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Finite temperature expectation values of boundary operators

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Abstract

A conjecture is presented for the thermal one-point function of boundary operators in integrable boundary quantum field theories in terms of form factors. It is expected to have applications in studying boundary critical phenomena and boundary flows, which are relevant in the context of condensed matter and string theory. The conjectured formula is verified by a low-temperature expansion developed using finite size techniques, which can also be used to evaluate higher point functions both in the bulk and on the boundary.

1 Introduction

The aim of the present work is to calculate the thermal one-point function of local boundary operators in integrable boundary quantum field theories. Such a theory can be specified with a Euclidean action of the form

$$\mathcal{A}=\int_{-\infty}^{\infty}d\tau\left(\int_{-\infty}^{0}dx\,\mathcal{L}\left(\Phi^{\alpha},\partial_{\tau}\Phi^{\alpha},\partial_{x}\Phi^{\alpha}\right)+\mathcal{L}_{B}\left(\Phi^{\alpha}(x=0),\partial_{\tau}\Phi^{\alpha}(x=0)\right)\right) \tag{1.1}$$

where the field variables are denoted Φ^{α}. The bulk equations of motion follow from the Euler-Lagrange equations specified by $\mathcal{L}$, while the boundary condition is obtained by varying $\mathcal{L}_B$; the possible choices for the action are restricted by requiring integrability [1].

For a finite temperature T the Euclidean time τ must be compactified to a volume

$$R=\frac{1}{T}$$

Consider a local operator $\mathcal{O}$ inserted at the boundary $x=0$ as shown in figure 1.1. The quantity of interest is the thermal average

$$\langle\mathcal{O}\rangle^{R}=\frac{\mathrm{Tr}\left(\mathrm{e}^{-RH}\mathcal{O}\right)}{\mathrm{Tr}\left(\mathrm{e}^{-RH}\right)} \tag{1.2}$$

where H is the Hamiltonian corresponding to the action (1.1) and the trace is taken on the space of states allowed by the boundary condition.

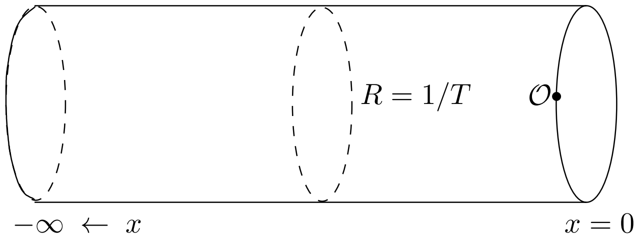

Figure 1.1: The finite temperature boundary quantum field theory with a local boundary insertion $\mathcal{O}$

The main motivation to study finite temperature correlators of boundary operators comes from boundary renormalization group flows, where the most useful quantity characterizing the space of the flows is the Affleck-Ludwig g-function or boundary entropy [2]. The original setting where this function was introduced already made use of finite temperature. Furthermore, as shown by Friedan and Konechny [3], the variation of this function along the flow can be computed via a sum rule that is expressed in terms of finite temperature boundary two-point functions. The present paper can be considered as a step towards constructing such correlators from field theory data. In addition, quantities like the thermal average (1.2) may have direct physical relevance to condensed matter systems.

Our goal is to express the thermal average in terms of matrix elements (form factors) of the operator $\mathcal{O}$. Therefore in section 2 the boundary form factor bootstrap is presented, slightly extended from its original formulation in [4] to include theories with more than one particle species. In section 3 we formulate a conjecture for the thermal average (1.2) based on the earlier work by Leclair and Mussardo [5] in the bulk case.

In order to provide evidence for the conjecture, the proposed formula is developed in a low-temperature series, with the details described in appendix A. The low-temperature expansion of (1.2) is then evaluated using an independent method developed in [6]. This approach requires the knowledge of boundary form factors in finite volume (up to corrections that decay exponentially with the volume). Section 4 presents the relevant results from the paper [7], and appendix B provides some further details on the evaluation of diagonal matrix elements. The calculation itself is presented in section 5, with a particularly complicated part relegated to appendix C. Section 6 is devoted to the conclusions.

2 The boundary form factor bootstrap

The relations satisfied by the form factors of a local boundary operator were derived in [4]. Compared to the equations in [4], the ones presented here are slightly generalized to allow for more than one particle species. Such an extension was first given in [8]; the derivation of these equations is straightforward using the methods of [4].

Here the equations are listed without much further explanation. Take an integrable boundary quantum field theory in the (infinite volume) domain $x < 0$, with N scalar particles of masses m_a $(a = 1 \ldots N)$. As usual in two-dimensional field theory, asymptotic particles are labeled with their rapidities θ, and their energy and momentum reads

$$E_a \pm p_a = m_a \mathrm{e}^{\pm\theta_a}$$

Both the bulk and boundary scattering are assumed to be diagonal and given by the two-particle S matrices

$$S_{a_1 a_2}(\theta_1 - \theta_2) = \mathrm{e}^{i\delta_{a_1 a_2}(\theta_1 - \theta_2)} \tag{2.1}$$

(where $\delta_{a_1 a_2}(\theta_1 - \theta_2)$ are the two-particle phase-shifts) and the one-particle reflection factors

$$R_a(\theta)$$

satisfying the boundary reflection factor bootstrap conditions of Ghoshal and Zamolodchikov [1]. For a local operator $\mathcal{O}(t)$ localized at the boundary (located at $x = 0$, and parametrized by the time coordinate t) the form factors are defined as

$$\begin{aligned} {}_{a_1' \dots a_m'}\langle \theta_1', \dots, \theta_m' | \mathcal{O}(t) | \theta_1, \dots, \theta_n \rangle_{a_1 \dots a_n} = \\ F^{\mathcal{O}}_{a_1' \dots a_n'; a_1 \dots a_n}(\theta_1', \dots, \theta_m'; \theta_1, \dots, \theta_n) e^{-imt(\sum \cosh\theta_i - \sum \cosh\theta_j')} \end{aligned}$$

using the asymptotic states introduced in [9]. They can be extended analytically to complex values of the rapidity variables. With the help of the crossing relations derived in [4] all form factors can be expressed in terms of the elementary form factors

$$\langle 0 | \mathcal{O}(0) | \theta_1, \dots, \theta_n \rangle_{in} = F^{\mathcal{O}}_{a_1 \dots a_n}(\theta_1, \dots, \theta_n) \tag{2.2}$$

which can be shown to satisfy the following equations:

I. Permutation:

$$\begin{aligned} F^{\mathcal{O}}_{a_1 \dots a_i a_{i+1} \dots a_n}(\theta_1, \dots, \theta_i, \theta_{i+1}, \dots, \theta_n) = \\ S_{a_i a_{i+1}}(\theta_i - \theta_{i+1}) F^{\mathcal{O}}_{a_1 \dots a_{i+1} a_i \dots a_n}(\theta_1, \dots, \theta_{i+1}, \theta_i, \dots, \theta_n) \end{aligned} \tag{2.3}$$

II. Reflection:

$$F^{\mathcal{O}}_{a_1 \dots a_n}(\theta_1, \dots, \theta_{n-1}, \theta_n) = R_{a_n}(\theta_n) F^{\mathcal{O}}_{a_1 \dots a_n}(\theta_1, \dots, \theta_{n-1}, -\theta_n) \tag{2.4}$$

III. Crossing reflection:

$$F^{\mathcal{O}}_{a_1 \dots a_n}(\theta_1, \theta_2, \dots, \theta_n) = R_{a_1}(i\pi - \theta_1) F^{\mathcal{O}}_{a_1 \dots a_n}(2i\pi - \theta_1, \theta_2, \dots, \theta_n) \tag{2.5}$$

IV. Kinematical singularity

$$\begin{aligned} -i \operatorname*{Res}_{\theta=\theta'} F^{\mathcal{O}}_{a a' a_1 \dots a_n}(\theta + i\pi, \theta', \theta_1, \dots, \theta_n) = \\ \mathbb{C}_{aa'} \left(1 - \prod_{i=1}^{n} S_{a a_i}(\theta - \theta_i) S_{a a_i}(\theta + \theta_i) \right) F^{\mathcal{O}}_{a_1 \dots a_n}(\theta_1, \dots, \theta_n) \end{aligned} \tag{2.6}$$

where $\mathbb{C}_{aa'} = \delta_{\bar{a}a'}$ is the charge conjugation matrix ($\bar{a}$ denotes the antiparticle of species a).

V. Boundary kinematical singularity

$$-i \operatorname*{Res}_{\theta=0} F^{\mathcal{O}}_{a a_1 \dots a_n}(\theta + \frac{i\pi}{2}, \theta_1, \dots, \theta_n) = \frac{g_a}{2} \Big(1 - \prod_{i=1}^{n} S_{a a_i}(\frac{i\pi}{2} - \theta_i) \Big) F^{\mathcal{O}}_{a_1 \dots a_n}(\theta_1, \dots, \theta_n) \tag{2.7}$$

where g_a is the one-particle coupling to the boundary

$$R_a(\theta) \sim \frac{i g_a^2}{2\theta - i\pi} \quad , \quad \theta \sim i\frac{\pi}{2} \tag{2.8}$$

There are also further equations corresponding to the bulk and boundary bootstrap structure (i.e. bound state singularities of the scattering amplitudes S and R), but they are not needed in the sequel. The equations are supplemented by the assumption of maximum analyticity i.e. that the form factors only have the minimal singularity structure consistent with the bootstrap equations. We remark that it is a general property of non-trivially interacting diagonal factorized scattering theories that their amplitudes are fermionic:

$$S_{aa}(0) = -1$$

and as a result of eqn. (2.3) all form factor functions satisfy an exclusion property (Pauli principle), i.e. they vanish when any two of their rapidity arguments coincide, together with the corresponding species indices.

It was shown in [10] that the space of solutions of the above equations is consistent with the operator spectrum predicted by boundary conformal field theory in the Lee-Yang and sinh-Gordon model. More recently the author gave a general procedure to construct solutions with a specific scaling dimension starting from an appropriate solution of the bulk form factor axioms [11].

We remark that using the bulk form factor bootstrap (cf. [12] for a review) as a guide it is straightforward to extend these axioms for non-diagonal scattering, i.e. particles with an internal degree of freedom. Some results for such theories (albeit only for diagonal boundary scattering) can be found in [13, 14].

3 A conjecture for the expectation values

Consider a theory with a spectrum that contains a single massive particle species of mass m. Leclair and Mussardo proposed the following expression for the bulk finite temperature one-point functions [5]:

$$\langle \mathcal{A} \rangle^R = \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{i=1}^{n} \left(\int_{-\infty}^{\infty} \frac{d\theta_i}{2\pi} \frac{\mathrm{e}^{-\epsilon(\theta_i)}}{1+\mathrm{e}^{-\epsilon(\theta_i)}} \right) f_{2n}^c(\theta_1, ..., \theta_n) \tag{3.1}$$

where f_{2n}^c is the connected diagonal form factor of the local bulk operator $\mathcal{A}$, $R = 1/T$ in terms of the temperature T, and $\epsilon(\theta)$ is the pseudo-energy function, which is the solution of the thermodynamic Bethe Ansatz (TBA) equation

$$\epsilon(\theta) = mR\cosh\theta - \int_{-\infty}^{\infty} \frac{d\theta'}{2\pi} \varphi(\theta - \theta') \log(1 + \mathrm{e}^{-\epsilon(\theta')}) \tag{3.2}$$

where

$$\varphi(\theta) = \frac{d}{d\theta}\delta(\theta)$$

is the derivative of the two-particle phase-shift introduced in (2.1). The factor $1/n!$ takes into account the fact that a complete set of n-particle in-states is obtained with the ordering

$\theta_1 \geq \theta_2 \geq \cdots \geq \theta_n$, but the integrals can be extended to the entire space using the fact that the functions $f^c_{2n}(\theta_1, ..., \theta_n)$ are symmetric in all of their arguments.

