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On the thermodynamic limit of form factors in the massless XXZ Heisenberg chain

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Abstract

We consider the problem of computing form factors of the massless XXZ Heisenberg spin-1/2 chain in a magnetic field in the (thermodynamic) limit where the size M of the chain becomes large. For that purpose, we take the particular example of the matrix element of the operator σ^z between the ground state and an excited state with one particle and one hole located at the opposite ends of the Fermi interval (umklapp-type term). We exhibit its power-law decrease in terms of the size of the chain M, and compute the corresponding exponent and amplitude. As a consequence, we show that this form factor is directly related to the amplitude of the leading oscillating term in the long-distance asymptotic expansion of the correlation function $\langle \sigma_1^z \sigma_{m+1}^z \rangle$.

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1 Introduction

The main purpose of this article is to open a way for the study of the form factors (or in general of the matrix elements of local operators) of the massless XXZ Heisenberg chain in a magnetic field in the limit where the size of the chain becomes large. For that purpose we will consider a particular matrix element of the local spin operator σ^z between the ground state and an excited state with one particle and one hole located at the opposite ends of the Fermi interval (umklapp-type term). Although the present article is devoted to this special case, it will be clear that the method we propose can be applied to more general cases as well.

As already mentioned in our recent work [1], this particular form factor is of direct interest for the computation of the asymptotic behavior of the σ^z two-point correlation function. Let us briefly recall how it appears in this context. In [1] we explained how to compute, from first principles, the long-distance asymptotic behavior of some two-point correlation functions: the longitudinal spin-spin correlation function in the massless phase of the XXZ spin-1/2 Heisenberg chain and also the density-density correlation function of the quantum one-dimensional Bose gas. In particular, for the spin chain, we obtained that the correlation function of the third components of spin behaves at large distance m as

$$\langle\sigma_1^z\sigma_{m+1}^z\rangle - \langle\sigma_1^z\rangle^2 = -\frac{2\mathcal{Z}^2}{\pi^2 m^2} + 2|F_\sigma|^2\cdot\frac{\cos(2mp_F)}{m^{2\mathcal{Z}^2}} \;+\; \text{corrections.} \tag{1.1}$$

In this formula p_F stands for the Fermi momentum and $\mathcal{Z}$ represents the value of the dressed charge on the Fermi boundary, the precise definition of these quantities being postponed to Section 2.2. We announced in [1] that the coefficient F_σ in (1.1) is related to the thermodynamic limit of the properly normalized aforementioned special form factor of the σ^z operator. We prove this statement in this article.

The fact that the coefficient F_σ should be related to this form factor is not really surprising. It is well known that the leading asymptotic behavior of the correlation functions is defined by low-energy excitations in the spectrum of the Hamiltonian. From this assumption, the form of the asymptotics (1.1) was predicted by the Luttinger liquid approach [2, 3, 4, 5, 6, 7, 8] and the conformal field theory [9, 11, 10, 12] together with the analysis of finite size corrections [13, 14, 15, 16, 17, 18, 19, 20, 21]. There the oscillating term in the asymptotic formula corresponds to the process of a particle jumping from one Fermi boundary to the other. One can expect therefore that the numerical coefficient in this term should be somehow related to the corresponding form factor.

However, the precise relationship between the coefficient F_σ and the form factor under consideration has been missing up to now. The first reason is that the methods mentioned above hardly give any prediction for the exact value of the coefficient F_σ: an expression for this amplitude was already given in [30, 31], but only for the case of zero magnetic field, and its physical meaning was not clear. The second reason is the absence of sufficient information about the thermodynamic limit of form factors in massless models. The matter is that, in distinction of massive models in infinite volume for which form factors were successfully calculated in series of works (see e.g. [22, 23, 24, 25]), the thermodynamic limit of the form factors in the massless case have a non-trivial behavior with respect to the size of the system. This phenomenon was observed, apparently for the first time, in [28] for the model of one dimensional bosons. Recently similar results were obtained in [29] for the free fermion limit of the XXZ spin chain. This non-trivial behavior of the form factors with respect to the size of the system makes very difficult their analysis directly in the infinite volume contrary to the case of massive models.

One of the main goal of the present article is to develop a method to resolve this problem. We start with determinant representations for form factors for the *finite* Heisenberg chain [36]. Then, acting in the spirit of works [28, 25], we proceed to the thermodynamic limit of the specific form factor under consideration. This method allows us to obtain its leading (power-law) behavior in terms of the size of the chain and to calculate the corresponding finite amplitude. Remarkably, the exponent governing the power-law decrease of the norm squared of this (umklapp-type) form factor in terms of the size M of the chain is equal to the critical exponent $2\mathcal{Z}^2$ for the corresponding oscillating term in (1.1).

The article is organized as follows. In Section 2, we recall some well known results concerning the XXZ chain, its algebraic Bethe ansatz solution and its thermodynamic limit. The main result of the article is discussed in Section 3: we define more precisely the form factor that we investigate and we write explicitly its relation with the amplitude appearing in (1.1); we also recall the exact expression of this amplitude as computed in [1]. The next sections are devoted to the proof of this result. In Section 4 we remind determinant representations for this form factor in the finite chain that are suited for our analysis. It enables us, in Section 5, to compute its thermodynamic limit. Several technical results concerning this limit are given in the appendices.

2 The XXZ chain: general results

The Hamiltonian of the integrable spin-1/2 XXZ chain, with anisotropy parameter Δ and in an external longitudinal magnetic field h, is given by

$$H = H^{(0)} - hS_z, \tag{2.1}$$

where

$$H^{(0)} = \sum_{m=1}^{M} \left\{ \sigma^x_m \sigma^x_{m+1} + \sigma^y_m \sigma^y_{m+1} + \Delta(\sigma^z_m \sigma^z_{m+1} - 1) \right\}, \tag{2.2}$$

$$S_z = \frac{1}{2} \sum_{m=1}^{M} \sigma^z_m, \qquad [H^{(0)}, S_z] = 0. \tag{2.3}$$

In this expression, as well as in (1.1), $\sigma^{x,y,z}_m$ stand for the local spin operators (in the spin-1/2 representation where they are represented by Pauli matrices) acting non-trivially on the m^{th} site of the chain. The quantum space of states is $\mathcal{H} = \otimes_{m=1}^{M} \mathcal{H}_m$ where $\mathcal{H}_m \sim \mathbb{C}^2$ is the local quantum space at site m. We assume periodic boundary conditions and, for simplicity, the length of the chain M is chosen to be even. Since the simultaneous reversal of all spins is equivalent to a change of sign of the magnetic field, it is enough to consider the case $h \geq 0$.

In the thermodynamic limit ($M \to \infty$) the model exhibits different regimes depending on the values of the anisotropy Δ and magnetic field h [32]. We focus on the massless regime ($|\Delta| < 1$) and assume that the magnetic field is below its critical value h_c [39]. All along this article we use the parameterization $\Delta = \cos\zeta$, $0 < \zeta < \pi$.

2.1 The finite XXZ chain in the algebraic Bethe Ansatz framework

The central object of the algebraic Bethe Ansatz method is the quantum monodromy matrix. In the case of the XXZ chain, it is a 2×2 matrix,

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}, \tag{2.4}$$

with operator-valued entries A, B, C and D acting on the quantum space of states $\mathcal{H}$ of the chain. These operators depend on a complex parameter λ and satisfy a set of quadratic commutation relations driven by the six-vertex R-matrix.

