\pm = \lambda_\pm(\beta^2)\) are given by (2.24). Notice that \(I_1(p), I_3(p)\) coincide with the vacuum eigenvalues of the first local integrals of motion in the quantum KdV theory [14]. At the same time \(\tilde{H}_1(p)\) is a vacuum eigenvalue of the first “dual unlocal” integral of motion [15].

If \(\beta^2 = \frac{2n}{1+2n}\) \((n = 1, 2, ...)\), the first order contribution of the “\(\lambda_+\)-term” interferes with the \(2n\) order of the perturbation expansion generated by the “\(\lambda\)-term”. The poles of the coupling constant \(\lambda_+ (2.24)\) at these points indicate this phenomena. The interference produces a logarithmic contribution. For example, at \(\beta^2 = \frac{2}{3}\) the specific free energy behaves as
\[
f_{XXZ} \bigg|_{\beta^2=\frac{2}{3}} = -\frac{2}{3\sqrt{3}a} - \frac{a}{96\pi} (16\pi^2 T^2 + 9h^2) \left\{ 1 + \frac{5}{6} a^2 T^2 + \frac{a^2}{192\pi^2} (16\pi^2 T^2 + 9h^2) \times \left[ \frac{11}{12} - \log(aT/12) - \Re \left( \psi\left(\frac{1}{2} + \frac{3ih}{8\pi T}\right) \right) \right] \right\} + ... ,
\tag{3.6}
\]
where \(\psi(t) = \partial_t \log(\Gamma(t))\).

If \(\beta^2 \approx 1\), Eq.(3.4) defines the leading asymptotic behavior in the very narrow domain of temperature and magnetic field,
\[
\log\left(\frac{1}{aT}\right), \quad \log\left(\frac{1}{ah}\right) \gg \frac{1}{1-\beta^2} .
\]
In the limit \(\beta^2 \to 1\) the domain of validity of (3.4) disappears completely. Hence the case of the XXX spin chain requires an additional analysis similar to the one of Refs. [3], [4].

Let us consider the Gaussian model with \(\beta^2 = 1\). The fields
\[
J_0 = \frac{1}{2} \partial_x \phi, \quad J_\pm = e^{\pm i\phi},
\]
\[
\bar{J}_0 = \frac{1}{2} \partial_x \bar{\phi}, \quad \bar{J}_\pm = e^{\mp i\bar{\phi}},
\tag{3.7}
\]
generate the right and left current algebras at the level \(k = 1\), and the Gaussian model coincides with the Wess-Zumino-Witten (WZW) model,
\[
H_{Gauss} \bigg|_{\beta^2=1} = H_{WZW} . \tag{3.8}
\]
In the vicinity of the point $\beta^2 = 1$ it is convenient to rewrite the effective XXZ Hamiltonian as the marginal current-current perturbation of the WZW Hamiltonian \[10\],

$$H_{XXZ} = a^{-1}L \mathcal{E}_0 + H_{WZW} + \int_0^L \frac{dx}{2\pi} \left\{ g_\parallel J_0 \bar{J}_0 + \frac{g_\perp}{2} (J_+ \bar{J}_- + J_- \bar{J}_+) + \ldots \right\}. \quad (3.9)$$

Here $g_\parallel \geq 0$ and $|g_\perp| \leq g_\parallel$ are small running coupling constants. The corresponding Renormalization Group (RG) equations are known exactly [4], [17]. Under a suitable diffeomorphism of $g_\parallel$ and $g_\perp$ (i.e. the renormalization scheme choice), one can set up

$$r \frac{dg_\parallel}{dr} = -\frac{2}{2-g_\parallel} g_\perp^2 - g_\parallel, \quad \frac{dg_\perp}{dr} = -\frac{2 g_\parallel g_\perp}{2-g_\parallel}. \quad (3.10)$$

Here $r$ is the RG length scale. These equations are solved as

$$g_\parallel = 2 (1 - \beta^2) \frac{1+q}{1-q}, \quad g_\perp = -4 (1 - \beta^2) \frac{q^2}{1-q}, \quad (3.11)$$

with

$$q (1-q)^{2\beta^2-2} = \left( \frac{r}{r_0} \right)^{4-\frac{1}{\beta^2}}, \quad (3.12)$$

while $r_0$ is a $r$-independent constant.