The main idea behind the formula (3.1) comes from the TBA expression of the free energy

$$f(R) = -\int_{-\infty}^{\infty} \frac{d\theta}{2\pi} m \cosh(\theta) \log(1 + \mathrm{e}^{-\epsilon(\theta)})$$

which shows that the finite temperature vacuum can be considered as a free Fermi gas of quasi-particles for which the thermal weight is given by the pseudo-energy function $\epsilon(\theta)$. The essential condition necessary for the validity of this picture is that the complete set of states used to derive (3.1) must be inserted at a position which is asymptotically far from any local operator insertion, so that their distribution is governed by the unperturbed finite temperature ground state. This is the reason why the Leclair-Mussardo conjecture does not work for the two-point functions [15], because the states inserted between the two local operators cannot be asymptotically far from the positions of the operators which are themselves located at a finite distance from each other.

From figure 1.1 it is obvious that a complete set of asymptotic states can be inserted at $x = -\infty$ where their distribution is unaffected by the presence of the boundary operator $\mathcal{O}$. The only difference to the bulk case is that the complete system of in-states is spanned by multi-particle states with all their rapidities positive (i.e. with all particles moving towards the boundary), so the natural generalization of (3.1) is

$$\langle \mathcal{O} \rangle^R = \sum_{n=0}^{\infty} \frac{1}{n!} \prod_{i=1}^{n} \left(\int_0^{\infty} \frac{d\theta_i}{2\pi} \frac{\mathrm{e}^{-\epsilon(\theta_i)}}{1 + \mathrm{e}^{-\epsilon(\theta_i)}} \right) F^c_{2n}(\theta_1, ..., \theta_n) \tag{3.3}$$

where F^c_{2n} is the connected part of the diagonal form factor of the local boundary operator $\mathcal{O}$:

$$F^c_{2n}(\theta_1, ..., \theta_n) = \langle \theta_1, \theta_2, \dots, \theta_n | \mathcal{O}(t = 0) | \theta_1, \theta_2, \dots, \theta_n \rangle^{connected} \tag{3.4}$$

which is again symmetric in all their variables as a result of equation (2.3). The precise definition of the connected matrix element (valid both for bulk and the boundary operators) is specified later in subsection 4.2.

The conjectured expression (3.3) can be checked against a calculation of the low-temperature expansion using the boundary form factors; this calculation is performed in the sequel. However, the kinematical residue equation (2.6) implies that diagonal matrix elements contain disconnected terms which are infinite, and therefore must be regularized. As shown in [6] a natural regularization can be obtained by putting the system in a finite volume, which was implemented for the bulk case in [16, 6] and for the boundary case in [7].

For completeness we note that the conjecture (3.3) can be extended to a theory with multiple particle species and diagonal scattering in the following form:

$$\langle \mathcal{O} \rangle^R = \sum_{n=0}^{\infty} \frac{1}{n!} \sum_{a_1} \cdots \sum_{a_n} \prod_{i=1}^{n} \left(\int_0^{\infty} \frac{d\theta_i}{2\pi} \frac{\mathrm{e}^{-\epsilon_{a_i}(\theta_i)}}{1 + \mathrm{e}^{-\epsilon_{a_i}(\theta_i)}} \right) F^c_{a_1 \dots a_n}(\theta_1, ..., \theta_n) \tag{3.5}$$

where

$$F^c_{a_1 \dots a_n}(\theta_1, ..., \theta_n) = {}_{a_1 \dots a_n}\langle \theta_1, \theta_2, \dots, \theta_n | \mathcal{O}(t = 0) | \theta_1, \theta_2, \dots, \theta_n \rangle^{connected}_{a_1 \dots a_n}$$

while the pseudo-energy functions satisfy

$$\epsilon_a(\theta) = m_a R \cosh\theta - \sum_b \int \frac{d\theta'}{2\pi} \varphi_{ab}(\theta - \theta') \log(1 + \mathrm{e}^{-\epsilon_{ab}(\theta')})$$

where

$$\varphi_{ab}(\theta) = \frac{d}{d\theta}\delta_{ab}(\theta) \tag{3.6}$$

are the derivatives of the two-particle phase-shifts introduced in (2.1). For the sake of simplicity the species labels will be omitted from now on, i.e. every formula will be written for the case of a single particle species; the extension to multiple species (with diagonal scattering) is rather straightforward.

Eqn. (3.3) can be expanded systematically order by order in e^{-mR} which yields a low temperature expansion, following the procedure implemented for the Leclair-Mussardo formula (3.1) in [6]. The detailed calculation is performed in Appendix A with the following result:

$$\langle\mathcal{O}\rangle^R = \sigma_1 + \sigma_2 + \sigma_3 + O\left(\mathrm{e}^{-4mR}\right) \tag{3.7}$$

where

$$\begin{aligned}
\sigma_1 &= \int_0^\infty \frac{d\theta_1}{2\pi}\left(\mathrm{e}^{-mR\cosh\theta_1} - \mathrm{e}^{-2mR\cosh\theta_1} + \mathrm{e}^{-3mR\cosh\theta_1}\right) F_2^c(\theta_1) \\
&\quad + \frac{1}{2}\int_0^\infty \frac{d\theta_1}{2\pi}\int_0^\infty \frac{d\theta_2}{2\pi}\mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2)}\Phi_{12}\left(F_2^c(\theta_1) + F_2^c(\theta_2)\right) \\
&\quad + \frac{1}{2}\int_0^\infty \frac{d\theta_1}{2\pi}\int_0^\infty \frac{d\theta_2}{2\pi}\int_0^\infty \frac{d\theta_3}{2\pi}\mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2+\cosh\theta_3)}\big(\Phi_{12}\Phi_{13} \\
&\quad + \Phi_{12}\Phi_{23} + \Phi_{13}\Phi_{23}\big)F_2^c(\theta_3) \\
&\quad - \int_0^\infty \frac{d\theta_1}{2\pi}\int_0^\infty \frac{d\theta_2}{2\pi}\mathrm{e}^{-mR(2\cosh\theta_1+\cosh\theta_2)}\left(2F_2^c(\theta_1) + \frac{1}{2}F_2^c(\theta_2)\right)\Phi_{12} \\
\sigma_2 &= \frac{1}{2}\int_0^\infty \frac{d\theta_1}{2\pi}\int_0^\infty \frac{d\theta_2}{2\pi}\mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2)}F_4^c(\theta_1,\theta_2) \\
&\quad - \int_0^\infty \frac{d\theta_1}{2\pi}\int_0^\infty \frac{d\theta_2}{2\pi}\mathrm{e}^{-mR(2\cosh\theta_1+\cosh\theta_2)}F_4^c(\theta_1,\theta_2) \\
&\quad + \frac{1}{2}\int_0^\infty \frac{d\theta_1}{2\pi}\int_0^\infty \frac{d\theta_2}{2\pi}\int_0^\infty \frac{d\theta_3}{2\pi}\mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2+\cosh\theta_3)}\left(\Phi_{12} + \Phi_{13}\right)F_4^c(\theta_2,\theta_3) \\
\sigma_3 &= \frac{1}{6}\int_0^\infty \frac{d\theta_1}{2\pi}\int_0^\infty \frac{d\theta_2}{2\pi}\int_0^\infty \frac{d\theta_3}{2\pi}\mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2+\cosh\theta_3)}F_6^c(\theta_1,\theta_2,\theta_3)
\end{aligned}$$

and

$$\Phi_{ij} = \varphi(\theta_i - \theta_j) + \varphi(\theta_i + \theta_j)$$

For later convenience some terms were reordered by reshuffling the integral variables.

In the sequel this result is compared to the result obtained from explicit evaluation of the finite temperature Gibbs average. In order to perform this calculation it is necessary to use finite volume as a regulator, and so now we turn to the issue of boundary form factors in finite volume, based on the results of [7].

4 Boundary form factors in finite volume

4.1 Bethe-Yang equations

Let us consider an integrable boundary quantum field theory with particles of species $a = 1,\dots,N$ and corresponding masses m_a in finite volume L as shown in figure 4.1. As in section

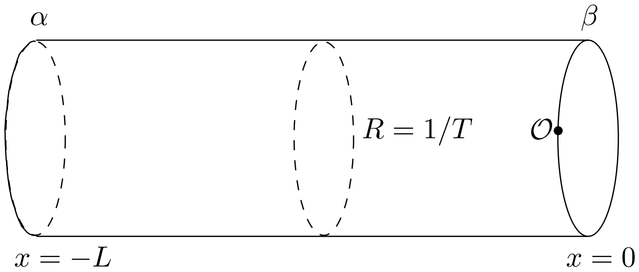

Figure 4.1: The setting of Fig. 1.1 in finite volume

2, the bulk and boundary scattering is assumed to be diagonal and given by the two-particle S matrices

$$S_{a_1a_2}(\theta_1-\theta_2)=\mathrm{e}^{i\delta_{a_1a_2}(\theta_1-\theta_2)}$$

and the one-particle reflection factors

$$R_a^{(\alpha)}(\theta)=\mathrm{e}^{i\delta_a^{(\alpha)}(\theta)}\qquad,\qquad R_a^{(\beta)}(\theta)=\mathrm{e}^{i\delta_a^{(\beta)}(\theta)}\tag{4.1}$$

where α and β denote the left and right boundary conditions, respectively.

In the diagonal case, the multi-particle energy levels in a finite volume L are described by the following Bethe-Yang equations [17]:

$$Q_j(\theta_1,\dots,\theta_n)_{a_1\dots a_n}\;=\;2\pi I_j\tag{4.2}$$

where the phases describing the wave function monodromies are

$$\begin{aligned}Q_j(\theta_1,\dots,\theta_n)_{a_1\dots a_n}\;=\;&2m_{a_j}L\sinh\theta_j+\delta_{a_j}^{(\alpha)}(\theta_j)+\delta_{a_j}^{(\beta)}(\theta_j)\\&+\sum_{k\neq j}\big(\delta_{a_ja_k}(\theta_j-\theta_k)+\delta_{a_ja_k}(\theta_j+\theta_k)\big)\end{aligned}$$

Here all rapidities θ_j (and accordingly all quantum numbers I_j) are taken to be positive[1]. The corresponding multi-particle state is denoted by

$$|\{I_1,\dots,I_n\}\rangle_{a_1\dots a_n,L}$$

and its energy (relative to the ground state) is

$$E_{I_1\dots I_n}(L)=\sum_{j=1}^{n}m_{a_j}\cosh\tilde{\theta}_j$$

where $\left\{\tilde{\theta}_j\right\}_{j=1,\dots,n}$ is the solution of eqns. (4.2) in volume L. The energy calculated from the Bethe-Yang equations is exact to all order in $1/L$; only finite size effects decaying exponentially with L are neglected.

[1]Boundary reflections change the sign of the momentum, so finite volume multi-particle states can be characterized by the absolute value of the rapidities.