The Hamiltonian $H^{(0)}$ of the XXZ chain is given by a trace identity [33] involving the transfer matrix

$$\mathcal{T}(\lambda) = \operatorname{tr} T(\lambda) = A(\lambda) + D(\lambda). \tag{2.5}$$

The transfer matrices commute for arbitrary values of the spectral parameter, $[\mathcal{T}(\lambda), \mathcal{T}(\mu)] = 0$, and their common eigenstates coincide with those of the Hamiltonian.

The solution of the quantum inverse scattering problem enables us to express local spin operators in terms of the entries of the monodromy matrix [36, 37]:

$$\sigma_k^\alpha = \mathcal{T}^{k-1}(-i\zeta/2) \cdot \operatorname{tr}\big(T(-i\zeta/2)\,\sigma^\alpha\big) \cdot \mathcal{T}^{-k}(-i\zeta/2). \tag{2.6}$$

In the l.h.s. σ_k^α denote a local spin operator at site k, whereas σ^α appearing in the r.h.s. should be understood as a 2×2 Pauli matrix multiplying the 2×2 monodromy matrix.

It turns out to be convenient to introduce a slightly more general object [26], the twisted transfer matrix

$$\mathcal{T}_\kappa(\lambda) = A(\lambda) + \kappa D(\lambda), \tag{2.7}$$

depending on an additional complex parameter κ. For a fixed value of κ, these twisted transfer matrices also commute with each others, $[\mathcal{T}_\kappa(\lambda), \mathcal{T}_\kappa(\mu)] = 0$, and hence possess a common eigenbasis. The latter goes to the one of the Hamiltonian (2.2) in the $\kappa \to 1$ limit.

In the framework of the algebraic Bethe Ansatz, an arbitrary quantum state can be obtained from the states generated by a multiple action of $B(\lambda)$ operators on the reference state $|\,0\,\rangle$ with all spins up (respectively by a multiple action of $C(\lambda)$ operators on the dual reference state $\langle\,0\,|$). Consider the subspace $\mathcal{H}^{(M/2-N)}$ of the space of states $\mathcal{H}$ with a fixed number N of spins down. In this subspace, the eigenstates $|\,\psi_\kappa(\{\mu\})\,\rangle$ (respectively the dual eigenstates $\langle\,\psi_\kappa(\{\mu\})\,|$) of the twisted transfer matrix $\mathcal{T}_\kappa(\nu)$ can be constructed in the form

$$|\,\psi_\kappa(\{\mu\})\,\rangle = \prod_{j=1}^{N} B(\mu_j)|\,0\,\rangle, \qquad \langle\,\psi_\kappa(\{\mu\})\,| = \langle\,0\,|\prod_{j=1}^{N} C(\mu_j)\,, \tag{2.8}$$

where the parameters $\mu_1, \dots, \mu_N$ satisfy the system of twisted Bethe equations

$$\mathcal{Y}_\kappa(\mu_j|\{\mu\}) = 0, \qquad j = 1, \dots, N. \tag{2.9}$$

Here, the function $\mathcal{Y}_\kappa$ is defined as

$$\mathcal{Y}_\kappa(\nu|\{\mu\}) = a(\nu)\prod_{k=1}^{N}\sinh(\mu_k - \nu - i\zeta) + \kappa\, d(\nu)\prod_{k=1}^{N}\sinh(\mu_k - \nu + i\zeta), \tag{2.10}$$

$a(\nu)$, $d(\nu)$ being the eigenvalues of the operators $A(\nu)$ and $D(\nu)$ on the reference state $|\,0\,\rangle$:

$$a(\nu) = \sinh^M\big(\nu - \tfrac{i\zeta}{2}\big), \qquad d(\nu) = \sinh^M\big(\nu + \tfrac{i\zeta}{2}\big). \tag{2.11}$$

The corresponding eigenvalue of $\mathcal{T}_\kappa(\nu)$ on $|\,\psi_\kappa(\{\mu\})\,\rangle$ (or on a dual eigenstate) is

$$\tau_\kappa(\nu|\{\mu\}) = a(\nu)\prod_{k=1}^{N}\frac{\sinh(\mu_k - \nu - i\zeta)}{\sinh(\mu_k - \nu)} + \kappa\, d(\nu)\prod_{k=1}^{N}\frac{\sinh(\nu - \mu_k - i\zeta)}{\sinh(\nu - \mu_k)}. \tag{2.12}$$

Note that all this construction is also valid at $\kappa = 1$, in which case we agree upon omitting the subscript κ in the corresponding quantities.

Not all the solutions to the system (2.9) yield eigenstates of the operator $\mathcal{T}_\kappa(\nu)$. The detailed classification of the pertinent solutions is given in [35] (see also [27]). For those solutions corresponding to the eigenstates (the so-called admissible solutions), the system of the twisted Bethe equations can be recast as

$$\frac{a(\mu_j)}{d(\mu_j)} \prod_{k=1}^{N} \frac{\sinh(\mu_k - \mu_j - i\zeta)}{\sinh(\mu_k - \mu_j + i\zeta)} = -\kappa, \qquad j = 1, \dots, N. \tag{2.13}$$

2.2 Thermodynamic limit

We outline here very briefly the thermodynamic limit of the model, more detailed analysis can be found in [40, 34, 39].

The ground state of the infinite chain with fixed magnetization $\langle\sigma^z\rangle$ can be constructed as the $M \to \infty$ limit of the finite chain ground state (2.8) at $\kappa = 1$. Hereby the limit of the ratio N/M is equal to an average density D whose value is related to the magnetization by $\langle\sigma^z\rangle = 1 - 2D$.

In order to construct the ground state, one first takes the logarithm of the system (2.13) at $\kappa = 1$ and N and M fixed,

$$Mp_0(\mu_j) - \sum_{k=1}^{N} \vartheta(\mu_j - \mu_k) = 2\pi n_j, \qquad j = 1, \dots, N. \tag{2.14}$$

Here $-M/2 < n_j \le M/2$, with $n_j \in \mathbb{Z}$ for N odd and $n_j \in \mathbb{Z} + 1/2$ for N even (recall that M is assumed even). The functions $p_0(\lambda)$ and $\vartheta(\lambda)$,

$$p_0(\lambda) = i \log\left(\frac{\sinh(\frac{i\zeta}{2} + \lambda)}{\sinh(\frac{i\zeta}{2} - \lambda)}\right), \qquad \vartheta(\lambda) = i \log\left(\frac{\sinh(i\zeta + \lambda)}{\sinh(i\zeta - \lambda)}\right), \tag{2.15}$$

are respectively called bare momentum and bare phase (we choose the principal branch of the logarithm). Among all the eigenstates obtained through (2.14), we define the N-particle ground state to be the state with the lowest energy in the sector with N spins down. It is characterized by the (half-)integers $n_j = I_j \equiv j - (N+1)/2$ [40], and the corresponding roots λ_j are real numbers belonging to some interval $[-q, q]$ called the Fermi zone.

At the next step the length of the chain M as well as the number of spins down N are sent to infinity at fixed limiting value of N/M. In this limit the Bethe roots λ_j corresponding to the N-particle ground state condensate, $\lambda_{j+1} - \lambda_j = O(M^{-1})$ (see e.g. [34]), and the system (2.14) turns into a linear integral equation for the spectral density $\rho(\lambda)$ [1].