The correction to the specific free energy, descended from the “$\lambda$-term” of (2.23), admits a power series expansion,

$$f_{XXZ} = \mathcal{E}_0 - \frac{a\pi T^2}{6} \left\{ 1 + u_{10} g_\parallel + u_{20} g_\parallel^2 + u_{02} g_\perp^2 + O(g^3) \right\} - \frac{ah^2}{16\pi} \left\{ 1 + v_{10} g_\parallel + v_{20} g_\parallel^2 + v_{02} g_\perp^2 + O(g^3) \right\} + \ldots. \quad (3.13)$$

To find values of the first coefficients $u_{kj}, v_{kj}$ we should compare the expansion of (3.13) and (3.4) in power series of $1 - \beta^2$ for a fixed value of the parameter $q$. According to (3.12), the latter can be chosen as a solution of the algebraic equation

$$q (1-q)^{2\beta^2-2} = \left[ \frac{aT e^{-\frac{4}{\pi^2}} \Gamma(1 + \frac{\beta^2}{2 - 2\beta^2})}{\Gamma(1 + \frac{1}{2 - 2\beta^2})} \right]^\frac{1}{2\beta^2-4} \left| \frac{\Gamma(\beta^2 - 2 + \frac{ih}{4\pi \beta^2 T})}{\Gamma(2 - \beta^2 - \frac{ih}{4\pi \beta^2 T})} \right|^2. \quad (3.14)$$

A simple calculation leads to the result

$$f_{XXZ} = \mathcal{E}_0 - \frac{\pi aT^2}{6} \left\{ 1 + \frac{3}{8} g_\parallel g_\perp + O(g^4) \right\} - \frac{ah^2}{16\pi} \left\{ 1 + \frac{g_\parallel}{2} + \frac{g_\perp^2}{4} - \frac{g_\parallel g_\perp}{8} \right\} + \ldots. \quad (3.15)$$
Now we can take the limit $\beta^2 \to 1$,

$$g\parallel \to g, \quad g\perp \to -g,$$  \hspace{1cm} (3.16)

of Eqs. (3.11), (3.14), (3.15) and obtain the low temperature behavior of the specific free energy of the XXX spin chain,

$$f_{XXX} = -2J \log(2) - \frac{T^2}{6J} \left\{ 1 + \frac{3}{8} g^3 + O(g^4) \right\} - \frac{h^2}{16\pi^2 J} \left\{ 1 + \frac{g}{2} + \frac{3}{32} g^3 + O(g^4) \right\} - \frac{\sqrt{3}}{16\pi^3 J^3} \left\{ \frac{h^4}{64\pi^2} + \frac{h^2 T^2}{4} + \frac{3\pi^2 T^4}{5} + O(g) \right\} + \ldots .$$  \hspace{1cm} (3.17)

The function $g = g(T, h)$ in (3.17) solves the equation

$$g^{-1} + \frac{1}{2} \log(g) = -\Re \left( \psi(1 + \frac{i h}{4\pi T}) \right) + \log \left( \sqrt{2\pi e} \frac{1}{J/T} \right),$$  \hspace{1cm} (3.18)

with $\psi(t) = \partial_t \log(\Gamma(t))$. In the formulas (3.17), (3.18) we use the original parameter $J$ of the Hamiltonian (2.1) with $\Delta = 1$. We also include the correction arising from the “$\lambda_\perp$-term” (3.3). From (3.18) one has the formula for the magnetic susceptibility,

$$\chi = -4 \partial_h^2 f_{XXX} \big|_{h = 0},$$  \hspace{1cm} (3.19)

as a function of temperature,

$$\chi(T) = \frac{1}{2J\pi^2} \left\{ 1 + \frac{g}{2} + \frac{3 g^3}{32} + O(g^4) + \frac{\sqrt{3} T^2}{4\pi J^2} \left( 1 + O(g) \right) + \ldots \right\} .$$  \hspace{1cm} (3.20)

Now the running constant depends on temperature only, $g = g(T)$,

$$g^{-1} + \frac{1}{2} \log(g) = \log \left( \sqrt{2\pi e} \gamma \frac{1}{J/T} \right)$$

and $\gamma = 0.577216...$ is the Euler constant. The leading $T$-dependence (the first order in $g$) of $\chi(T)$ was obtained previously in [18]. In Fig. 1, (3.20) is compared against the result of numerical solution of the Thermodynamic Bethe Ansatz equations [18].
Fig. 1. Magnetic susceptibility of the XXX antiferromagnetic spin chain. The continuous line represents (3.20). The bullets were obtained by the numerical solution of the Thermodynamic Bethe Ansatz equations [18].