4.2 Matrix elements in finite volume

In general infinite volume and finite volume matrix elements are just related by the square root of the ratio of normalization of the corresponding states [7, 16]. This results in the following relation:

$$
\begin{aligned}
&{}_{b_1\dots b_m}\langle\{I'_1,\dots,I'_m\}|\mathcal{O}(0)|\{I_1,\dots,I_n\}\rangle_{a_1\dots a_n,L} = \\
&\frac{F^{\mathcal{O}}_{\bar{b}_m\dots\bar{b}_1 a_1\dots a_n}(\tilde{\theta}'_m+i\pi,\dots,\tilde{\theta}'_1+i\pi,\tilde{\theta}_1,\dots,\tilde{\theta}_n)}{\sqrt{\rho_{a_1\dots a_n}(\tilde{\theta}_1,\dots,\tilde{\theta}_n)\rho_{b_1\dots b_m}(\tilde{\theta}'_1,\dots,\tilde{\theta}'_m)}}+O(\mathrm{e}^{-\mu L})
\end{aligned}
\tag{4.3}
$$

where $F^{\mathcal{O}}_{a_1\dots a_n}(\tilde{\theta}_1,\dots,\tilde{\theta}_n)$ is the form factor of the operator $\mathcal{O}$ (in the infinite volume theory, i.e. on the half-line $x<0$), $\left\{\tilde{\theta}_j\right\}_{j=1,\dots,n}$ is the solution of eqns. (4.2) in volume L for the set of quantum numbers $\{I_1,\dots,I_n\}$ (similarly for $\left\{\tilde{\theta}'_j\right\}_{j=1,\dots,m}$ and $\{I'_1,\dots,I'_m\}$), and

$$
\rho_{a_1\dots a_n}(\theta_1,\dots,\theta_n)=\det\left\{\frac{\partial Q_k(\theta_1,\dots,\theta_n)_{a_1\dots a_n}}{\partial\theta_l}\right\}_{k,l=1,\dots,n}
\tag{4.4}
$$

is the finite volume density of states, which is the Jacobi determinant of the mapping between the space of quantum numbers and the space of rapidities specified by the Bethe-Yang equations (4.2). An explicit expression for the derivative matrix of the Bethe-Yang equations (4.2) is

$$
\begin{aligned}
\frac{\partial Q_k}{\partial\theta_k} &= 2m_{a_k}L\cosh\theta_k+\psi^{(\alpha)}_{a_k}(\theta_k)+\psi^{(\beta)}_{a_k}(\theta_k)+\sum_{j\neq k}[\varphi_{a_j a_k}(\theta_j-\theta_k)+\varphi_{a_j a_k}(\theta_j+\theta_k)] \\
\frac{\partial Q_k}{\partial\theta_j} &= -\varphi_{a_j a_k}(\theta_j-\theta_k)+\varphi_{a_j a_k}(\theta_j+\theta_k) \qquad , \qquad j\neq k
\end{aligned}
\tag{4.5}
$$

where

$$
\psi^{(\alpha)}_a(\theta)=\frac{d}{d\theta}\delta^{(\alpha)}_a(\theta)\ ,\ \psi^{(\beta)}(\theta)=\frac{d}{d\theta}\delta^{(\beta)}_a(\theta)
$$

are the derivatives of the boundary phase-shifts defined in (4.1), while the φ are the derivatives of the bulk ones as written in (3.6).

Eqn. (4.3) is valid as long as the sets of the rapidities corresponding to the two states, $\left\{\tilde{\theta}_j\right\}_{j=1,\dots,n}$ and $\left\{\tilde{\theta}'_j\right\}_{j=1,\dots,m}$, are disjoint i.e. when there are no disconnected contributions. For diagonal matrix elements

$$
{}_{a_1\dots a_n}\langle\{I_1,\dots,I_n\}|\mathcal{O}(0)|\{I_1,\dots,I_n\}\rangle_{a_1\dots a_n,L}
$$

a more careful analysis is required [6, 7]. According to (4.3) for this case it is necessary to consider

$$
F_{\bar{a}_n\dots\bar{a}_1 a_1\dots a_n}(\theta_n+i\pi,\dots,\theta_1+i\pi,\theta_1,\dots,\theta_n)
$$

Because of the kinematical poles the above expression is not well-defined. The bulk kinematical singularity axiom (2.6) implies that the regularized version

$$
F_{\bar{a}_n\dots\bar{a}_1 a_1\dots a_n}(\theta_n+i\pi+\epsilon_n,\dots,\theta_1+i\pi+\epsilon_1,\theta_1,\dots,\theta_n)
$$

has a finite limit when $\epsilon_i \to 0$ simultaneously. However, the end result depends on the direction of the limit, i.e. on the ratio of the ϵ_i parameters. The terms that are relevant in this limit can be written in the following general form:

$$F_{\bar{a}_n\dots\bar{a}_1 a_1\dots a_n}(\theta_n + i\pi + \epsilon_n, ..., \theta_1 + i\pi + \epsilon_1, \theta_1, ..., \theta_n) = \prod_{i=1}^{n} \frac{1}{\epsilon_i} \cdot \sum_{i_1=1}^{n} \dots \sum_{i_n=1}^{n} \mathcal{A}^{a_1\dots a_n}_{i_1\dots i_n}(\theta_1, \dots, \theta_n)\epsilon_{i_1}\epsilon_{i_2}\dots\epsilon_{i_n} + \dots \tag{4.6}$$

where $\mathcal{A}^{a_1\dots a_n}_{i_1\dots i_n}$ is a tensor of rank n in the indices $i_1, \dots, i_n$ which is symmetric under the exchange of indices that correspond to particles of the same species, and the ellipsis denote terms that vanish when taking $\epsilon_i \to 0$ simultaneously.

The connected matrix element can be defined as the ϵ_i independent part of eqn. (4.6), i.e. the part which does not diverge whenever any of the ϵ_i is taken to zero:

$$F^c_{a_1\dots a_n}(\theta_1, ..., \theta_n) = \sum_{(p_1\dots p_n)} \mathcal{A}^{a_1\dots a_n}_{p_1\dots p_n}(\theta_1, \dots, \theta_n) \tag{4.7}$$

where the summation goes over all permutations $(p_1, \dots, p_n)$ of the numbers $1, \dots, n$. As shown in appendix B, all other evaluations of the diagonal matrix elements (4.6) can be readily expressed in terms of the connected amplitudes.

It was shown in [7] that a natural generalization of an expression proposed earlier by Saleur [15] for bulk diagonal matrix elements can be extended to the boundary case in the following way[2]:

$$_{a_1\dots a_n}\langle\{I_1 \dots I_n\}|\mathcal{O}(0)|\{I_1 \dots I_n\}\rangle_{a_1\dots a_n,L} = \frac{1}{\rho_{a_1\dots a_n}(\tilde{\theta}_1, \dots, \tilde{\theta}_n)} \sum_{A\subset\{1,2,\dots n\}} F^c_{a(A)}(\{\tilde{\theta}_k\}_{k\in A})\tilde{\rho}_{a_1\dots a_n}(\tilde{\theta}_1, \dots, \tilde{\theta}_n|A) + O(\mathrm{e}^{-\mu L}) \tag{4.8}$$

The summation runs over all subsets A of $\{1, 2, \dots n\}$ and again $\left\{\tilde{\theta}_j\right\}_{j=1,\dots,n}$ is the solution of eqns. (4.2) in volume L for the set of quantum numbers $\{I_1, \dots, I_n\}$. For any such subset the corresponding species index list is defined as

$$a(A) = \{a_k\}_{k\in A}$$

and

$$\tilde{\rho}_{a_1\dots a_n}(\theta_1, \dots, \theta_n|A) = \det \mathcal{J}^{a_1\dots a_n}_A(\theta_1, \dots, \theta_n) \tag{4.9}$$

is the appropriate sub-determinant of the $n \times n$ Bethe-Yang Jacobi matrix

$$\mathcal{J}_{a_1\dots a_n}(\theta_1, \dots, \theta_n)_{kl} = \frac{\partial Q_k(\theta_1, \dots, \theta_n)_{a_1\dots a_n}}{\partial\theta_l} \tag{4.10}$$

obtained by deleting the rows and columns corresponding to the subset of indices A. The determinant of the empty sub-matrix (i.e. when $A = \{1, 2, \dots n\}$) is defined to equal 1 by convention. It is also shown in appendix B that the symmetric evaluation which gave a very convenient alternative to (4.8) in the bulk [6], behaves rather differently in the boundary case.

[2]Note that here the original result of [7] is extended to the case of several particle species.

5 Expansion of finite temperature expectation values

5.1 Low-temperature expansion for one-point functions

The procedure leading to a well-defined low-temperature expansion was outlined in section 7 of [6]; details about the validity of the method and the existence of the limits taken are omitted (the interested reader is referred to the above paper for details). Let us evaluate the finite temperature expectation value of an operator $\mathcal{O}$ located at $x = 0$ in a finite but large volume L, according to the setting introduced in section 4:

$$\langle \mathcal{O} \rangle_L^R = \frac{\mathrm{Tr}_L \left(\mathrm{e}^{-RH_L} \mathcal{O} \right)}{\mathrm{Tr}_L \left(\mathrm{e}^{-RH_L} \right)} \qquad , \; T = 1/R \tag{5.1}$$

H_L is the finite volume Hamiltonian, and Tr_L means that the trace is now taken over the finite volume Hilbert space. The expectation value $\langle \mathcal{O} \rangle^R$ can be recovered in the limit $L \to \infty$ which means that the left boundary condition α in figure 4.1 plays an auxiliary role, and the end result can only depend on the $x = 0$ boundary condition β; this issue will be taken up again in subsection 5.5.

In the calculation below particle species labels are dropped for simplicity (they can be easily reinstated if necessary) and we use the simplified notation F_{2n} for the n-particle diagonal matrix element introduced in (3.4). It is also convenient to introduce a new notation:

$$|\theta_1, \ldots, \theta_n\rangle_L = |\{I_1, \ldots, I_n\}\rangle_L$$

where $\theta_1, \ldots, \theta_n$ solve the Bethe-Yang equations (4.2) for n particles with quantum numbers $I_1, \ldots, I_n$ in volume L; as remarked in subsection 2.1, all of the rapidities can be taken positive. The low temperature expansion of (5.1) can be developed in orders of e^{-mR} using

$$\begin{aligned}
\mathrm{Tr}_L \left(\mathrm{e}^{-RH_L} \mathcal{O} \right) &= \langle \mathcal{O} \rangle_L + \sum_{\theta^{(1)}} \mathrm{e}^{-mR\cosh\theta^{(1)}} \langle \theta^{(1)} | \mathcal{O} | \theta^{(1)} \rangle_L \\
&+ \frac{1}{2} \sum_{\theta_1^{(2)}, \theta_2^{(2)}}{}' \mathrm{e}^{-mR(\cosh\theta_1^{(2)} + \cosh\theta_2^{(2)})} \langle \theta_1^{(2)}, \theta_2^{(2)} | \mathcal{O} | \theta_1^{(2)}, \theta_2^{(2)} \rangle_L + \\
&+ \frac{1}{6} \sum_{\theta_1^{(3)}, \theta_2^{(3)}, \theta_3^{(3)}}{}' \mathrm{e}^{-mR(\cosh\theta_1^{(3)} + \cosh\theta_2^{(3)} + \cosh\theta_3^{(3)})} \langle \theta_1^{(3)}, \theta_2^{(3)}, \theta_3^{(3)} | \mathcal{O} | \theta_1^{(3)}, \theta_2^{(3)}, \theta_3^{(3)} \rangle_L \\
&+ O(\mathrm{e}^{-4mR})
\end{aligned} \tag{5.2}$$

and

$$\begin{aligned}
\mathrm{Tr}_L \left(\mathrm{e}^{-RH_L} \right) &= 1 + \sum_{\theta^{(1)}} \mathrm{e}^{-mR\cosh(\theta^{(1)})} + \frac{1}{2} \sum_{\theta_1^{(2)}, \theta_2^{(2)}}{}' \mathrm{e}^{-mR(\cosh(\theta_1^{(2)}) + \cosh(\theta_2^{(2)}))} \\
&+ \frac{1}{6} \sum_{\theta_1^{(3)}, \theta_2^{(3)}, \theta_3^{(3)}}{}' \mathrm{e}^{-mR(\cosh\theta_1^{(3)} + \cosh\theta_2^{(3)} + \cosh\theta_3^{(3)})} + O(\mathrm{e}^{-4mR})
\end{aligned} \tag{5.3}$$