A standard way to derive this integral equation is to introduce a ground state counting function $\hat{\xi}(\lambda)$. Namely, let $\lambda(\hat{\xi})$ satisfy the functional equation

$$p_0\big(\lambda(\hat{\xi})\big) - \frac{1}{M}\sum_{k=1}^{N} \vartheta\big(\lambda(\hat{\xi}) - \lambda_k\big) = 2\pi\left(\hat{\xi} - \frac{N+1}{2M}\right), \tag{2.16}$$

[1] Although there are evidences that the ground state can be described in that way, strictly speaking, to our knowledge, this statement has been proved only in the case $\Delta \le 0$ [40, 34].

for a given value of $\hat{\xi}$ and with parameters λ_k corresponding to the N-particle ground state. Evidently, $\hat{\xi}(\lambda)$ is the counting function, since $\lambda(\frac{j}{M}) = \lambda_j$ and $\hat{\xi}(\lambda_j) = j/M$ due to equation (2.14). The (finite-size) density of the N-particle ground state is defined by $\hat{\rho}(\lambda) = \mathrm{d}\hat{\xi}/\mathrm{d}\lambda$. From (2.16), it is equal to

$$2\pi\hat{\rho}(\lambda) = p_0'(\lambda) - \frac{1}{M}\sum_{k=1}^{N} K(\lambda - \lambda_k), \tag{2.17}$$

with

$$K(\lambda) = \vartheta'(\lambda) = \frac{\sin 2\zeta}{\sinh(\lambda + i\zeta)\sinh(\lambda - i\zeta)}. \tag{2.18}$$

In the thermodynamic limit, the N-particle density $\hat{\rho}(\lambda)$ goes to the spectral density $\rho(\lambda)$ of the infinite chain with support on a finite interval $[-q, q]$. In this limit, discrete sums of piecewise continuous functions can be replaced by integrals *via* the Euler–Maclaurin summation formula

$$\lim_{N,M\to\infty} \frac{1}{M}\sum_{k=1}^{N} f(\lambda_k) = \lim_{N,M\to\infty} \frac{1}{M}\sum_{k=1}^{N} f\big(\hat{\xi}^{-1}(\tfrac{k}{M})\big) = \int_{-q}^{q} f(\lambda)\,\rho(\lambda)\,\mathrm{d}\lambda. \tag{2.19}$$

Thus, replacing the sum over k by an integral in (2.17), we obtain the integral equation for the density of the infinite chain,

$$\rho(\lambda) + \frac{1}{2\pi}\int_{-q}^{q} K(\lambda - \mu)\,\rho(\mu)\,\mathrm{d}\mu = \frac{1}{2\pi}p_0'(\lambda). \tag{2.20}$$

The average density $D = \lim_{N,M\to\infty} N/M$ is then given by

$$D = \lim_{N,M\to\infty} \frac{1}{M}\sum_{k=1}^{N} 1 = \int_{-q}^{q} \rho(\lambda)\,\mathrm{d}\lambda, \tag{2.21}$$

which defines the integration boundary q in (2.20).

Observe that the definition of the discrete density $\hat{\rho}(\lambda)$ implies that $\rho(\lambda)$ can also be defined as the limiting value

$$\rho(\lambda_j) = \lim_{N,M\to\infty} \frac{\hat{\xi}(\lambda_{j+1}) - \hat{\xi}(\lambda_j)}{\lambda_{j+1} - \lambda_j} = \lim_{N,M\to\infty} \frac{1}{M(\lambda_{j+1} - \lambda_j)}. \tag{2.22}$$

The method described above allows one to construct the ground state of the infinite XXZ chain at fixed magnetization. For the XXZ chain in an external magnetic field, the magnetization of the ground state is not an independent variable but depends on the magnetic field h. Then the boundary of the Fermi zone q in the equation (2.20) is defined from the condition $\varepsilon(q) = 0$ (instead of from (2.21)), where $\varepsilon(\lambda)$ is the dressed energy satisfying an integral equation similar to (2.20):

$$\varepsilon(\lambda) + \frac{1}{2\pi}\int_{-q}^{q} K(\lambda - \mu)\,\varepsilon(\mu)\,\mathrm{d}\mu = h - 2p_0'(\lambda)\sin\zeta\ . \tag{2.23}$$

The condition $\varepsilon(q) = 0$ provides the positiveness of the energy of any excited state. We see from (2.23) that the Fermi boundary q depends on the anisotropy parameter Δ and on the magnetic field h, *i.e.* that q is a function of the parameters of the Hamiltonian (2.1). We remind that q remains finite for non-zero magnetic fields, while it tends to infinity when $h \to 0$. Throughout the present article, q will be kept finite in all the computations.

Let us finally recall the definitions of the dressed momentum and charge, which are two important functions characterizing the ground state. The dressed momentum is closely related to the density as

$$p(\lambda) = 2\pi \int_0^\lambda \rho(\mu)\, \mathrm{d}\mu. \tag{2.24}$$

Obviously, the thermodynamic limit $\xi(\lambda)$ of the counting function $\hat{\xi}(\lambda)$ can be expressed in terms of the dressed momentum according to $\xi(\lambda) = [p(\lambda) + p(q)]/2\pi$. The dressed charge satisfies the integral equation

$$Z(\lambda) + \frac{1}{2\pi} \int_{-q}^{q} K(\lambda - \mu)\ Z(\mu)\, \mathrm{d}\mu = 1, \tag{2.25}$$

and can be interpreted in the XXZ model as the intrinsic magnetic moment of the elementary excitations [39]. The quantities $\mathcal{Z} = Z(q)$ and $p_{_F} = p(q) = \pi D$ (Fermi momentum) enter the asymptotic formula (1.1).

The excitations above the ground state can be constructed by adjoining particles and holes to the Dirac sea [41, 42, 43, 44, 45, 40, 46]. In other words, an excited state above the ground state corresponds to the replacement of a finite number of the (half-)integers $I_j = j - (N+1)/2$ parameterizing the ground state by some different ones, not belonging to the original sequence. In general, this induces a shift of the Bethe parameters $\{\mu\}$ describing this excited state with respect to the ground state Bethe roots $\{\lambda\}$, and possible appearance of complex roots.

3 Statement of the result

We are now in position to be more precise about the result we prove in this article.

We study a particular form factor of the σ^z operator, involving a very specific excited state, namely the one with one particle and one hole located on the opposite ends of the Fermi zone. For definiteness, we consider the case where the spectral parameters of the particle and hole are respectively equal to $\pm q$. This means that the (half-)integers which characterize this state through (2.14), that we will denote I'_j ($j = 1, \dots, N$), coincide with the ground state ones ($I'_j = I_j$) for $j = 2, \dots, N$, but differ at $j = 1$: $I'_1 = N + 1 - (N+1)/2$. There exists another way of describing the same eigenstate: by shifting the ground state (half-)integers by 1, *i.e.* by setting $I'_j = j + 1 - (N+1)/2$. In the framework of this approach, we can consider the aforementioned excited state as a limit of a *twisted ground state*. Indeed, similarly to (2.14) different eigenstates of the twisted transfer matrix are characterized by sets of (half-)integers $\tilde{n}_j$ in the logarithmic form of the twisted Bethe equations (2.13),

$$Mp_0(\mu_j) - \sum_{k=1}^{N} \vartheta(\mu_j - \mu_k) = 2\pi\tilde{n}_j - i\beta, \qquad j = 1, \dots, N, \tag{3.1}$$

where $\kappa = e^{\beta}$. In the case $\tilde{n}_j = I_j$, we call the corresponding eigenstate the twisted ground state. In that case and at $\beta = 2\pi i$, the equations (3.1) reduce to (2.14) with $n_j = I'_j = j+1-(N+1)/2$, and, thus, the twisted ground state becomes the excited state described above.