4. Finite size corrections to vacuum energies

In this Section we consider the XXZ spin chain at zero magnetic field and temperature. If $T = 0$, the function $f_{\text{XXZ}}$ (1.1) coincides with the specific ground state energy $E_{\text{XXZ}}^{(0)}/N$ and Eqs.(3.2) are useful to study finite size effects. In fact, the calculation can be easily generalized to obtain the finite size corrections to an arbitrary vacuum eigenvalue (not only ground state) $E_{\text{XXZ}}^{(s)}$ in the sector with a given value $s$ of the total spin $S^z$ (2.22). Let us parameterize $E_{\text{XXZ}}^{(s)}/N$ by the form,

$$E_{\text{XXZ}}^{(s)}/N = E_0 + \frac{2\pi}{aN^2} \delta(s, \theta, N), \quad (4.1)$$

Then,

$$\delta = \frac{s^2 \beta^2}{2} + \frac{\theta^2}{2 \beta^2} - \frac{1}{12} \delta \cos + \delta^T + \ldots \quad (4.2)$$

The function $\delta^T$ gives the first order contribution of the “$\lambda_\perp$-terms” in (2.23). It reads
\[ \delta^T = -\frac{4\pi^2}{N^2} \left\{ \lambda_+ I_1 \left( \frac{s\beta}{2} + \theta \right) I_1 \left( \frac{s\beta}{2} - \theta \right) + \lambda_- \left( I_3 \left( \frac{s\beta}{2} + \theta \right) + I_3 \left( \frac{s\beta}{2} - \theta \right) \right) \right\} . \tag{4.3} \]

The term \( \delta^\cos \) in (4.2) arises from the second order perturbation theory generated by the field \( \cos(\tilde{\varphi}/\beta) \),

\[ \delta^\cos = -\frac{2}{\pi} \beta^8 \sin \left( \frac{2\pi}{\beta^2} \right) \left[ \frac{\sqrt{\pi} \Gamma(1 + \frac{\beta^2}{2 - 2\beta^2})}{N \Gamma(1 + \frac{1}{2 - 2\beta^2})} \right] \frac{1}{\beta^4} \tilde{H}_1 \left( \frac{s\beta}{2} + \theta \right) \tilde{H}_1 \left( \frac{s\beta}{2} - \theta \right) . \tag{4.4} \]

The auxiliary functions in (4.3), (4.4) are given by (3.5). For \( \beta^2 \) sufficiently close to unity the finite size corrections require an additional RG consideration. In a similar way to (3.13), an appropriate RG analysis leads to the following expression for (4.2),

\[ \delta(s, \theta, N) = \delta^{RG} + \delta^T + \ldots . \tag{4.5} \]

The function \( \delta^{RG} \) is a RG improved contribution of the “\( \lambda \)-term”,

\[ \delta^{RG} = -\frac{1}{12} \left\{ 1 + \frac{3}{8} g^2 \right\} + \frac{s^2}{2} \left\{ 1 - \frac{g^2}{2} + \frac{1}{4} g^2 - \frac{7}{32} g^2 - \frac{27}{32} \right\} + \frac{|s|}{16} \left\{ 2g^2 - g^2 \right\} + \frac{\theta^2}{2} \left\{ 1 + \frac{g^2}{2} + \frac{g^2}{4} - \frac{g^2}{8} - \frac{9}{32} g^2 \right\} + O(g^4) , \tag{4.6} \]

where the running constants are given by (3.11) with

\[ q (1 - q)^{\beta - 2} = \left[ \frac{\sqrt{\pi} e^{-\frac{1}{2}} \Gamma(1 + \frac{\beta^2}{2 - 2\beta^2})}{N \Gamma(1 + \frac{1}{2 - 2\beta^2})} \right] \frac{1}{\beta^4} \times \frac{\Gamma(\beta^2 - s + \theta \beta - 2)}{\Gamma(\beta^2 - s - \theta \beta - 2)} \frac{\Gamma(2 - \beta^2 + s + \theta \beta - 2)}{\Gamma(2 - \beta^2 + s - \theta \beta - 2)} . \tag{4.7} \]