The denominator of (5.1) can then be easily expanded:

$$\begin{aligned}
\frac{1}{\mathrm{Tr}_L\left(\mathrm{e}^{-RH_L}\right)} &= 1-\sum_{\theta^{(1)}}\mathrm{e}^{-mR\cosh\theta^{(1)}}+\left(\sum_{\theta^{(1)}}\mathrm{e}^{-mR\cosh\theta^{(1)}}\right)^2-\frac{1}{2}\sum_{\theta_1^{(2)},\theta_2^{(2)}}{}'\,\mathrm{e}^{-mR(\cosh\theta_1^{(2)}+\cosh\theta_2^{(2)})}\\
&\quad-\left(\sum_{\theta^{(1)}}\mathrm{e}^{-mR\cosh\theta^{(1)}}\right)^3+\left(\sum_{\theta^{(1)}}\mathrm{e}^{-mR\cosh\theta^{(1)}}\right)\sum_{\theta_1^{(2)},\theta_2^{(2)}}{}'\,\mathrm{e}^{-mR(\cosh\theta_1^{(2)}+\cosh\theta_2^{(2)})}\\
&\quad-\frac{1}{6}\sum_{\theta_1^{(3)},\theta_2^{(3)},\theta_3^{(3)}}{}'\,\mathrm{e}^{-mR(\cosh\theta_1^{(3)}+\cosh\theta_2^{(3)}+\cosh\theta_3^{(3)})}+O(\mathrm{e}^{-4mR})
\end{aligned} \tag{5.4}$$

The primes in the multi-particle sums serve as a reminder that there exist only states for which all quantum numbers are distinct. Since it was assumed that there is a single particle species, this means that terms in which any two of the rapidities coincide are excluded. All n-particle terms in (5.2) and (5.3) have a $1/n!$ prefactor which takes into account that different ordering of the same rapidities give the same state; as the expansion contains only diagonal matrix elements, phases resulting from reordering the particles cancel. It is also crucial to remember that in the boundary case the summations only run over positive values of the rapidities (cf. section 3). The upper indices of the rapidity variables indicate the number of particles in the original finite volume states which helps to keep track which multi-particle state density is relevant.

It is also necessary to extend the finite volume matrix elements to rapidities that are not necessarily solutions of the appropriate Bethe-Yang equations. The required analytic continuation can be written down using eqn. (4.8):

$$\langle\theta_1,\dots,\theta_n|\mathcal{O}|\theta_1,\dots,\theta_n\rangle_L=\frac{1}{\rho_n(\theta_1,\dots,\theta_n)_L}\sum_{A\subset\{1,2,\dots n\}}F^c_{2|A|}(\{\theta_i\}_{i\in A})\tilde{\rho}(\theta_1,\dots,\theta_n|A)_L+O(\mathrm{e}^{-\mu L}) \tag{5.5}$$

where the volume dependence of the n-particle density factors was made explicit and the form factors are computed from solutions of the bootstrap equations in section 2 with the boundary condition β. It is apparent that the continuation is specified only up to terms decaying exponentially with the volume L but this is sufficient for the evaluation of the $L\to\infty$ limit of (5.1).

It is useful to notice that unitarity and real analyticity imply that all the phase-shift derivatives

$$\varphi(\theta)=\frac{d}{d\theta}\delta(\theta)\ ,\ \psi^{(\alpha)}(\theta)=\frac{d}{d\theta}\delta^{(\alpha)}(\theta)\ ,\ \psi^{(\beta)}(\theta)=\frac{d}{d\theta}\delta^{(\beta)}(\theta) \tag{5.6}$$

are real and even functions. Another important observation is that the exclusion principle (cf. section 2) implies that the amplitudes $F^c_{2n}(\theta_1,\dots,\theta_n)$ vanish whenever any two of their rapidity arguments coincide. In addition, the connected form factor functions are symmetric under permutations of their arguments according to their definition (4.7) and (in contrast to the bulk case) they are even functions in all of their rapidity arguments separately i.e.

$$F^c_{2n}(\theta_1,\theta_2,\dots,\theta_n)=F^c_{2n}(-\theta_1,\theta_2,\dots,\theta_n)$$

which is a result of the reflection equation (2.4) satisfied by the form factors.

5.2 Lowest order terms

The leading correction is

$$\langle\mathcal{O}\rangle_L^R = \langle\mathcal{O}\rangle_L + \sum_{\theta^{(1)}} \mathrm{e}^{-mR\cosh\theta^{(1)}} \left(\langle\theta^{(1)}|\mathcal{O}|\theta^{(1)}\rangle_L - \langle\mathcal{O}\rangle_L \right) + O(\mathrm{e}^{-2mR})$$

From (5.5)

$$\langle\theta|\mathcal{O}|\theta\rangle_L - \langle\mathcal{O}\rangle = \frac{1}{\rho_1(\theta)} F_2^c(\theta) + O\left(\mathrm{e}^{-\mu L}\right)$$

Note also that the difference between the finite volume vacuum expectation value and the infinite volume one decays exponentially with L

$$\langle\mathcal{O}\rangle_L - \langle\mathcal{O}\rangle \sim O\left(\mathrm{e}^{-\mu L}\right)$$

From now on such exponential corrections will simply be omitted. In the large L limit the summation can be replaced by the integral

$$\sum_{\theta^{(1)}} \to \int \frac{d\theta}{2\pi} \rho_1(\theta)$$

and therefore

$$\langle\mathcal{O}\rangle^R = \langle\mathcal{O}\rangle + \int_0^\infty \frac{d\theta}{2\pi} F_2^c(\theta) \mathrm{e}^{-mR\cosh\theta} + O(\mathrm{e}^{-2mR}) \tag{5.7}$$

5.3 Corrections of order e^{-2mR}

To this order one has

$$\begin{aligned}
\langle\mathcal{O}\rangle_L^R &= \langle\mathcal{O}\rangle_L + \sum_{\theta^{(1)}} \mathrm{e}^{-mR\cosh\theta^{(1)}} \left(\langle\theta^{(1)}|\mathcal{O}|\theta^{(1)}\rangle_L - \langle\mathcal{O}\rangle_L \right) \\
&- \left(\sum_{\theta_1^{(1)}} \mathrm{e}^{-mR\cosh\theta_1^{(1)}} \right) \left(\sum_{\theta_2^{(1)}} \mathrm{e}^{-mR\cosh\theta_2^{(1)}} \left(\langle\theta_2^{(1)}|\mathcal{O}|\theta_2^{(1)}\rangle_L - \langle\mathcal{O}\rangle_L \right) \right) \\
&+ \frac{1}{2} \sum_{\theta_1^{(2)},\theta_2^{(2)}}{}' \mathrm{e}^{-mR(\cosh\theta_1^{(2)} + \cosh\theta_2^{(2)})} \left(\langle\theta_1^{(2)},\theta_2^{(2)}|\mathcal{O}|\theta_1^{(2)},\theta_2^{(2)}\rangle_L - \langle\mathcal{O}\rangle_L \right) + O(\mathrm{e}^{-3mR})
\end{aligned}$$

Using the symmetry of the first term in the rapidities and separating the diagonal contribution from the double summation on the last line leads to

$$\begin{aligned}
&-\frac{1}{2} \left(\sum_{\theta_1^{(1)}} \mathrm{e}^{-mR\cosh\theta_1^{(1)}} \right) \left(\sum_{\theta_2^{(1)}} \mathrm{e}^{-mR\cosh\theta_2^{(1)}} \left(\langle\theta_1^{(1)}|\mathcal{O}|\theta_1^{(1)}\rangle_L + \langle\theta_2^{(1)}|\mathcal{O}|\theta_2^{(1)}\rangle_L - 2\langle\mathcal{O}\rangle_L \right) \right) \\
&+\frac{1}{2} \sum_{\theta_1^{(2)},\theta_2^{(2)}} \mathrm{e}^{-mR(\cosh\theta_1^{(2)} + \cosh\theta_2^{(2)})} \left(\langle\theta_1^{(2)},\theta_2^{(2)}|\mathcal{O}|\theta_1^{(2)},\theta_2^{(2)}\rangle_L - \langle\mathcal{O}\rangle_L \right) \\
&-\frac{1}{2} \sum_{\theta_1^{(2)}=\theta_2^{(2)}} \mathrm{e}^{-2mR\cosh\theta_1^{(2)}} \left(\langle\theta_1^{(2)},\theta_1^{(2)}|\mathcal{O}|\theta_1^{(2)},\theta_1^{(2)}\rangle_L - \langle\mathcal{O}\rangle_L \right)
\end{aligned}$$

The terms containing two independent rapidity sums can be written as

$$\Sigma_2^{(2)} = \frac{1}{2}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}e^{-mR(\cosh\theta_1+\cosh\theta_2)}\Bigg(-\rho_1(\theta_1)\rho_1(\theta_2)\left(\frac{1}{\rho_1(\theta_1)}F_2^c(\theta_1)+\frac{1}{\rho_1(\theta_2)}F_2^c(\theta_2)\right)$$
$$+F_4^c(\theta_1,\theta_2)+\tilde{\rho}(\theta_1,\theta_2|\{1\})F_2^c(\theta_1)+\tilde{\rho}(\theta_1,\theta_2|\{2\})F_2^c(\theta_2)\Bigg)$$

where

$$\rho_1(\theta)=2mL\cosh\theta+\psi^{(\alpha)}(\theta)+\psi^{(\beta)}(\theta)$$

is the one-particle state density, while

$$\begin{aligned}\tilde{\rho}(\theta_1,\theta_2|\{2\}) &= 2mL\cosh\theta_1+\psi^{(\alpha)}(\theta_1)+\psi^{(\beta)}(\theta_1)+\varphi(\theta_1-\theta_2)+\varphi(\theta_1+\theta_2)\\ \tilde{\rho}(\theta_1,\theta_2|\{1\}) &= 2mL\cosh\theta_2+\psi^{(\alpha)}(\theta_2)+\psi^{(\beta)}(\theta_2)+\varphi(\theta_2-\theta_1)+\varphi(\theta_2+\theta_1)\end{aligned} \quad (5.8)$$

are the corresponding sub-determinants of the two-particle Bethe-Yang Jacobian, evaluated according to (4.9). Taking $L\to\infty$

$$\Sigma_2^{(2)}=\frac{1}{2}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}e^{-mR(\cosh\theta_1+\cosh\theta_2)}\left[F_4^c(\theta_1,\theta_2)+\left(\varphi(\theta_1-\theta_2)+\varphi(\theta_1+\theta_2)\right)\left(F_2^c(\theta_1)+F_2^c(\theta_2)\right)\right]$$

The diagonal contribution contains a single rapidity sum

$$\Sigma_2^{(1)}=-\frac{1}{2}\sum_{\theta_1^{(2)}=\theta_2^{(2)}}e^{-2mR\cosh\theta_1^{(2)}}\left(\langle\theta_1^{(2)},\theta_1^{(2)}|\mathcal{O}|\theta_1^{(2)},\theta_1^{(2)}\rangle_L-\langle\mathcal{O}\rangle_L\right)$$

for which one needs to evaluate the density of states for a degenerate two-particle state. The appropriate Bethe-Yang equation reads

$$2mL\sinh\theta_1^{(2)}+\delta(0)+\delta\left(2\theta_1^{(2)}\right)+\delta^{(\alpha)}\left(\theta_1^{(2)}\right)+\delta^{(\beta)}\left(\theta_1^{(2)}\right)=2\pi I_1 \quad (5.9)$$

and so the summation can be replaced by

$$\sum_{\theta_1^{(2)}=\theta_2^{(2)}} \rightarrow \int\frac{d\theta}{2\pi}\bar{\rho}_{12}(\theta)$$
$$\bar{\rho}_{12}(\theta)=2mL\cosh\theta+2\varphi(2\theta)+\psi^{(\alpha)}(\theta_1)+\psi^{(\beta)}(\theta_1) \quad (5.10)$$