Our result is the following :

In the thermodynamic limit, the normalized form factor of the σ^z operator between the ground state $|\,\psi(\{\lambda\})\,\rangle$ and the excited state $\langle\,\psi(\{\mu\})\,|$ defined above is related to the amplitude $|F_\sigma|^2$ (which is a finite number) appearing in the asymptotic formula (1.1) *for the longitudinal spin-spin correlation function as*

$$\lim_{N,M\to\infty}\left(\frac{M}{2\pi}\right)^{2\mathcal{Z}^2}\frac{|\langle\psi(\{\mu\})|\sigma^z|\psi(\{\lambda\})\rangle|^2}{\|\psi(\{\mu\})\|^2\cdot\|\psi(\{\lambda\})\|^2}=|F_\sigma|^2. \tag{3.2}$$

In other words, it means that the modulus squared of the corresponding form factor behaves as $|F_\sigma|^2\left(\frac{M}{2\pi}\right)^{-2\mathcal{Z}^2}$ for M large. It is remarkable that the exponent $2\mathcal{Z}^2$ governing the modulus squared of the form factor power-law decrease in terms of the size M of the chain is exactly equal to the exponent for the power-law behavior of the corresponding oscillating term in the correlation function (1.1)*, but there in terms of the distance m separating the two spin operators.*

This result will be proven throughout Sections 4 and 5. There, the above special form factor will be computed and its thermodynamic limit will be taken.

In order to complete this statement, let us recall the explicit value of the amplitude $|F_\sigma|^2$ obtained in [1]:

$$|F_\sigma|^2=\left(\frac{2G(2,\mathcal{Z})\,\sin p_F}{\pi\mathcal{Z}}\right)^2\cdot\left[2\pi\,\rho(q)\,\sinh(2q)\right]^{-2\mathcal{Z}^2}\cdot e^{C_1-C_0}\cdot\widetilde{\mathcal{A}}(\beta)\big|_{\beta=2\pi i}. \tag{3.3}$$

Here the notation $G(a,x)$ represents the product of Barnes functions $G(a,x)=G(a+x)G(a-x)$ (*cf* A.2). The constants C_0 and C_1 are defined in terms of the dressed charge Z:

$$C_0=\int_{-q}^{q}\frac{Z(\lambda)\,Z(\mu)}{\sinh^2(\lambda-\mu-i\zeta)}\,\mathrm{d}\lambda\,\mathrm{d}\mu\,, \tag{3.4}$$

$$C_1=\frac{1}{2}\int_{-q}^{q}\frac{Z'(\lambda)\,Z(\mu)-Z(\lambda)\,Z'(\mu)}{\tanh(\lambda-\mu)}\,\mathrm{d}\lambda\,\mathrm{d}\mu+2\mathcal{Z}\int_{-q}^{q}\frac{\mathcal{Z}-Z(\lambda)}{\tanh(q-\lambda)}\,\mathrm{d}\lambda\,. \tag{3.5}$$

Finally, the coefficient $\widetilde{\mathcal{A}}(\beta)$ is given in terms of a ratio of Fredholm determinants:

$$\widetilde{\mathcal{A}}(\beta)=\left|\,e^{\frac{\beta}{2}[\tilde{z}(q-i\zeta)-\tilde{z}(-q-i\zeta)]}\,\frac{\det\left[I+\frac{1}{2\pi i}U_{-q}^{(\lambda)}(w,w')\right]}{\det\left[I+\frac{1}{2\pi}K\right]}\,\right|^2. \tag{3.6}$$

In this expression, the integral operator $I+K/2\pi$ occurring in the denominator acts on the interval $[-q,q]$ with kernel (2.18), whereas the integral operator appearing in the numerator acts on a contour surrounding $[-q,q]$ with kernel

$$U_{-q}^{(\lambda)}(w,w')=-\frac{e^{\beta\tilde{z}(w)}\,[K_\kappa(w-w')-K_\kappa(-q-w')]}{e^{\beta\tilde{z}(w+i\zeta)}-e^{\beta+\beta\tilde{z}(w-i\zeta)}}, \tag{3.7}$$

where

$$K_\kappa(\lambda) = \coth(\lambda + i\zeta) - \kappa \coth(\lambda - i\zeta), \qquad \kappa = e^\beta. \tag{3.8}$$

The function $\tilde{z}(w)$ appearing (3.6), (3.7), is the $i\pi$-periodic Cauchy transform of the dressed charge Z,

$$\tilde{z}(w) = \frac{1}{2\pi i} \int_{-q}^{q} \coth(\lambda - w)\, Z(\lambda)\, \mathrm{d}\lambda. \tag{3.9}$$

Observe that it has a cut on the interval $[-q, q]$ and satisfies the following properties:

$$\tilde{z}(w + i\zeta) - \tilde{z}(w - i\zeta) = 1 - Z(w)\,, \tag{3.10}$$

$$\tilde{z}_+(w) - \tilde{z}_-(w) = Z(w)\,, \qquad w \in [-q, q]\,. \tag{3.11}$$

The equation (3.10) follows from (2.25). In (3.11), $\tilde{z}_\pm$ stand for the limiting values of $\tilde{z}$ when $\mathbb{R}$ is approached from the upper and lower half planes.

Remark 3.1. Equation (3.3) contains the limiting value of $\widetilde{\mathcal{A}}(\beta)$ at $\beta = 2\pi i$. We did not set $\beta = 2\pi i$ directly in (3.6)–(3.8), as it may cause problems at some particular values of Δ. For example, at $\Delta = 0$ ($\zeta = \frac{\pi}{2}$, $Z(\lambda) = 1$), the kernel (3.7) becomes ill-defined when $\beta = 2\pi i$. It should therefore be understood in the sense of the limit $\beta \to 2i\pi$, the latter being well defined.

4 Special form factor for the finite chain

The solution of the quantum inverse scattering problem (2.6) and determinant representations for scalar products [38, 36] give a possibility to express, for the finite chain, arbitrary form factors of local spin operators as finite-size determinants [36]. We explain here how to obtain such a representation for the special form factor defined above. Then, following the ideas of [25, 1], we transform the obtained determinant to a new one, more convenient for the calculation of the thermodynamic limit.

From now on, we will consider eigenstates of the twisted transfer matrix only for κ belonging to the unit circle, *i.e.* $\kappa = e^\beta$, where β is pure imaginary. This restriction is not crucial, but convenient. The matter is that, due to the involution $A^\dagger(\bar{\lambda}) = D(\lambda)$ ($\dagger$ means Hermitian conjugation), the operator $e^{-\beta/2}\mathcal{T}_\kappa(\lambda)$ becomes self-adjoint for $|\kappa| = 1$ and $\lambda \in \mathbb{R}$. In such a case, the roots of the twisted Bethe equations (3.1) are real or contain complex conjugated pairs. In its turn, the involution $B^\dagger(\bar{\lambda}) = -C(\lambda)$ guarantees the duality of eigenstates $\langle \psi_\kappa(\{\mu\})| = (-1)^N |\psi_\kappa(\{\mu\})\rangle^\dagger$.