The function

\[ \delta(s, \theta, N) - \delta(0, 0, N) \]

was calculated in [11] by the numerical solution of the Algebraic Bethe Ansatz equations for \( \beta^2 = \frac{5}{6} \) and some vacuum energies. In Table 1 the numerical results are compared against the derived formula. The following comment is appropriate here. The function

\[ 3 \text{ In writing (4.2), we assume that } \beta^2 \neq \frac{2n}{2n+1}, \ n = 2, 3, \ldots \text{ (see comment to the equation (3.4)).} \]
as well as the right hand side of (4.7), has the pole at $s = 0$, $\theta = 1$. The reason of the singularity is rather simple; We have developed the perturbation theory starting with the Fock vacuum states $|p, \bar{p}\rangle$ (2.11), with
\[
p = \frac{\theta}{2\beta} + \frac{s}{2\beta}, \quad \bar{p} = \frac{\theta}{2\beta} - \frac{s}{2\beta}.
\]
But for $s = 0$ and $\theta$ sufficiently close to unity, the contribution of the vacuum state with $p = \bar{p} = \frac{\theta - 2}{2\beta}$ to the true ground state of the XXZ spin chain becomes significant. It seems reasonable that the disagreement between the numerical data and obtained asymptotics for the case $s = 0$, $\theta = \frac{1}{2}$ in Table 1 is due to this effect.

The finite size corrections for the XXX spin chain can be derived by taking the limit (3.16) of Eqs. (4.6), (4.3). In particular,
\[
\delta^T|_{\beta^2 = 1} = -\frac{\pi \sqrt{3}}{8N^2} \left\{ s^4 + \theta^4 + 6s^2\theta^2 - s^2 - \theta^2 + \frac{3}{20} \right\},
\]
\[
\delta^{RG}|_{\beta^2 = 1} = -\frac{1}{12} \left\{ 1 + \frac{3}{8} g^3 \right\} \frac{s^2}{2} \left\{ 1 - \frac{g}{2} + \frac{g^2}{4} - \frac{7}{32} g^3 \right\} + \frac{|s|}{16} \left\{ 2g^2 - g^3 \right\} + O(g^4),
\]
with
\[
g^{-1} + \frac{1}{2} \log(g) = \log \left( 2^{\frac{\pi}{2}} \pi^{-\frac{1}{4}} e^{-\frac{1}{4}N} \right) - \frac{1}{2} \left( \psi(1 + s + \theta) + \psi(1 + s - \theta) \right).
\]
The leading terms in (4.8) for $\theta = 0$, $s = 0, 1$ are in agreement with the results of the work [19].

|     | $s = 0, \theta = \frac{1}{2}$ | $s = 1, \theta = 0$ | $s = 1, \theta = \frac{1}{4}$ |
|-----|------------------------------|----------------------|-----------------------------|
| $N$ | \begin{tabular}{c|c|c|c|c|c} \hline & BA & RG & BA & RG & BA & RG \\ \hline 8   & 0.15519 & 0.15467 & 0.39793 & 0.395... & 0.43606 & 0.433... \\ 16  & 0.15217 & 0.15185 & 0.40594 & 0.40555 & 0.44606 & 0.44406 \\ 32  & 0.15104 & 0.15081 & 0.41063 & 0.41060 & 0.44897 & 0.44883 \\ 64  & 0.15055 & 0.15037 & 0.41327 & 0.41327 & 0.45128 & 0.45121 \\ 128 & 0.15030 & 0.15015 & 0.41474 & 0.41474 & 0.45254 & 0.45250 \\ 256 & 0.15017 & 0.15003 & 0.41557 & 0.41557 & 0.45324 & 0.45321 \\ \infty & 0.15000 & 0.41600 & & & 0.45416 \\ \hline \end{tabular} | \begin{tabular}{c|c|c|c|c|c} \hline & BA & RG & BA & RG & BA & RG \\ \hline 8   & 0.15519 & 0.15467 & 0.39793 & 0.395... & 0.43606 & 0.433... \\ 16  & 0.15217 & 0.15185 & 0.40594 & 0.40555 & 0.44606 & 0.44406 \\ 32  & 0.15104 & 0.15081 & 0.41063 & 0.41060 & 0.44897 & 0.44883 \\ 64  & 0.15055 & 0.15037 & 0.41327 & 0.41327 & 0.45128 & 0.45121 \\ 128 & 0.15030 & 0.15015 & 0.41474 & 0.41474 & 0.45254 & 0.45250 \\ 256 & 0.15017 & 0.15003 & 0.41557 & 0.41557 & 0.45324 & 0.45321 \\ \infty & 0.15000 & 0.41600 & & & 0.45416 \\ \hline \end{tabular} |