On the other hand from (5.5) it follows that

$$\langle\theta,\theta|\mathcal{O}|\theta,\theta\rangle_L-\langle\mathcal{O}\rangle_L = \frac{1}{\rho_2(\theta,\theta)}\Big[F_4^c(\theta_1,\theta_2)+\tilde{\rho}(\theta_1,\theta_2|\{1\})F_2^c(\theta_1)$$
$$+\tilde{\rho}(\theta_1,\theta_2|\{2\})F_2^c(\theta_2)\Big]_{\theta_1=\theta_2=\theta}+O\left(e^{-\mu L}\right)$$

where the $\tilde{\rho}$ are given in (5.8) and the factor at the front can be calculated from (4.4)

$$\rho_2(\theta,\theta)=4m^2L^2\cosh^2\theta+O(L)$$

In addition, the exclusion property can be used to substitute $F_c^4(\theta,\theta)=0$. Taking the limit $L\to\infty$ results in

$$\Sigma_2^{(1)} = -\frac{1}{2}\int\frac{d\theta}{2\pi}\mathrm{e}^{-2mR\cosh\theta}2F_2^c(\theta)$$

and so the total contribution at this order reads

$$\begin{aligned}\Sigma_2 &= \Sigma_2^{(1)}+\Sigma_2^{(2)}\\ &= -\int_0^\infty\frac{d\theta}{2\pi}\mathrm{e}^{-2mR\cosh\theta}F_2^c(\theta)\\ &+ \frac{1}{2}\int_0^\infty\frac{d\theta_1}{2\pi}\int_0^\infty\frac{d\theta_2}{2\pi}\mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2)}\Big[F_4^c(\theta_1,\theta_2)\\ &\quad+\left(\varphi(\theta_1-\theta_2)+\varphi(\theta_1+\theta_2)\right)\left(F_2^c(\theta_1)+F_2^c(\theta_2)\right)\Big]\end{aligned}\qquad(5.11)$$

5.4 Corrections of order e^{-3mR}

This calculation proceeds in a similar way but it is rather long and so it is relegated to appendix C. The net result is

$$\begin{aligned}\Sigma_3 = &\frac{1}{6}\int_0^\infty\frac{d\theta_1}{2\pi}\int_0^\infty\frac{d\theta_2}{2\pi}\int_0^\infty\frac{d\theta_3}{2\pi}\mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2+\cosh\theta_3)}[F_6^c(\theta_1,\theta_2,\theta_3)\\ &+3F_4^c(\theta_2,\theta_3)(\Phi_{12}+\Phi_{13})+3F_2^c(\theta_3)(\Phi_{12}\Phi_{13}+\Phi_{12}\Phi_{23}+\Phi_{13}\Phi_{23})]\\ &-\int_0^\infty\frac{d\theta_1}{2\pi}\int_0^\infty\frac{d\theta_2}{2\pi}\mathrm{e}^{-mR(2\cosh\theta_1+\cosh\theta_2)}\Big[F_4^c(\theta_1,\theta_2)\\ &+\left(2F_2^c(\theta_1)+\frac{1}{2}F_2^c(\theta_2)\right)\Phi_{12}\Big]+\int_0^\infty\frac{d\theta_1}{2\pi}\mathrm{e}^{-3mR\cosh\theta_1}F_2^c(\theta_1)\end{aligned}\qquad(5.12)$$

where $\Phi_{ij}=\varphi(\theta_i-\theta_j)+\varphi(\theta_i+\theta_j)$.

5.5 Discussion of the results

It is very important to note that in the order by order corrections (5.7), (5.11) and (5.12), the dependence on the boundary condition β at $x=0$ is only carried by the form factors F_{2n}^c. However, in the intermediate calculations the Bethe-Yang determinants enter, which depend on the boundary conditions α and β in a symmetrical way: according to eqn. (4.5), the boundary phase-shift derivatives always appear in the combination

$$\psi^{(\alpha)}(\theta)+\psi^{(\beta)}(\theta)$$

The fact that all such terms drop in the $L\to\infty$ limit is necessary for consistency since the end result can only depend on the boundary condition β imposed at $x=0$, but not on the auxiliary (and indeed arbitrary) boundary condition α imposed at $x=-L$ (cf. figure 4.1).

Summarizing the results, the expansion of the one-point function reads

$$\langle\mathcal{O}\rangle^R=\langle\mathcal{O}\rangle+\Sigma_1+\Sigma_2+\Sigma_3+O\left(\mathrm{e}^{-4mR}\right)$$

where

$$\Sigma_1=\int_0^\infty\frac{d\theta}{2\pi}F_2^c(\theta)\mathrm{e}^{-mR\cosh\theta}$$

while Σ_2 and Σ_3 are given in eqns. (5.11) and (5.12), respectively. Note that this result exactly coincides with the expansion (3.7) of the conjectured formula (3.3), which is a strong reason to believe that the conjecture is indeed correct to all orders (especially in view of the very nontrivial structure of the third-order correction terms).

There is a rather obvious structural similarity between the bulk formula (3.1) and the boundary one (3.3). Taking into account the symmetry of the pseudo-energy function exploited in appendix A, it is possible to bring the bulk and boundary cases into correspondence by interchanging the following ingredients:

bulk	boundary
$\int_{-\infty}^{\infty}\frac{d\theta_i}{2\pi}$	$\int_{0}^{\infty}\frac{d\theta_i}{2\pi}$
$f_{2n}^c(\theta_1,\dots\theta_n)$	$F_{2n}^c(\theta_1,\dots\theta_n)$
$\varphi(\theta_j-\theta_k)$	$\varphi(\theta_j-\theta_k)+\varphi(\theta_j+\theta_k)$

(some care must be taken on the second line to follow properly the particle labels of f_2^c, since the bulk connected two-particle form factor is actually independent of the rapidity and thus the argument is usually omitted). Since Theorem 1 of appendix B is related to the corresponding bulk theorem of [6] via the correspondence implied by the last two lines in the above table, it is also possible to express the expansion (3.7) in terms of symmetric form factors analogously to the result obtained in [6]:

$$\begin{aligned}\langle\mathcal{O}\rangle^R &= \langle\mathcal{O}\rangle+\int_0^\infty\frac{d\theta}{2\pi}F_2^s(\theta)\left[\mathrm{e}^{-mR\cosh\theta}-\mathrm{e}^{-2mR\cosh\theta}+\mathrm{e}^{-3mR\cosh\theta}\right]\\ &+\frac{1}{2}\int_0^\infty\frac{d\theta_1}{2\pi}\int_0^\infty\frac{d\theta_2}{2\pi}F_4^s(\theta_1,\theta_2)\left[\mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2)}-2\mathrm{e}^{-mR(2\cosh\theta_1+\cosh\theta_2)}\right]\\ &+\frac{1}{6}\int_0^\infty\frac{d\theta_1}{2\pi}\int_0^\infty\frac{d\theta_2}{2\pi}\int_0^\infty\frac{d\theta_3}{2\pi}F_6^s(\theta_1,\theta_2,\theta_3)\mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2+\cosh\theta_3)}\\ &-\int_0^\infty\frac{d\theta_1}{2\pi}\int_0^\infty\frac{d\theta_2}{2\pi}\left[F_2^s(\theta_1)-\frac{1}{2}F_2^s(\theta_2)\right]\Phi_{12}\mathrm{e}^{-mR(2\cosh\theta_1+\cosh\theta_2)}+O\left(\mathrm{e}^{-4mR}\right)\end{aligned}$$

where eqns. (B.5,B.6,B.7) were used, together with the freedom to relabel some integration variables. However, note that this is not automatically guaranteed in the finite volume formalism used in the present section, since the computation makes use of the various Bethe-Yang determinants which depend explicitly on the combination $\varphi(\theta_j-\theta_k)-\varphi(\theta_j+\theta_k)$ as pointed out in appendix B. The agreement between (3.7) and the corrections in eqns. (5.7,5.11,5.12) shows that this dependence drops out after the limit $L\to\infty$, which is far from trivial, albeit required for overall consistency.

6 Conclusions and outlook

The main result of this paper is eqn. (3.3) (or its generalization (3.5)) which provides a way to evaluate finite temperature expectation values of boundary operators in terms of form factors.

At first sight all the rest of the argument (i.e. the low-temperature expansion using the finite volume regularization) is only developed in order to verify this conjecture. However, as already pointed out for the bulk case discussed in [6], the finite volume regulator can be used to evaluate two-point (or even higher) correlation functions at finite temperature. There has been some development in the bulk case [5, 15, 18, 19, 20], but there is a general problem that the regulator imposed to deal with the disconnected contributions is rather ad hoc. The failure of Delfino's proposal for the bulk finite temperature expectation values [22, 23] shows that the ambiguity inherent in the regularization procedure (which is manifested in the directional dependence of the diagonal limit discussed in subsection 4.2 and appendix B) must be taken seriously.

However, as pointed out already in [6], finite volume as a regulator is guaranteed to give a correct answer as a matter of principle, since it provides a physical way to regularize the form factors entering the expansion. Therefore it would be very interesting to apply the ideas presented in [6] and here to compute bulk and boundary two-point functions, respectively.

Another interesting issue is to obtain an extension of the finite volume description of form factors to non-diagonal scattering theories, both in the bulk and on the boundary. Since the description of finite volume energy levels is known and is not very complicated (one obtains scalar Bethe-Yang equations after suitably diagonalizing a family of commuting transfer matrices, cf. [21] and references therein), it can be expected that the necessary description of form factors is not too difficult to find. One can then use these results to evaluate finite temperature averages and correlators in the non-diagonal case as well.

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A Low-temperature expansion of the conjectured formula (3.1)

First the pseudo-energy function $\epsilon(\theta)$ must be expanded to the necessary order. Using the fact that $\epsilon(\theta)$ is an even function, the TBA equation can be written in the form

$$\epsilon(\theta) = mR\cosh(\theta) - \int_0^\infty \frac{d\theta'}{2\pi}\left[\varphi(\theta-\theta')+\varphi(\theta+\theta')\right]\log(1+\mathrm{e}^{-\epsilon(\theta')})$$

Iterating this equation twice with the starting value $\epsilon^{(0)}(\theta) = mR\cosh(\theta)$ and taking care to expand the logarithm one obtains

$$\begin{aligned}\epsilon(\theta_1) &= RE_1 - \int_0^\infty \frac{d\theta_2}{2\pi}\Phi_{12}\mathrm{e}^{-RE_2} - \frac{1}{2}\int_0^\infty \frac{d\theta_2}{2\pi}\Phi_{12}\mathrm{e}^{-2RE_2} \\ &- \int_0^\infty \frac{d\theta_2}{2\pi}\int_0^\infty \frac{d\theta_3}{2\pi}\Phi_{12}\Phi_{23}\mathrm{e}^{-R(E_2+E_3)} + O\left(\mathrm{e}^{-3mR}\right)\end{aligned}$$

where

$$E_i = m\cosh\theta_i \quad , \quad \Phi_{ij} = \varphi(\theta_i-\theta_j)+\varphi(\theta_i+\theta_j)$$

which leads to

$$\begin{aligned}\mathrm{e}^{-\epsilon(\theta_1)} &= \mathrm{e}^{-RE_1} + \mathrm{e}^{-RE_1}\int_0^\infty \frac{d\theta_2}{2\pi}\Phi_{12}\mathrm{e}^{-RE_2} \\ &+\frac{1}{2}\mathrm{e}^{-RE_1}\left(\int_0^\infty \frac{d\theta_2}{2\pi}\Phi_{12}\mathrm{e}^{-RE_2}\right)^2 - \frac{1}{2}\mathrm{e}^{-RE_1}\int_0^\infty \frac{d\theta_2}{2\pi}\Phi_{12}\mathrm{e}^{-2RE_2} \\ &+\mathrm{e}^{-RE_1}\int_0^\infty \frac{d\theta_2}{2\pi}\int_0^\infty \frac{d\theta_3}{2\pi}\Phi_{12}\Phi_{23}\mathrm{e}^{-R(E_2+E_3)} + O\left(\mathrm{e}^{-4mR}\right)\end{aligned} \tag{A.1}$$