4.1 Special form factor and scalar product

Consider the following operator $\mathcal{Q}_m$, giving the number of spins down in the first m sites of the chain:

$$\mathcal{Q}_m = \frac{1}{2} \sum_{n=1}^{m} (1 - \sigma_n^z)\,. \tag{4.1}$$

It is easy to see that

$$e^{\beta \mathcal{Q}_m} = \prod_{n=1}^{m} \left(\frac{1+\kappa}{2} + \frac{1-\kappa}{2} \cdot \sigma_n^z \right), \qquad \kappa = e^\beta, \tag{4.2}$$

and we have

$$2D_m\,\frac{\partial}{\partial\beta}e^{\beta\mathcal{Q}_m}\bigg|_{\beta=2\pi in}=1-\sigma^z_{m+1},\qquad n\in\mathbb{Z},\tag{4.3}$$

where the symbol D_m stands for the lattice derivative: $D_mf(m)=f(m+1)-f(m)$. Also, note that $e^{\beta\mathcal{Q}_m}$ is a polynomial in κ which becomes the identity operator whenever $\beta=2\pi in$, $n\in\mathbb{Z}$.

The operator (4.2) admits, through the solution of the inverse problem (2.6), a simple representation in terms of the twisted and standard transfer matrices:

$$e^{\beta\mathcal{Q}_m}=\mathcal{T}_\kappa^m\big(-\tfrac{i\zeta}{2}\big)\,\mathcal{T}^{-m}\big(-\tfrac{i\zeta}{2}\big).\tag{4.4}$$

We use this representation and consider the following matrix element of $e^{\beta\mathcal{Q}_m}$:

$$\langle\psi_\kappa(\{\mu\})|e^{\beta\mathcal{Q}_m}|\psi(\{\lambda\})\rangle=\langle\psi_\kappa(\{\mu\})|\mathcal{T}_\kappa^m\big(-\tfrac{i\zeta}{2}\big)\,\mathcal{T}^{-m}\big(-\tfrac{i\zeta}{2}\big)|\psi(\{\lambda\})\rangle,\tag{4.5}$$

where $|\psi(\{\lambda\})\rangle$ is the ground state in the N-particle sector, and $\langle\psi_\kappa(\{\mu\})|$ is an eigenstate of the twisted transfer matrix $\mathcal{T}_\kappa$. Then

$$\langle\psi_\kappa(\{\mu\})|e^{\beta\mathcal{Q}_m}|\psi(\{\lambda\})\rangle=\left(\frac{\tau_\kappa(\frac{-i\zeta}{2}|\{\mu\})}{\tau(\frac{-i\zeta}{2}|\{\lambda\})}\right)^m\langle\psi_\kappa(\{\mu\})|\psi(\{\lambda\})\rangle.\tag{4.6}$$

Setting $\nu=-\frac{i\zeta}{2}$ in (2.12), we obtain

$$\langle\psi_\kappa(\{\mu\})|e^{\beta\mathcal{Q}_m}|\psi(\{\lambda\})\rangle=e^{im\sum_{j=1}^N[p_0(\mu_j)-p_0(\lambda_j)]}\langle\psi_\kappa(\{\mu\})|\psi(\{\lambda\})\rangle.\tag{4.7}$$

Let us now differentiate (4.7) with respect to β at $\beta=2\pi i$. Hereby, at $\beta=2\pi i$, the state $\langle\psi_\kappa(\{\mu\})|$ becomes an eigenstate of the standard transfer matrix. As it does not coincide with the ground state, it is orthogonal to the last one, and thus,

$$\langle\psi(\{\mu\})|\mathcal{Q}_m|\psi(\{\lambda\})\rangle=\left(e^{im\sum_{j=1}^N[p_0(\mu_j)-p_0(\lambda_j)]}-1\right)\frac{\partial}{\partial\beta}\langle\psi_\kappa(\{\mu\})|\psi(\{\lambda\})\rangle\bigg|_{\beta=2\pi i}.\tag{4.8}$$

Using also (4.3) we find that the special form factor we want to compute can be obtained in terms of the normalized scalar product between the ground state $|\,\psi(\{\lambda\})\,\rangle$ and the twisted ground state $\langle\,\psi_\kappa(\{\mu\})\,|$ given by (3.1) with $\tilde{n}_j=I_j$:

$$\frac{|\langle\psi(\{\mu\})|\sigma^z_{m+1}|\psi(\{\lambda\})\rangle|^2}{\|\psi(\{\mu\})\|^2\cdot\|\psi(\{\lambda\})\|^2}=-8\sin^2\left(\frac{\mathcal{P}_{ex}}{2}\right)\cdot\frac{\partial^2}{\partial\beta^2}S_N^{(\kappa)}(\{\mu\},\{\lambda\})\bigg|_{\beta=2\pi i},\tag{4.9}$$

with

$$S_N^{(\kappa)}(\{\mu\},\{\lambda\})=\left(\frac{\langle\psi_\kappa(\{\mu\})|\psi(\{\lambda\})\rangle}{\|\psi_\kappa(\{\mu\})\|\cdot\|\psi(\{\lambda\})\|}\right)^2,\tag{4.10}$$

and where $\mathcal{P}_{ex}=\sum_{j=1}^N[p_0(\mu_j)-p_0(\lambda_j)]$ is the total momentum of the excitation. Deriving (4.9) we have used that $\langle\psi_\kappa(\{\mu\})|\psi(\{\lambda\})\rangle$ is real at $|\kappa|=1$.

In (4.10), the parameters μ_j satisfy the system of twisted Bethe equations (3.1) with $\tilde{n}_j=I_j$ and, hence, are functions of β. In particular, they are taken to be

$$\mu_j(\beta)\big|_{\beta=0}=\lambda_j,\qquad j=1,\dots,N.\tag{4.11}$$

Then, in the l.h.s. of (4.9), the set $\{\mu_j(\beta=2\pi i)\}$ describes the excited state considered in Section 3 with a particle at q and a hole at $-q$.

4.2 Determinant representation

Thus, in order to study our special form factor, we can use the determinant representations for the scalar product between an eigenstate of the twisted transfer matrix with any arbitrary state of the form (2.8). Let us recall these representations.

Proposition 4.1. *[38, 36] Let $\mu_1,\dots,\mu_N$ satisfy the system* (2.9) *and $\lambda_1,\dots,\lambda_N$ be generic complex numbers. Then*

$$\langle 0|\prod_{j=1}^{N} C(\lambda_j)|\psi_\kappa(\{\mu\})\rangle = \langle\psi_\kappa(\{\mu\})|\prod_{j=1}^{N} B(\lambda_j)|0\rangle = \frac{\prod_{a=1}^{N} d(\mu_a)}{\prod\limits_{a>b}^{N}\sinh(\mu_a-\mu_b)\sinh(\lambda_b-\lambda_a)}\cdot \det{}_N\,\Omega_\kappa(\{\mu\},\{\lambda\}|\{\mu\}), \quad (4.12)$$

where the $N\times N$ matrix $\Omega_\kappa(\{\mu\},\{\lambda\}|\{\mu\})$ is defined as

$$(\Omega_\kappa)_{jk}(\{\mu\},\{\lambda\}|\{\mu\}) = a(\lambda_k)\,t(\mu_j,\lambda_k)\prod_{a=1}^{N}\sinh(\mu_a-\lambda_k-i\zeta) - \kappa\, d(\lambda_k)\,t(\lambda_k,\mu_j)\prod_{a=1}^{N}\sinh(\mu_a-\lambda_k+i\zeta), \quad (4.13)$$

with

$$t(\mu,\lambda) = \frac{-i\sin\zeta}{\sinh(\mu-\lambda)\sinh(\mu-\lambda-i\zeta)}. \quad (4.14)$$