Table 1. The function $\delta(s, \theta, N) - \delta(0, 0, N)$ for $\beta^2 = \frac{5}{6}$. The “BA” columns were obtained by means of the numerical solution of the Algebraic Bethe Ansatz equations [11]. The “RG” columns follow from (4.3), (4.4), (4.3).
5. Subleading asymptotics of correlation functions

As well as the Hamiltonian density (2.23), the formulas (2.19) give only leading terms of the expansions in local quantum fields of the spin operators. The leading terms allow one to obtain the leading asymptotic behavior of correlation functions of the spin operators. Subleading asymptotics are the result of the two effects: next terms in the expansion (2.19) and XXZ corrections of the Gaussian ground state, which defined by the effective Hamiltonian (2.23). Therefore, to derive the subleading asymptotics of the correlation functions systematically, one needs to know next terms in the expansion (2.19). Unfortunately, this problem admits only a qualitative analysis at the moment. Nevertheless, some interesting quantitative predictions for the subleading asymptotics can be obtained based on the effective Hamiltonian (2.23) only. As an example we consider the equal time correlator

\[ W(n) = \frac{\langle \text{vac} | \sigma^x_{k} \sigma^x_{k+n} | \text{vac} \rangle}{\langle \text{vac} | \text{vac} \rangle}, \quad n = 1, 2, \ldots , \quad (5.1) \]

for the infinite spin chain \( (L = \infty) \). Simple arguments [16] show that the most important correction of the bosonization formula for \( \sigma^\pm_{k+n} \) has the form

\[ \sigma^\pm_{k+n} = a \frac{\beta^2}{2} \sqrt{\frac{F}{2}} e^{\pm i \frac{\beta^2}{2}}(x) \left( 1 \pm i (-1)^n a A \partial_x \varphi(x) + \ldots \right) \quad (x = na) . \quad (5.2) \]

The exact value of the coefficient \( A \) is not known nowadays. It is instructive to note that due to the sign factor \((-1)^n\) in (5.2) a linear contribution of the “A-term” in \( W(n) \) is canceled out exactly for odd integer \( n \) and the subleading asymptotic is determined by the effective Hamiltonian only. We conclude that for \( \frac{2}{3} < \beta^2 < 1 \),

\[ W(n) = F n^{-\beta^2} \left\{ 1 - C n^{4 - \frac{4}{\pi^2}} - 2 \beta A ((-1)^n + 1) n^{-1} + \ldots \right\} , \quad \text{as} \ n \to +\infty . \quad (5.3) \]

Here the constant \( F \) is given by (2.21), \( A = A(\beta) \) is not known, while the constant \( C = C(\beta^2) \) can be obtained by the second order perturbation theory based on the effective Hamiltonian (2.23). The calculation leads to the formula

\[ C = \frac{\Gamma^2(\beta^{-2})}{\Gamma^2(1 - \beta^{-2})} \left[ \frac{\Gamma(1 + \frac{\beta^2}{2 - 2\beta^2})}{2\sqrt{\pi} \Gamma(1 + \frac{1}{2 - 2\beta^2})} \right] \beta^4 \left( \frac{2 \pi^2}{\sin^2(2\pi \beta^{-2})} - \frac{\beta^4}{(1 - \beta^2)(2 - \beta^2)} - \psi'(\beta^{-2}) - \psi'(\frac{3}{2} - \beta^{-2}) \right) , \quad (5.4) \]
with $\psi'(t) = \partial_t^2 \log (\Gamma(t))$. Eq.(5.3) defines the subleading asymptotic behavior of the correlation function for

$$\log(n) \gg \frac{1}{1 - \beta^2}.$$ 

In order to study the limit $\beta^2 \to 1$, it is useful to rearrange the expansion of $W(n)$. To do it, let us introduce $g_\parallel$ and $g_\perp$ by Eqs.(3.11), while

$$q (1-q) \frac{\beta^2}{2} - 2 = \left[ \frac{e^{-\gamma-1} \Gamma \left( 1 + \frac{\beta^2}{2 - 2\beta^2} \right)}{2 \sqrt{\pi} n \Gamma \left( 1 + \frac{1}{2 \beta^2} \right)} \right] ^{\frac{4}{\beta^2} - 4},$$