Recall that (3.3) reads

$$\langle\mathcal{O}\rangle^R = \sum_{n=0}^{\infty}\frac{1}{n!}\prod_{i=1}^{n}\left(\int_0^{\infty}\frac{d\theta_i}{2\pi}\frac{\mathrm{e}^{-\epsilon(\theta_i)}}{1+\mathrm{e}^{-\epsilon(\theta_i)}}\right)F_{2n}^c(\theta_1,...,\theta_n)$$

Using (A.1) and the geometric series

$$\frac{\mathrm{e}^{-\epsilon}}{1+\mathrm{e}^{-\epsilon}} = \mathrm{e}^{-\epsilon}-\mathrm{e}^{-2\epsilon}+\mathrm{e}^{-3\epsilon}+\dots$$

this can be expanded in orders of e^{-mR}. One obtains

$$\langle\mathcal{O}\rangle^R = \sigma_1+\sigma_2+\sigma_3+O\left(\mathrm{e}^{-4mR}\right) \tag{A.2}$$

where

$$\begin{aligned}
\sigma_1 &= \int_0^{\infty}\frac{d\theta_1}{2\pi}\left(\mathrm{e}^{-RE_1}-\mathrm{e}^{-2RE_1}+\mathrm{e}^{-3RE_1}\right)F_2^c(\theta_1)+\int_0^{\infty}\frac{d\theta_1}{2\pi}\int_0^{\infty}\frac{d\theta_2}{2\pi}\mathrm{e}^{-R(E_1+E_2)}\Phi_{12}F_2^c(\theta_1)\\
&+\frac{1}{2}\int_0^{\infty}\frac{d\theta_1}{2\pi}\int_0^{\infty}\frac{d\theta_2}{2\pi}\int_0^{\infty}\frac{d\theta_3}{2\pi}\mathrm{e}^{-R(E_1+E_2+E_3)}\left(\Phi_{12}\Phi_{13}+\Phi_{12}\Phi_{23}+\Phi_{13}\Phi_{23}\right)F_2^c(\theta_1)\\
&-\int_0^{\infty}\frac{d\theta_1}{2\pi}\int_0^{\infty}\frac{d\theta_2}{2\pi}\left(2\mathrm{e}^{-R(2E_1+E_2)}+\frac{1}{2}\mathrm{e}^{-R(E_1+2E_2)}\right)\Phi_{12}F_2^c(\theta_1)\\
\sigma_2 &= \frac{1}{2}\int_0^{\infty}\frac{d\theta_1}{2\pi}\int_0^{\infty}\frac{d\theta_2}{2\pi}\mathrm{e}^{-R(E_1+E_2)}F_4^c(\theta_1,\theta_2)\\
&-\int_0^{\infty}\frac{d\theta_1}{2\pi}\int_0^{\infty}\frac{d\theta_2}{2\pi}\mathrm{e}^{-R(2E_1+E_2)}F_4^c(\theta_1,\theta_2)\\
&+\frac{1}{2}\int_0^{\infty}\frac{d\theta_1}{2\pi}\int_0^{\infty}\frac{d\theta_2}{2\pi}\int_0^{\infty}\frac{d\theta_3}{2\pi}\mathrm{e}^{-R(E_1+E_2+E_3)}\left(\Phi_{13}+\Phi_{23}\right)F_4^c(\theta_1,\theta_2)\\
\sigma_3 &= \frac{1}{6}\int_0^{\infty}\frac{d\theta_1}{2\pi}\int_0^{\infty}\frac{d\theta_2}{2\pi}\int_0^{\infty}\frac{d\theta_3}{2\pi}\mathrm{e}^{-R(E_1+E_2+E_3)}F_6^c(\theta_1,\theta_2,\theta_3)
\end{aligned} \tag{A.3}$$

are the one/two/three-particle contributions expanded to $O(\mathrm{e}^{-4mR})$.

B Relation between different evaluations of the diagonal matrix element

Here the arguments of [6] are generalized to the case of boundary form factors. The goal is to compute the general expression

$$F_{a_1\dots a_n}(\theta_1,\dots,\theta_n|\epsilon_1,\dots,\epsilon_n) = F_{\bar{a}_n\dots\bar{a}_1a_1\dots a_n}(\theta_n+i\pi+\epsilon_n,...,\theta_1+i\pi+\epsilon_1,\theta_1,...,\theta_n) \tag{B.1}$$

for infinitesimal values of the ϵ_i. It is also interesting to consider the symmetric evaluation

$$F^s_{a_1\dots a_n}(\theta_1,\dots,\theta_n) = \lim_{\epsilon\to 0}F_{\bar{a}_n\dots\bar{a}_1a_1\dots a_n}(\theta_n+i\pi+\epsilon,...,\theta_1+i\pi+\epsilon,\theta_1,...,\theta_n) \tag{B.2}$$

Let us take n vertices labeled by the numbers $1,2,\dots,n$ and let G be the set of the directed graphs G_i with the following properties:

- G_i is tree-like.
- For each vertex there is at most one outgoing edge.

For an edge going from i to j we use the notation E_{ij}.

Theorem 1 (B.1) can be evaluated as a sum over all graphs in G, where the contribution of a graph G_i is given by the following two rules:

- Let $A_i = \{\alpha_1, \alpha_2, \dots, \alpha_m\}$ be the set of vertices from which there are no outgoing edges in G_i. The form factor associated to G_i is

$$F^c_{a_{\alpha_1} \dots a_{\alpha_m}}(\theta_{a_1}, \theta_{a_2}, \dots, \theta_{a_m}) \tag{B.3}$$

- For each edge E_{jk} the form factor above has to be multiplied by

$$\frac{\epsilon_j}{\epsilon_k}\Phi_{jk}$$

  where

$$\Phi_{jk} = \varphi_{a_j a_k}(\theta_j - \theta_k) + \varphi_{a_j a_k}(\theta_j + \theta_k) = \Phi_{kj}$$

Proof The proof goes by induction in n. For $n = 1$ there is only a single way to take the limit and so

$$F_a(\theta_1|\epsilon_1) = F^c_a(\theta_1) = F_{\bar{a}a}(i\pi + \theta_1, \theta_1)$$

This is in accordance with the theorem, because for $n = 1$ there is only the trivial graph which contains no edges and a single node.

Now assume that the theorem is true for $n - 1$ and let us take the case of n particles. Consider the residue of the matrix element (B.1) at $\epsilon_n = 0$ while keeping all the ϵ_i finite

$$R = \operatorname*{Res}_{\epsilon_n = 0} F_{a_1 \dots a_n}(\theta_1..\theta_n|\epsilon_1..\epsilon_n)$$

According to the theorem the graphs contributing to this residue are exactly those for which the vertex n has an outgoing edge and no incoming edges. Let R_j be sum of the diagrams where the outgoing edge is E_{nj} for some $j = 1, \dots, n-1$, and so

$$R = \sum_{j=1}^{n-1} R_j$$

The form factors appearing in R_j do not depend on θ_n. Therefore one gets exactly the diagrams that are needed to evaluate $F_{2(n-1)}(\theta_1..\theta_{n-1}|\epsilon_1..\epsilon_{n-1})$, apart from the proportionality factor associated to the link E_{nj} and so

$$R_j = \epsilon_j \Phi_{jn} F_{a_1 \dots a_{n-1}}(\theta_1..\theta_{n-1}|\epsilon_1..\epsilon_{n-1})$$

and summing over j yields

$$R = (\epsilon_1\Phi_{1n} + \epsilon_2\Phi_{2n} + \dots + \epsilon_{n-1}\Phi_{n-1\,n}) F_{a_1 \dots a_{n-1}}(\theta_1..\theta_{n-1}|\epsilon_1..\epsilon_{n-1}) \tag{B.4}$$

In order to prove the theorem, one only needs to show that the residue indeed takes this form. On the other hand, using the kinematical residue axiom (2.6)

$$\begin{aligned} R &= i\left(1 - \prod_{j=1}^{n-1} S_{a_n a_j}(\theta_n - \theta_j) S_{a_n a_j}(\theta_n - \theta_j - i\pi - \epsilon_j) S_{a_n a_j}(\theta_n + \theta_i) S_{a_n a_j}(\theta_n + \theta_j + i\pi + \epsilon_j)\right) \\ &\quad \times F_{a_1 \dots a_{n-1}}(\theta_1..\theta_{n-1}|\epsilon_1..\epsilon_{n-1}) \end{aligned}$$

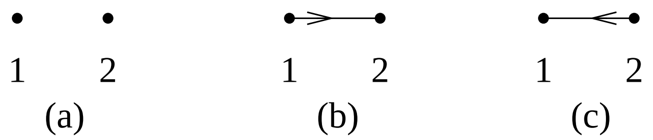

Figure B.1: The graphs relevant for $n = 2$

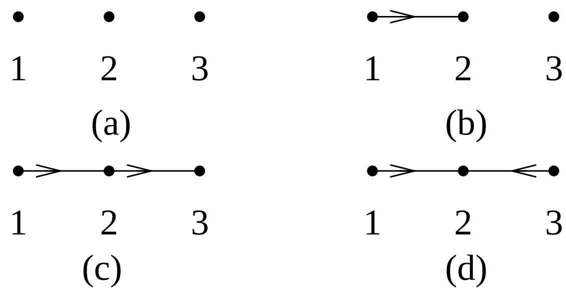

Figure B.2: The graphs relevant for $n = 3$

which is exactly the same as eqn. (B.4) when expanded to first order in ϵ_j.