Note that, due to the Bethe equations (2.9), the entries of the matrix $\Omega_\kappa(\{\mu\},\{\lambda\}\mid\{\mu\})$ are not singular at $\lambda_k=\mu_j$. In particular, if $\lambda_j=\mu_j$ for all $j=1,\dots,N$, then we obtain the square of the norm of the twisted eigenstate $\langle\psi_\kappa(\{\mu\})|\psi_\kappa(\{\mu\})\rangle$ (recall that $|\kappa|=1$), which reduces to

$$\langle\psi_\kappa(\{\mu\})|\psi_\kappa(\{\mu\})\rangle = (-1)^N\prod_{j=1}^{N}\left[2\pi i M\,\hat\rho_\kappa(\mu_j)\,a(\mu_j)\,d(\mu_j)\right]\frac{\prod\limits_{a,b=1}^{N}\sinh(\mu_a-\mu_b-i\zeta)}{\prod\limits_{\substack{a,b=1\\ a\neq b}}^{N}\sinh(\mu_a-\mu_b)} \times \det{}_N\,\Theta^{(\mu)}_{jk}, \quad (4.15)$$

with

$$\Theta^{(\mu)}_{jk} = \delta_{jk} + \frac{K(\mu_j-\mu_k)}{2\pi M\hat\rho_\kappa(\mu_k)}, \qquad 2\pi M\hat\rho_\kappa(\mu) = -i\log'\frac{a(\mu)}{d(\mu)} - \sum_{a=1}^{N}K(\mu-\mu_a). \quad (4.16)$$

In the case of interest (scalar product of the untwisted ground state $|\,\psi(\{\lambda\})\,\rangle$ with the κ-twisted one $\langle\,\psi_\kappa(\{\mu\})\,|$), one has two different representations for the scalar product. On the one hand, it is possible to apply equation (4.12) when $|\,\psi(\{\lambda\})\,\rangle$ in understood as an arbitrary state. On the other hand, one can consider $|\,\psi(\{\lambda\})\,\rangle$ as an eigenstate (for $\kappa=1$), interpret $\langle\,\psi_\kappa(\{\mu\})\,|$

as an arbitrary state, and apply formula (4.12) with $\lambda \leftrightarrow \mu$. Thus, one can obtain two different, but equivalent representations for the scalar product $\langle\, \psi_\kappa(\{\mu\})\,|\psi(\{\lambda\})\rangle$. We do not give here the explicit formulae (which can be easily derived from (4.12)–(4.14)) as these representations are not convenient for the calculation of thermodynamic limits. In order to obtain new formulae that are appropriate for such goal, one can extract the products of $\sinh^{-1}(\mu_k - \lambda_j)$ from the determinant of the matrix Ω_κ (see [1, 28, 25]). As a result, one obtains two new representations containing Fredholm determinants of integral operators of the form $I + \frac{1}{2\pi i}\widehat{U}_\theta^{(\lambda,\mu)}(w,w')$, with kernels

$$\widehat{U}_\theta^{(\lambda)}(w,w') = -\prod_{a=1}^{N}\frac{\sinh(w-\mu_a)}{\sinh(w-\lambda_a)}\cdot\frac{K_\kappa(w-w')-K_\kappa(\theta-w')}{V_+^{-1}(w)-\kappa V_-^{-1}(w)}, \tag{4.17}$$

$$\widehat{U}_\theta^{(\mu)}(w,w') = \prod_{a=1}^{N}\frac{\sinh(w'-\lambda_a)}{\sinh(w'-\mu_a)}\cdot\frac{K_\kappa(w-w')-K_\kappa(w-\theta)}{V_-(w')-\kappa V_+(w')}. \tag{4.18}$$

Here θ is an arbitrary complex number, K_κ is given by (3.8), and

$$V_\pm(w) \equiv V_\pm\left(w \mid \begin{matrix}\{\lambda\}_N\\ \{\mu\}_N\end{matrix}\right) = \prod_{a=1}^{N}\frac{\sinh(w-\lambda_a \pm i\zeta)}{\sinh(w-\mu_a \pm i\zeta)}. \tag{4.19}$$

These integral operators act on a contour surrounding the points $\{\lambda\}$ (resp.$\{\mu\}$) but no any other singularity of $\widehat{U}_\theta^{(\lambda,\mu)}(w,w')$. More precisely, one has the following proposition (see Appendix A of [1] for the proof):

Proposition 4.2. *[1] Let $\lambda_1,\dots,\lambda_N$ satisfy the system of untwisted Bethe equations and $\mu_1,\dots,\mu_N$ satisfy the system of κ-twisted Bethe equations* (2.9)*. Then*

$$\begin{aligned}\langle\psi(\{\lambda\})|\psi_\kappa(\{\mu\})\rangle = \prod_{a,b=1}^{N}\frac{\sinh(\mu_a-\lambda_b-i\zeta)}{\sinh(\lambda_a-\mu_b)}\cdot\prod_{j=1}^{N}\left\{d(\mu_j)\,d(\lambda_j)\left[\kappa\frac{V_+(\lambda_j)}{V_-(\lambda_j)}-1\right]\right\}\\ \times\frac{1-\kappa}{V_+^{-1}(\theta)-\kappa V_-^{-1}(\theta)}\cdot\det\left[I+\frac{1}{2\pi i}\widehat{U}_\theta^{(\lambda)}(w,w')\right],\end{aligned} \tag{4.20}$$

and

$$\begin{aligned}\langle\psi(\{\lambda\})|\psi_\kappa(\{\mu\})\rangle = \prod_{a,b=1}^{N}\frac{\sinh(\lambda_a-\mu_b-i\zeta)}{\sinh(\mu_a-\lambda_b)}\cdot\prod_{j=1}^{N}\left\{d(\mu_j)\,d(\lambda_j)\left[\frac{V_-(\mu_j)}{V_+(\mu_j)}-\kappa\right]\right\}\\ \times\frac{1-\kappa}{V_-(\theta)-\kappa V_+(\theta)}\cdot\det\left[I+\frac{1}{2\pi i}\widehat{U}_\theta^{(\mu)}(w,w')\right].\end{aligned} \tag{4.21}$$

We would like to emphasize that equations (4.20) and (4.21) describe scalar products for the *finite* XXZ chain even though they contain Fredholm determinants of integral operators. In fact, it is not difficult to see that the integral operators $\widehat{U}_\theta^{(\lambda,\mu)}$ are of finite rank and hence the Fredholm determinants can be reduced to usual determinants of $N \times N$ matrices [1].

Remark 4.1. We gave here two different representations for the same quantity, because we will use both of them. Namely, we will substitute (4.20) for one scalar product $\langle\psi_\kappa(\{\mu\})|\psi(\{\lambda\})\rangle$ in (4.10) and (4.21) for the other one, despite the evident fact that these scalar products are the same. This way seems to be slightly strange, but it leads directly to equation (3.3). Due to the equivalence of the representations (4.20) and (4.21) one can use, of course, only one of them, coming eventually to the same result. The last way, however, requires some additional identities, since the equivalence of the representations (4.20) and (4.21) is non-trivial.