(5.5)

and $\gamma$ is the Euler constant. Using (5.3), (5.4), one obtains

$$W(n) = \sqrt{\frac{2}{\pi^3}} \frac{Z(g_\parallel, g_\perp)}{n \sqrt{|g_\parallel|}} \left\{ 1 - \frac{g_\parallel^2}{8} - \frac{g_\perp^2}{16} - \frac{4 \zeta(3) + 3}{192} g_\parallel^3 + \frac{164 \zeta(3) - 67}{384} g_\parallel^2 g_\perp^2 + O(g^4) - \frac{A}{2n} ((-1)^n + 1 + O(g)) + O(n^{-2}) \right\},$$

(5.6)

where $A = 4\beta A \big|_{\beta^2 = 1}$ and $\zeta(s)$ is the Riemann zeta function. The non-perturbative function $Z$ in (5.6) reads

$$Z(g_\parallel, g_\perp) = \left[ \frac{|g_\perp|}{2 e^{\frac{\pi}{\beta^2}} g_\parallel} \right] \sqrt{g_\parallel^2 - g_\perp^2} / 4.$$ 

We can derive the asymptotic of the correlation function of the XXX spin chain by taking the limit $g_\parallel \to g$, $g_\perp \to -g$. Finally one has

$$W(n) \big|_{\beta^2 = 1} = \sqrt{\frac{2}{\pi^3}} \frac{1}{n \sqrt{g}} \left\{ 1 - \frac{3}{16} g^2 + \frac{156 \zeta(3)}{384} g^3 + O(g^4) - \frac{A}{2n} ((-1)^n + 1 + O(g)) + O(n^{-2}) \right\},$$

(5.7)

and

$$g^{-1} + \frac{1}{2} \log(g) = \log \left( 2\sqrt{2\pi e^{\gamma+1} n} \right).$$

The correlation function $W(n) \big|_{\beta^2 = 1}$ ($1 \leq n \leq 30$) was calculated numerically in the works [21], [22]. In Table 2 the numerical data are compared against (5.7) for odd integers

4 The coefficient $\sqrt{\frac{2}{\pi^3}}$ in Eq.(5.7) was derived previously in [20] based on the explicit form of the constant $F$ (2.21). I am grateful to I. Affleck for communications concerning this calculation.

5 K.A. Hallberg et al. [22] used the notations $\omega(n) = W(n)/4 \big|_{\beta^2 = 1}$. 

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Fig. 2. The correlation function $\frac{n}{4} \langle \text{vac} | \sigma^x_i \sigma^x_{i+n} | \text{vac} \rangle / \langle \text{vac} | \text{vac} \rangle$ for the XXX spin chain.

The bullets (see Table 2) were obtained in [22]. The continuous line I follows from (5.7) for odd integers $n$. The line II represents (5.7) for even $n$ ($A = 0.4$).

Unfortunately, we can not directly compare the numerics for even integers $n$, since the value of the constant $A$ in (5.7) is not known. Fitting of the data gives

$$A \approx 0.4 .$$

(5.8)

The corresponding plots are presented on Fig. 2.

Finally we note that there are two different approaches to exact calculation of correlation functions like (5.1) at the moment. In the first one the correlation functions are expressed in terms of Fredholm determinants [3], [23], [24]. Recently M. Jimbo and T. Miwa [25] found another representation for the correlation functions in terms of $n$-fold integrals. It would be interesting to derive the large $n$ asymptotics (5.3), (5.7) via these approaches.

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Table 2. The correlation function $\frac{n}{4} \frac{\langle \text{vac} | \sigma^x_k \sigma^x_{k+n} | \text{vac} \rangle}{\langle \text{vac} | \text{vac} \rangle}$ for the XXX spin chain. The column “NUM” were obtained in [22]. The column “RG” follows from (5.1) and (5.7) for odd integers $n$. 