Therefore the procedure described in the theorem gives the correct result for the terms that include a $1/\epsilon_n$ singularity. Using symmetry in the rapidity variables this is true for all the terms that include at least one $1/\epsilon_i$ for an arbitrary i. There is only one diagram that cannot be generated by the inductive procedure, namely the empty graph. However, there are no singularities ($1/\epsilon_i$ factors) associated to it, and it is identical to $F^c_{2n}(\theta_1, \ldots, \theta_n)$ by definition. *Qed.*

Let us now illustrate how the theorem works for the case of a theory with a single particle species. In this case one can use the simplified notation introduced in (3.4) and similarly denote

$$F_{2n}(\theta_1, \ldots, \theta_n|\epsilon_1, \ldots, \epsilon_n) = F(\theta_n + i\pi + \epsilon_n, ..., \theta_1 + i\pi + \epsilon_1, \theta_1, ..., \theta_n)$$

The case $n = 1$ is trivial:

$$F^c_2(\theta) = F^s_2(\theta) \tag{B.5}$$

For $n = 2$, there are only three graphs, depicted in figure B.1. Applying the rules yields

$$F_4(\theta_1, \theta_2|\epsilon_1, \epsilon_2) = F^c_4(\theta_1, \theta_2) + \Phi_{12}\left(\frac{\epsilon_1}{\epsilon_2}F^c_2(\theta_2) + \frac{\epsilon_2}{\epsilon_1}F^c_2(\theta_1)\right)$$

which yields

$$F^s_4(\theta_1, \theta_2) = F^c_4(\theta_1, \theta_2) + \Phi_{12}\left(F^c_2(\theta_2) + F^c_2(\theta_1)\right) \tag{B.6}$$

upon putting $\epsilon_1 = \epsilon_2$. For $n = 3$ there are 4 different kinds of graphs, the representatives of which are shown in figure B.2; all other graphs can be obtained by permuting the node labels $1, 2, 3$. The contributions of these graphs are

$$\begin{aligned}
(a) &\;:\; F_6^c(\theta_1,\theta_2,\theta_3) \\
(b) &\;:\; \frac{\epsilon_2}{\epsilon_1}\Phi_{12}F_4^c(\theta_2,\theta_3) \\
(c) &\;:\; \frac{\epsilon_2}{\epsilon_1}\frac{\epsilon_3}{\epsilon_2}\Phi_{12}\Phi_{23}F_2^c(\theta_3) = \frac{\epsilon_3}{\epsilon_1}\Phi_{12}\Phi_{23}F_2^c(\theta_3) \\
(d) &\;:\; \frac{\epsilon_2}{\epsilon_1}\frac{\epsilon_2}{\epsilon_3}\Phi_{12}\Phi_{23}F_2^c(\theta_2)
\end{aligned}$$

Adding up all the contributions and putting $\epsilon_1 = \epsilon_2 = \epsilon_3$:

$$\begin{aligned}
F_6^s(\theta_1,\theta_2,\theta_3) &= F_6^c(\theta_1,\theta_2,\theta_3) \\
&+ (\Phi_{12}+\Phi_{13})F_4^c(\theta_2,\theta_3) + (\Phi_{12}+\Phi_{23})F_4^c(\theta_1,\theta_3) + (\Phi_{13}+\Phi_{23})F_4^c(\theta_1,\theta_2) \\
&+ (F_2^c(\theta_1)+F_2^c(\theta_2)+F_2^c(\theta_3))(\Phi_{12}\Phi_{13}+\Phi_{12}\Phi_{23}+\Phi_{13}\Phi_{23}) \qquad \text{(B.7)}
\end{aligned}$$

It can be seen that these results are a natural generalization of the bulk ones obtained in [6] with φ replaced by Φ. It is also important to keep in mind that contrary to the bulk situation F_2^c depends on the rapidity (in the bulk it is a constant since Lorentz invariance entails that all form factors depend only on rapidity differences).

Now the finite volume diagonal matrix elements (4.8) can also be re-expressed in terms of the symmetric evaluation. The first nontrivial case is $n = 2$ for which

$$\begin{aligned}
\langle\{I_1,I_2\}|\mathcal{O}(0)|\{I_1,I_2\}\rangle &= \frac{1}{\rho_2(\tilde\theta_1,\tilde\theta_2)}\Big(F_4^c(\tilde\theta_1,\tilde\theta_2) + \tilde\rho(\tilde\theta_1,\tilde\theta_2|\{1\})F_2^c(\tilde\theta_1) \\
&\quad +\tilde\rho(\tilde\theta_1,\tilde\theta_2|\{2\})F_2^c(\tilde\theta_2)\Big) + \langle\mathcal{O}\rangle + O(\mathrm{e}^{-\mu L})
\end{aligned}$$

where $\tilde\theta_1, \tilde\theta_2$ are the solutions of the 2-particle Bethe-Yang equations with quantum numbers I_1, I_2. $\tilde\rho$ denotes the appropriate sub-determinants (4.10) of the two-particle Jacobian matrix, while ρ_n is the full n-particle Jacobi determinant (4.4). It is straightforward to verify that

$$\begin{aligned}
F_4^c(\theta_1,\theta_2) + \tilde\rho(\theta_1,\theta_2|\{1\})F_2^c(\theta_1) + \tilde\rho(\theta_1,\theta_2|\{2\})F_2^c(\theta_2) = \\
F_4^s(\theta_1,\theta_2) + \rho_1(\theta_1)F_2^s(\theta_1) + \rho_1(\theta_2)F_2^s(\theta_2) \\
+2\varphi(\theta_1+\theta_2)\left(F_2^s(\theta_1)+F_2^s(\theta_2)\right) \qquad \text{(B.8)}
\end{aligned}$$

The term on the last line shows that the analogue of Theorem 2 in [6] (which would make the expressions on the first two lines identical) fails in the boundary case. This results from the fact that the derivative matrix (4.5) of the Bethe-Yang equations (4.2) carries a dependence not only on the combination $\varphi(\theta_j-\theta_k)+\varphi(\theta_j+\theta_k)$, but also on $\varphi(\theta_j-\theta_k)-\varphi(\theta_j+\theta_k)$.

The relations (B.6), (B.7) and (B.8) were also verified numerically using the explicit form factor solutions presented in [7].

C e^{-3mR} corrections to the finite temperature one-point function

In order to keep the calculation manageable, let us introduce the following shortened notations:

$$\begin{aligned}
&E_i = m\cosh\theta_i \\
&\langle\theta_1,\dots,\theta_n|\mathcal{O}|\theta_1,\dots,\theta_n\rangle_L = \langle 1\dots n|\mathcal{O}|1\dots n\rangle_L \\
&\rho(\theta_1,\dots,\theta_n) = \rho(1\dots n) \\
&\tilde{\rho}(\theta_1,\dots,\theta_n|\{a_1,\dots,a_k\}) = \tilde{\rho}(1\dots n|\{a_1,\dots,a_k\})
\end{aligned}$$

Summations will be shortened to

$$\begin{aligned}
\sum_{\theta_1\dots\theta_n} &\to \sum_{1\dots n} \\
\sum_{\theta_1\dots\theta_n}{}' &\to \sum_{1\dots n}{}'
\end{aligned}$$

and for later convenience also denote

$$\Phi_{ij} = \varphi(\theta_i-\theta_j)+\varphi(\theta_i+\theta_j)$$

which satisfies $\Phi_{ij}=\Phi_{ji}$.

Multiplying (5.2) with (5.4) and collecting the third order correction terms:

$$\begin{aligned}
&\frac{1}{6}\sum_{123}{}'\mathrm{e}^{-R(E_1+E_2+E_3)}\left(\langle 123|\mathcal{O}|123\rangle_L-\langle\mathcal{O}\rangle_L\right) \\
-\;&\left(\sum_1 \mathrm{e}^{-RE_1}\right)\frac{1}{2}\sum_{23}{}'\mathrm{e}^{-R(E_2+E_3)}\left(\langle 23|\mathcal{O}|23\rangle_L-\langle\mathcal{O}\rangle_L\right) \\
+\;&\left\{\left(\sum_1 \mathrm{e}^{-RE_1}\right)\left(\sum_2 \mathrm{e}^{-RE_2}\right)-\frac{1}{2}\sum_{12}{}'\mathrm{e}^{-R(E_1+E_2)}\right\}\left(\sum_3 \mathrm{e}^{-RE_3}\right)\left(\langle 3|\mathcal{O}|3\rangle_L-\langle\mathcal{O}\rangle_L\right)
\end{aligned}$$

To keep trace of the state densities it is important to avoid combining rapidity sums. The constrained summations can be replaced by free sums with the diagonal contributions subtracted:

$$\begin{aligned}
\sum_{12}{}' &= \sum_{12}-\sum_{1=2} \\
\sum_{123}{}' &= \sum_{123}-\left(\sum_{1=2,3}+\sum_{2=3,1}+\sum_{1=3,2}\right)+2\sum_{1=2=3}
\end{aligned}$$

where the diagonal contributions are labeled according to which diagonal the summation corresponds to, but otherwise the given sum is free, e.g.

$$\sum_{1=2,3}$$

shows a summation over all triplets $\theta_1^{(3)}, \theta_2^{(3)}, \theta_3^{(3)}$ where $\theta_1^{(3)} = \theta_2^{(3)}$ and $\theta_3^{(3)}$ runs free (it can also be equal with the other two). Finally denote

$$F(12\dots n) = F_{2n}^c(\theta_1, \dots, \theta_n)$$

so from (5.5) the necessary matrix elements can be written in the form

$$\begin{aligned}
\rho(123)\left(\langle 123|\mathcal{O}|123\rangle_L - \langle\mathcal{O}\rangle_L\right) &= F(123) + \tilde{\rho}(123|\{1,2\})F(12) \\
&\quad + \tilde{\rho}(123|\{1,3\})F(13) + \tilde{\rho}(123|\{2,3\})F(23) \\
&\quad + \tilde{\rho}(123|\{1\})F(1) + \tilde{\rho}(123|\{2\})F(2) + \tilde{\rho}(123|\{3\})F(3) \\
\rho(122)\left(\langle 122|\mathcal{O}|122\rangle_L - \langle\mathcal{O}\rangle_L\right) &= 2\tilde{\rho}(122|\{1,2\})F(12) + \tilde{\rho}(122|\{1\})F(1) + 2\tilde{\rho}(122|\{2\})F(2) \\
\rho(111)\left(\langle 111|\mathcal{O}|111\rangle_L - \langle\mathcal{O}\rangle_L\right) &= 3\tilde{\rho}(111|\{1\})F(1) \\
\rho(12)\left(\langle 12|\mathcal{O}|12\rangle_L - \langle\mathcal{O}\rangle_L\right) &= F(12) + \tilde{\rho}(12|\{1\})F(1) + \tilde{\rho}(12|\{2\})F(2) \\
\rho(11)\left(\langle 11|\mathcal{O}|11\rangle_L - \langle\mathcal{O}\rangle_L\right) &= 2\tilde{\rho}(11|\{1\})F(1) \\
\rho(1)\left(\langle 1|\mathcal{O}|1\rangle_L - \langle\mathcal{O}\rangle_L\right) &= F(1)
\end{aligned} \tag{C.1}$$

where the exclusion property was already used to eliminate form factors with equal rapidity arguments.

One can now proceed by collecting terms according to the number of free rapidity variables. The terms containing threefold summation are

$$\begin{aligned}
\Sigma_3^{(3)} &= \frac{1}{6}\sum_{123} \mathrm{e}^{-R(E_1+E_2+E_3)}\left(\langle 123|\mathcal{O}|123\rangle_L - \langle\mathcal{O}\rangle_L\right) - \frac{1}{2}\sum_{1}\sum_{2,3}\left(\langle 23|\mathcal{O}|23\rangle_L - \langle\mathcal{O}\rangle_L\right) \\
&+ \left(\sum_1\sum_2\sum_3 - \frac{1}{2}\sum_{1,2}\sum_3\right)\left(\langle 3|\mathcal{O}|3\rangle_L - \langle\mathcal{O}\rangle_L\right)
\end{aligned}$$

Replacing the sums with integrals

$$\begin{aligned}
\sum_1 &\to \int \frac{d\theta_1}{2\pi}\rho(1) \\
\sum_{1,2} &\to \int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\rho(12) \\
\sum_{1,2,3} &\to \int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}\rho(123)
\end{aligned}$$

and using (C.1)

$$\begin{aligned}
\Sigma_3^{(3)} &= \frac{1}{6}\int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}\mathrm{e}^{-R(E_1+E_2+E_3)}\left(F(123) + 3\tilde{\rho}(123|\{2,3\})F(23) + 3\tilde{\rho}(123|\{3\})F(3)\right) \\
&- \frac{1}{2}\int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}\mathrm{e}^{-R(E_1+E_2+E_3)}\rho(1)\left(F(23) + 2\rho(23|\{3\})F(3)\right) \\
&+ \int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\frac{d\theta_3}{2\pi}\mathrm{e}^{-R(E_1+E_2+E_3)}\left(\rho(1)\rho(2) - \frac{1}{2}\rho(12)\right)F(3)
\end{aligned}$$

where some of the integration variables were reshuffled. The result is

$$\begin{aligned}\Sigma_3^{(3)} &= \frac{1}{6}\int_0^\infty \frac{d\theta_1}{2\pi}\int_0^\infty \frac{d\theta_2}{2\pi}\int_0^\infty \frac{d\theta_3}{2\pi} \mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2+\cosh\theta_3)}\Big[F_6^c(\theta_1,\theta_2,\theta_3)\\ &+3F_4^c(\theta_2,\theta_3)(\Phi_{12}+\Phi_{13})+3F_2^c(\theta_3)(\Phi_{12}\Phi_{13}+\Phi_{12}\Phi_{23}+\Phi_{13}\Phi_{23})\Big] \qquad \text{(C.2)}\end{aligned}$$

(to derive the term on the second line note that the $F(3)$ terms in the integrand of $\Sigma_3^{(3)}$ can be symmetrized in θ_1 and θ_2 without changing the value of the integral).