It remains to apply all these results to our special form factor, which was expressed in terms of the normalized scalar product $S_N^{(\kappa)}$ through (4.9). Substituting (4.20), (4.21), (4.15) in (4.10), and using the Bethe equations (2.13), we obtain a representation for $S_N^{(\kappa)}$ as a product of three factors:

$$S_N^{(\kappa)}(\{\mu\},\{\lambda\}) = \mathcal{A}_N^{(\kappa)} \cdot D_N^{(\kappa)} \cdot \exp C_{0,N}^{(\kappa)}\,, \tag{4.22}$$

with

$$D_N^{(\kappa)} = \left(\det_N \frac{1}{\sinh(\mu_j-\lambda_k)}\right)^2 \cdot \prod_{j=1}^{N} \frac{\left(\frac{\kappa V_+(\lambda_j)}{V_-(\lambda_j)}-1\right)\left(\frac{V_-(\mu_j)}{\kappa V_+(\mu_j)}-1\right)}{4\pi^2 M^2\,\hat\rho(\lambda_j)\,\hat\rho_\kappa(\mu_j)}, \tag{4.23}$$

$$C_{0,N}^{(\kappa)} = \sum_{a,b=1}^{N} \log\frac{\sinh(\lambda_a-\mu_b-i\zeta)\,\sinh(\mu_b-\lambda_a-i\zeta)}{\sinh(\lambda_a-\lambda_b-i\zeta)\,\sinh(\mu_a-\mu_b-i\zeta)}, \tag{4.24}$$

and

$$\mathcal{A}_N^{(\kappa)} = \frac{(\kappa-1)^2\,\det\left[I+\frac{1}{2\pi i}\widehat{U}_{\theta_1}^{(\lambda)}(w,w')\right]\,\det\left[I+\frac{1}{2\pi i}\widehat{U}_{\theta_2}^{(\mu)}(w,w')\right]}{\left(V_+^{-1}(\theta_1)-\kappa V_-^{-1}(\theta_1)\right)\left(V_-(\theta_2)-\kappa V_+(\theta_2)\right)\cdot \det_N \Theta_{jk}^{(\lambda)} \cdot \det_N \Theta_{jk}^{(\mu)}}. \tag{4.25}$$

Recall that the representations (4.20), (4.21) contain an arbitrary complex parameter θ. Here we have used two different parameters θ_1 and θ_2 for each of the scalar products. In the following, we shall set $\theta_1 = -q$ and $\theta_2 = q$.

5 Thermodynamic limit of the special form factor

We compute now the large size behavior ($N, M \to \infty$, $N/M \to D$) of the special form factor represented in (4.9), (4.22). We need first to characterize how the parameters μ_j of the κ-twisted ground state Bethe Ansatz equations behave in this limit. More precisely, how they are shifted with respect to the parameters λ_j of the untwisted ground state. This will enable us to take the thermodynamic limit in the expression (4.22) for the normalized scalar product. Whereas it is quite straightforward to evaluate the limit of the factors $\mathcal{A}_N^{(\kappa)}$ and $C_{0,N}^{(\kappa)}$ (see Subsection 5.2), we will see in Subsection 5.3 that the factor $D_N^{(\kappa)}$ (4.23) requires more attention.

5.1 Twisted ground state and shift functions

In order to study the κ-twisted ground state $|\,\psi_\kappa(\{\mu\})\,\rangle$ in the thermodynamic limit, it is convenient to introduce, similarly as for the untwisted case (see (2.16)), a twisted counting function $\hat\xi_\kappa(\mu)$ satisfying $\hat\xi_\kappa(\mu_j) = j/M$. Its explicit expression is given by

$$\hat\xi_\kappa(\omega) = \frac{1}{2\pi}p_0(\omega) - \frac{1}{2\pi M}\sum_{k=1}^{N}\vartheta(\omega-\mu_k) + \frac{N+1}{2M} + \frac{i\beta}{2\pi M}\,, \tag{5.1}$$

with p_0 and ϑ given by (2.15). The corresponding discrete N-particle density $\hat{\rho}_\kappa(\mu) = \frac{\mathrm{d}\hat{\xi}_\kappa}{\mathrm{d}\mu}$ coincides with the function defined in (4.16). It also coincides, at $\beta = 0$, with the N-particle density of the ground state $\hat{\rho}(\lambda)$. It is easy to check that both functions $\hat{\rho}_\kappa(\lambda)$ (for $\kappa \neq 1$) and $\hat{\rho}(\lambda)$ go to the same function $\rho(\lambda)$ (2.22) in the thermodynamic limit.

Using the counting functions for the ground state (2.16) and twisted ground state (5.1), one can define shift functions describing the displacement of the spectral parameters $\{\mu\}$ with respect to ground state ones $\{\lambda\}$. One can actually introduce two shift functions:

$$\hat{F}(\lambda_j) = M\big[\hat{\xi}(\mu_j) - \hat{\xi}(\lambda_j)\big], \qquad \hat{F}_\kappa(\mu_j) = M\big[\hat{\xi}_\kappa(\mu_j) - \hat{\xi}_\kappa(\lambda_j)\big]. \tag{5.2}$$

Both have the same thermodynamic limit which we, from now on, denote by $F(\lambda)$. One can easily verify that

$$F(\lambda_j) = \lim_{N,M\to\infty} \frac{\mu_j - \lambda_j}{\lambda_{j+1} - \lambda_j}. \tag{5.3}$$

The subtraction of the equation (2.14) with $n_j = I_j$ (Bethe equation for the ground state) from (3.1) (Bethe equation for the twisted ground state, corresponding to the same number $\tilde{n}_j = I_j$) and a replacement of finite differences by derivatives and of sums by integrals as in (2.19), leads to the integral equation for the shift function F:

$$F(\lambda) + \frac{1}{2\pi}\int_{-q}^{q} K(\lambda-\mu)F(\mu)\,\mathrm{d}\mu = \frac{\beta}{2\pi i}. \tag{5.4}$$

Comparing this equation with the one for the dressed charge (2.25), one obtains

$$F(\lambda) = \frac{\beta Z(\lambda)}{2\pi i}. \tag{5.5}$$

Thence, for M large enough, the spectral parameters μ_j are shifted with respect to the ground state ones λ_j by a quantity $\epsilon_j = \mu_j - \lambda_j$ which can be computed for large M

$$\epsilon_j = \frac{\beta Z(\lambda_j)}{2\pi i M \rho(\lambda_j)} + O(M^{-2}), \qquad j = 1, \dots, N. \tag{5.6}$$

5.2 Thermodynamic limit of $\mathcal{A}_N^{(\kappa)}$ and $C_{0,N}^{(\kappa)}$

We first compute the limits of $C_{0,N}^{(\kappa)}$ and $\mathcal{A}_N^{(\kappa)}$. These limits are quite simple to calculate since it is enough to take into account only the leading order of the shift (5.6).

We have already seen that, in the thermodynamic limit $N, M \to \infty$, discreet sums over the parameters λ_j can be replaced by integrals *via* (2.19). It is also easy to see that

$$\lim_{N,M\to\infty} \prod_{j=1}^{N}\left(1 + \frac{1}{M}f(\lambda_j)\right) = \exp\left\{\int_{-q}^{q} f(\lambda)\,\rho(\lambda)\,\mathrm{d}\lambda\right\}, \tag{5.7}$$

$$\lim_{N,M\to\infty} \det{}_N\left[\delta_{jk} + \frac{1}{M}V(\lambda_j,\lambda_k)\right] = \det[I + V\rho], \tag{5.8}$$

provided $f(\lambda)$ and $V(\lambda,\mu)$ are piecewise continuous on $[-q,q]$. In (5.8), $\det[I+V\rho]$ refers to the Fredholm determinant of the integral operator $I + V\rho$ acting on the interval $[-q,q]$ with kernel $V(\lambda,\mu)\rho(\mu)$.