| $n$ | NUM | RG |
|-----|-----|----|
| 1   | 0.1477 | 0.1239 |
| 2   | 0.1214 |    |    |
| 3   | 0.1510 | 0.1427 |
| 4   | 0.1384 |    |    |
| 5   | 0.1541 | 0.1505 |
| 6   | 0.1463 |    |    |
| 7   | 0.1567 | 0.1554 |
| 8   | 0.1513 |    |    |
| 9   | 0.1596 | 0.1589 |
| 10  | 0.1550 |    |    |
| 11  | 0.1620 | 0.1616 |
| 12  | 0.1581 |    |    |
| 13  | 0.1641 | 0.1639 |
| 14  | 0.1606 |    |    |
| 15  | 0.1659 | 0.1658 |
| 16  | 0.1628 |    |    |
| 17  | 0.1676 | 0.1674 |
| 18  | 0.1646 |    |    |
| 19  | 0.1689 | 0.1689 |
| 20  | 0.1661 |    |    |
| 21  | 0.1700 | 0.1702 |
| 22  | 0.1674 |    |    |
| 23  | 0.1712 | 0.1713 |
| 24  | 0.1687 |    |    |
| 25  | 0.1723 | 0.1724 |
| 26  | 0.1699 |    |    |
| 27  | 0.1734 | 0.1733 |
| 28  | 0.1710 |    |    |
| 29  | 0.1746 | 0.1742 |
| 30  | 0.1722 |    |    |
6. Appendix

The calculation of the coupling constants in the effective Hamiltonian \((2.23)\) is based on the technique developed in the works [2], [3], [4]. We discuss it very briefly.

Let us consider the XXZ spin chain \((2.1)\) with infinite number of sites \(N\) in the magnetic field \(h\) \((3.1)\). The specific ground state energy

\[
E(h) = \lim_{N \to \infty} \frac{E_{X X Z}^{(0)}(h)}{N},
\]

reads [12], [6]

\[
E(h) = -\frac{h^4}{4} + J \int_{-\Lambda}^{\Lambda} \frac{d\alpha}{2\pi} \frac{\sin(\pi\beta^2)}{\cosh(2\alpha) + \cos(\pi\beta^2)},
\]

where \(\epsilon(\alpha)\) satisfies the Yang-Yang equation

\[
\epsilon(\alpha) - \int_{-\Lambda}^{\Lambda} \frac{d\alpha'}{\pi} \frac{\sin(2\pi\beta^2)}{\cosh(2\alpha - 2\alpha') - \cos(2\pi\beta^2)} = h - \frac{4\sin^2(\pi\beta^2)}{J\cosh(\alpha) + \cos(2\pi\beta^2)},
\]

\(\epsilon(\pm\Lambda) = 0\).

Solving \((6.3)\) by the Wiener-Hopf method, we obtain for the weak magnetic field

\[
E(h) = E_0 - \frac{a h^2}{16\pi \beta^2} \left( 1 + \kappa \left| ah \right|^4 + (\kappa_+ + \kappa_-) \left( ah \right)^2 \right) \left( \frac{|h|}{J} \ll 1 \right),
\]

where the constant \(a\) and \(E_0\) are given by \((2.6), (2.9)\), and

\[
\kappa = \frac{\Gamma^2(\beta^{-2}) \tan(\pi\beta^{-2})}{2\beta^2 \Gamma^2(\frac{1}{2} + \beta^{-2})} \left[ \frac{\Gamma\left(\frac{\beta^2}{2-2\beta^2}\right)}{\sqrt{8\pi} \Gamma\left(\frac{1}{2-2\beta^2}\right)} \right]^{\frac{2}{\beta^2}-2},
\]

\[
\kappa_+ = \frac{1}{64\pi \beta^2} \tan\left( \frac{\pi}{2 - 2\beta^2} \right),
\]

\[
\kappa_- = \frac{1}{192\pi} \frac{\Gamma\left(\frac{3}{2-2\beta^2}\right)}{\Gamma\left(\frac{3\beta^2}{2-2\beta^2}\right)} \frac{\Gamma\left(\frac{\beta^2}{2-2\beta^2}\right)}{\Gamma\left(\frac{1}{2-2\beta^2}\right)}.\]

Now, we should compare \((6.4)\) with the result of the perturbation theory based on the effective Hamiltonian \((2.23)\). This allows to extract the values of the constant \(\lambda\) and the combination \(\lambda_+ + 2\lambda_-\). The “\(\lambda_+\)” and “\(\lambda_-\)-terms” in the effective Hamiltonian \((2.23)\) differ essentially. The operator \(TT\) has Lorenz spin 0, while \(T^2 (\bar{T}^2)\) has Lorenz spin 4 (-4). Hence, the \(\lambda_-\)-term preserves the Lorenz invariance, whereas the “\(\lambda_-\)-term” destroys the rotational symmetry. A careful analysis of the expansion \((6.4)\) based on this simple observation makes it possible to split contributions of the operators \(TT\) and \(T^2 + \bar{T}^2\) and leads to \((2.24)\).
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