It is also easy to deal with terms containing a single integral. The only term of this form is

$$\Sigma_3^{(1)} = \frac{1}{3}\sum_{1=2=3} \mathrm{e}^{-R(E_1+E_2+E_3)}\left(\langle 123|\mathcal{O}|123\rangle_L - \langle\mathcal{O}\rangle_L\right)$$

When all rapidities $\theta_1^{(3)},\theta_2^{(3)},\theta_3^{(3)}$ are equal, the three-particle Bethe-Yang equations reduce to[3]

$$2mL\sinh\theta_1^{(3)} + 2\delta\left(2\theta_1^{(3)}\right) + \delta^{(\alpha)}\left(\theta_1^{(3)}\right) + \delta^{(\beta)}\left(\theta_1^{(3)}\right) = 2\pi I_1$$

Therefore the relevant state density is

$$\bar\rho_{123}(\theta) = 2mL\cosh\theta + 4\varphi(2\theta) + \psi^{(\alpha)}(\theta) + \psi^{(\beta)}(\theta)$$

and

$$\begin{aligned}\Sigma_3^{(1)} &= \frac{1}{3}\int\frac{d\theta_1}{2\pi}\mathrm{e}^{-3RE_1}\bar\rho_{123}(\theta_1)\left(\langle 111|\mathcal{O}|111\rangle_L - \langle\mathcal{O}\rangle_L\right)\\ &= \int\frac{d\theta_1}{2\pi}\mathrm{e}^{-3RE_1}\rho(1)\frac{\tilde\rho(111|\{1\})}{\rho(111)}F(1) \underset{L\to\infty}{\to} \int\frac{d\theta_1}{2\pi}\mathrm{e}^{-3mR\cosh\theta_1}F_2^c(\theta_1) \qquad \text{(C.3)}\end{aligned}$$

where it was used that

$$\rho(1)\frac{\tilde\rho(111|\{1\})}{\rho(111)} \to 1$$

when $L\to\infty$.

The calculation of double integral terms is much more involved. The contributions containing two rapidity summations are

$$\begin{aligned}\Sigma_3^{(2)} &= -\frac{1}{6}\left(\sum_{1=2,3}+\sum_{1=3,2}+\sum_{2=3,1}\right)\mathrm{e}^{-R(E_1+E_2+E_3)}\left(\langle 123|\mathcal{O}|123\rangle_L - \langle\mathcal{O}\rangle_L\right)\\ &+\frac{1}{2}\sum_{1}\sum_{2=3}\mathrm{e}^{-R(E_1+E_2+E_3)}\left(\langle 23|\mathcal{O}|23\rangle_L - \langle\mathcal{O}\rangle_L\right)\\ &+\frac{1}{2}\sum_{1=2}\sum_{3}\mathrm{e}^{-R(E_1+E_2+E_3)}\left(\langle 3|\mathcal{O}|3\rangle_L - \langle\mathcal{O}\rangle_L\right) \qquad \text{(C.4)}\end{aligned}$$

The density of partially degenerate two-particle states was already computed in (5.10), but the density of partially degenerate three-particle states is also needed. The relevant Bethe-Yang

[3]Just as in (5.9) there are also contributions of the form $\delta(0)$, but these can be absorbed into a redefinition of I_1.

equations are[4]

$$\begin{aligned} 2mL\sinh\theta_1+\delta(\theta_1-\theta_2)+\delta(\theta_1+\theta_2)+\delta(2\theta_1)+\delta^{(\alpha)}(\theta_1)+\delta^{(\beta)}(\theta_1) &= 2\pi I_1 \\ 2mL\sinh\theta_2+2\delta(\theta_2-\theta_1)+2\delta(\theta_2+\theta_1)+\delta^{(\alpha)}(\theta_2)+\delta^{(\beta)}(\theta_2) &= 2\pi I_2 \end{aligned}$$

where the first and the third particles are put as degenerate (i.e. $I_3 = I_1$). The density of these degenerate states is then

$$\begin{aligned} \bar\rho_{13,2}(12) &= \det\begin{pmatrix} r_{11} & r_{12} \\ r_{21} & r_{22}\end{pmatrix} \qquad \text{(C.5)} \\ & r_{11} = 2LE_1+\varphi(\theta_1-\theta_2)+\varphi(\theta_1+\theta_2)+2\varphi(2\theta_1)+\psi^{(\alpha)}(\theta)+\psi^{(\beta)}(\theta) \\ & r_{22} = 2LE_2+2\varphi(\theta_1-\theta_2)+2\varphi(\theta_1+\theta_2)+\psi^{(\alpha)}(\theta)+\psi^{(\beta)}(\theta) \\ & r_{12} = -\varphi(\theta_1-\theta_2)+\varphi(\theta_1+\theta_2) \quad , \quad r_{21} = -2\varphi(\theta_1-\theta_2)+2\varphi(\theta_1+\theta_2) \end{aligned}$$

where it was used that $\varphi(\theta) = \varphi(-\theta)$. Using the above result and substituting integrals for the sums, eqn. (C.4) can be rewritten in the form

$$\begin{aligned} &- \frac{1}{6}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\mathrm{e}^{-R(2E_1+E_2)}\frac{\bar\rho_{13,2}(12)}{\rho(112)}\Big[2\tilde\rho(112|\{2,3\})F(12) \\ &\quad +2\tilde\rho(112|\{1\})F(1)+\tilde\rho(112|\{3\})F(2)+\dots\Big] \\ &+ \frac{1}{2}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\mathrm{e}^{-R(E_1+2E_2)}\rho(1)\bar\rho_{12}(2)\frac{2\tilde\rho(22|\{1\})}{\rho(22)}F(2) \\ &+ \frac{1}{2}\int\frac{d\theta_1}{2\pi}\frac{d\theta_3}{2\pi}\mathrm{e}^{-R(2E_1+E_3)}\bar\rho_{12}(1)\rho(3)\frac{1}{\rho(3)}F(3) \end{aligned}$$

where the ellipsis denote additional contributions that can be obtained by cyclical permutation of the indices $1,2,3$ from those explicitly displayed inside the square bracket. These three sets of contributions can be shown to be equal to each other by relabeling the integration variables:

$$\begin{aligned} &- \frac{1}{2}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\mathrm{e}^{-R(2E_1+E_2)}\frac{\bar\rho_{13,2}(12)}{\rho(112)}\Big[2\tilde\rho(112|\{2,3\})F(12) \\ &\quad +2\tilde\rho(112|\{1\})F(1)+\tilde\rho(112|\{3\})F(2)\Big] \\ &+ \frac{1}{2}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\mathrm{e}^{-R(2E_1+E_2)}\rho(2)\bar\rho_{12}(1)\frac{2\tilde\rho(11|\{1\})}{\rho(11)}F(1) \\ &+ \frac{1}{2}\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\mathrm{e}^{-R(2E_1+E_2)}\bar\rho_{12}(1)F(2) \qquad \text{(C.6)} \end{aligned}$$

The terms containing $F(12)$ contribute

$$-\int\frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}F_4^c(\theta_1,\theta_2)\mathrm{e}^{-mR(\cosh\theta_1+2\cosh\theta_2)} \qquad \text{(C.7)}$$

where it was used that

$$\frac{\bar\rho_{13,2}(12)}{\rho(112)}\tilde\rho(112|\{2,3\}) = 1+O(L^{-1})$$

[4]Just as in (5.9) there are also contributions of the form $\delta(0)$, but these can be absorbed into a redefinition of I_1.

which results from (C.5) and

$$\tilde{\rho}(112|\{2,3\}) = 2mL\cosh\theta_1 + 2\varphi(0) + 2\varphi(2\theta_1) + +\psi^{(\alpha)}(\theta) + \psi^{(\beta)}(\theta)$$

The terms containing $F(1)$ and $F(2)$ combine to

$$\int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\mathrm{e}^{-R(2E_1+E_2)}\left(-\frac{\bar{\rho}_{13,2}(12)}{\rho(112)}\tilde{\rho}(112|\{1\}) + \rho(2)\bar{\rho}_{12}(1)\frac{\tilde{\rho}(11|\{1\})}{\rho(11)}\right)F(1) +$$
$$\frac{1}{2}\int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\mathrm{e}^{-R(2E_1+E_2)}\left(-\frac{\bar{\rho}_{13,2}(12)}{\rho(112)}\tilde{\rho}(112|\{3\}) + \bar{\rho}_{12}(1)\right)F(2)$$

A straightforward (albeit tedious) calculation leads to

$$\begin{aligned}
-\frac{\bar{\rho}_{13,2}(12)}{\rho(112)}\tilde{\rho}(112|\{1\}) + \rho(2)\bar{\rho}_{12}(1)\frac{\tilde{\rho}(11|\{1\})}{\rho(11)} &= -2(\varphi(\theta_1-\theta_2)+\varphi(\theta_1+\theta_2)) + O\left(L^{-1}\right)\\
-\frac{\bar{\rho}_{13,2}(12)}{\rho(112)}\tilde{\rho}(112|\{3\}) + \bar{\rho}_{12}(1) &= -\varphi(\theta_1-\theta_2)-\varphi(\theta_1+\theta_2) + O\left(L^{-1}\right)
\end{aligned}$$

Note that the individual terms in these sums are proportional to L but their contributions drops out. For a more detailed discussion of such "anomalous" density contributions the reader is referred to [6].

The total contribution in the $L\to\infty$ limit turns out to be just

$$-\int \frac{d\theta_1}{2\pi}\frac{d\theta_2}{2\pi}\mathrm{e}^{-mR(\cosh\theta_1+2\cosh\theta_2)}(2F_2^c(\theta_1)+\frac{1}{2}F_2^c(\theta_2))(\varphi(\theta_1-\theta_2)+\varphi(\theta_1+\theta_2)) \qquad (C.8)$$

Summing up the contributions (C.2), (C.3), (C.7) and (C.8) the end result is

$$\begin{aligned}
\Sigma_3 = &\frac{1}{6}\int_0^\infty \frac{d\theta_1}{2\pi}\int_0^\infty \frac{d\theta_2}{2\pi}\int_0^\infty \frac{d\theta_3}{2\pi}\mathrm{e}^{-mR(\cosh\theta_1+\cosh\theta_2+\cosh\theta_3)}[F_6^c(\theta_1,\theta_2,\theta_3)\\
&+3F_4^c(\theta_2,\theta_3)(\Phi_{12}+\Phi_{13}) + 3F_2^c(\theta_3)(\Phi_{12}\Phi_{13}+\Phi_{12}\Phi_{23}+\Phi_{13}\Phi_{23})]\\
&-\int_0^\infty \frac{d\theta_1}{2\pi}\int_0^\infty \frac{d\theta_2}{2\pi}\mathrm{e}^{-mR(2\cosh\theta_1+\cosh\theta_2)}[F_4^c(\theta_1,\theta_2) + (2F_2^c(\theta_1)+\frac{1}{2}F_2^c(\theta_2))\Phi_{12}]\\
&+\int_0^\infty \frac{d\theta_1}{2\pi}\mathrm{e}^{-3mR\cosh\theta_1}F_2^c(\theta_1)
\end{aligned} \qquad (C.9)$$

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