The thermodynamic limit of $C_{0,N}^{(\kappa)}$ is straightforward to obtain using (5.6):

$$\lim_{N,M\to\infty} C_{0,N}^{(\kappa)} = \lim_{N,M\to\infty} \sum_{j,k=1}^{N} \log \frac{\sinh(\lambda_j-\lambda_k-\epsilon_k-i\zeta)\,\sinh(\lambda_j-\lambda_k+\epsilon_j-i\zeta)}{\sinh(\lambda_j-\lambda_k-i\zeta)\,\sinh(\lambda_j-\lambda_k+\epsilon_j-\epsilon_k-i\zeta)}$$
$$= -\lim_{N,M\to\infty} \sum_{j,k=1}^{N} \epsilon_j\,\epsilon_k\,\partial_{\lambda_j}\partial_{\lambda_k} \log\sinh(\lambda_j-\lambda_k-i\zeta) = \frac{\beta^2}{4\pi^2} C_0, \tag{5.9}$$

where C_0 is given by (3.4).

Let us now consider the different factors in (4.25). As the limit of $\hat{\rho}(\lambda)$ and $\hat{\rho}_\kappa(\lambda)$ coincides with the ground state density $\rho(\lambda)$, both determinants $\det_N \Theta_{jk}^{(\lambda,\mu)}$ go to the Fredholm determinant of the operator $I+K/2\pi$:

$$\lim_{N,M\to\infty} \det_N \Theta_{jk}^{(\lambda,\mu)} = \det\left[I+K/2\pi\right]. \tag{5.10}$$

A direct application of (5.7) leads to

$$\lim_{N,M\to\infty} V_{\pm}(w) = e^{-\beta\tilde{z}(w\pm i\zeta)}. \tag{5.11}$$

Similarly,

$$\lim_{N,M\to\infty} \prod_{a=1}^{N} \frac{\sinh(w-\lambda_a)}{\sinh(w-\mu_a)} = e^{-\beta\tilde{z}(w)}, \qquad w \text{ uniformly away from } [-q,q]. \tag{5.12}$$

Substituting (5.11) and (5.12) into (4.17) we have that, at $\theta_1=-q$,

$$\lim_{N,M\to\infty} \frac{1}{2\pi i}\widehat{U}_{-q}^{(\lambda)}(w,w') = \frac{1}{2\pi i} U_{-q}^{(\lambda)}(w,w'), \tag{5.13}$$

where the kernel $U_{-q}^{(\lambda)}(w,w')$ is given by (3.7). It is also easy to see that, when $\theta_2=q$ and β is purely imaginary,

$$\lim_{N,M\to\infty} \frac{1}{2\pi i}\widehat{U}_{q}^{(\mu)}(w,w') = \left(\frac{1}{2\pi i} U_{-q}^{(\lambda)}\right)^{\dagger}(-\bar{w},-\bar{w}'), \tag{5.14}$$

where $\dagger$ means hermitian conjugation. A simple algebra based on (3.10) leads to

$$\lim_{N,M\to\infty} \mathcal{A}_N^{(\kappa)} = \left(\frac{\sinh\frac{\beta}{2}}{\sinh\frac{\beta\mathcal{Z}}{2}}\right)^2 \widetilde{\mathcal{A}}(\beta), \tag{5.15}$$

where $\widetilde{\mathcal{A}}(\beta)$ is given by (3.6).

5.3 Thermodynamic limit of the Cauchy determinant

As already mentioned, the thermodynamic limit of the factor $D_N^{(\kappa)}$ (4.23) is the most complicated to obtain. Although the final result for this quantity can be expressed in terms of the limiting value of the shift function (5.5), the approximation (5.6) is not enough for the intermediate analysis. The reason is that $D_N^{(\kappa)}$ contains the square of a Cauchy determinant which has poles at $\mu_j = \lambda_k$. These singularities are compensated by the zeros of

$$\prod_{j=1}^{N} \left(\frac{\kappa V_+(\lambda_j)}{V_-(\lambda_j)} - 1 \right) \left(\frac{V_-(\mu_j)}{\kappa V_+(\mu_j)} - 1 \right) . \tag{5.16}$$

However, this compensation takes place if and only if the parameters μ_j *exactly* solve the set of twisted Bethe equations, which means that it is not enough to consider only the first order of the shift function as in (5.6). Therefore, to compute the limit of $D_N^{(\kappa)}$, we should work with the exact formulae for the N-particle shift functions $\hat{F}$ and $\hat{F}_\kappa$ (5.2) defined in terms of the two counting functions $\hat{\xi}(\omega)$ and $\hat{\xi}_\kappa(\omega)$ (2.16), (5.1), their limiting values being only taken at the end of the computation.

In order to re-write (4.23) in terms of the shift functions $\hat{F}$ and $\hat{F}_\kappa$, we also introduce the functions

$$\hat{\varphi}(\lambda, \mu) = \frac{\sinh(\lambda - \mu)}{\hat{\xi}(\lambda) - \hat{\xi}(\mu)}, \qquad \hat{\varphi}_\kappa(\lambda, \mu) = \frac{\sinh(\lambda - \mu)}{\hat{\xi}_\kappa(\lambda) - \hat{\xi}_\kappa(\mu)}, \tag{5.17}$$

which fulfill

$$\hat{\varphi}^{-1}(\lambda, \lambda) = \hat{\xi}'(\lambda) = \hat{\rho}(\lambda), \qquad \hat{\varphi}_\kappa^{-1}(\lambda, \lambda) = \hat{\xi}'_\kappa(\lambda) = \hat{\rho}_\kappa(\lambda). \tag{5.18}$$

Note that $\hat{\varphi}$ and $\hat{\varphi}_\kappa$ have the same thermodynamic limit denoted by φ.

Proposition 5.1. *The product* $D_N^{(\kappa)}$ (4.23) *admits the following factorization:*

$$D_N^{(\kappa)} = H[\hat{F}] \cdot H[-\hat{F}_\kappa] \cdot \Phi[\hat{\varphi}] \cdot \Phi[\hat{\varphi}_\kappa] \cdot \prod_{j=1}^{N} \frac{\hat{\varphi}(\lambda_j, \lambda_j)\, \hat{\varphi}_\kappa(\mu_j, \mu_j)}{\hat{\varphi}(\lambda_j, \mu_j)\, \hat{\varphi}_\kappa(\mu_j, \lambda_j)}. \tag{5.19}$$

The functions $H[\hat{F}]$ *and* $\Phi[\hat{\varphi}]$ *are defined as*

$$H[\hat{F}] = \prod_{j>k}^{N} \left(1 + \frac{\hat{F}(\lambda_j) - \hat{F}(\lambda_k)}{j - k} \right) \prod_{\substack{j,k=1 \\ j \neq k}}^{N} \left(1 + \frac{\hat{F}(\lambda_j)}{j - k} \right)^{-1} \prod_{j=1}^{N} \frac{\sin\bigl(\pi \hat{F}(\lambda_j)\bigr)}{\pi \hat{F}(\lambda_j)}, \tag{5.20}$$

$$\Phi[\hat{\varphi}] = \frac{\prod\limits_{j>k}^{N} \left[\hat{\varphi}(\lambda_j, \lambda_k)\, \hat{\varphi}(\mu_k, \mu_j) \right]}{\prod\limits_{\substack{j,k=1 \\ j \neq k}}^{N} \hat{\varphi}(\mu_j, \lambda_k)}, \tag{5.21}$$

and the function $H[-\hat{F}_\kappa]$ *(respectively* $\Phi[\hat{\varphi}_\kappa]$*) can be obtained from* (5.20) *(resp.* (5.21)*) by the replacement* $\hat{F}(\lambda) \to -\hat{F}_\kappa(\mu)$ *(resp.* $\hat{\varphi} \to \hat{\varphi}_\kappa$*).*

Proof — Using the definition (2.16), (5.1) of the counting functions, one can easily see that

$$\frac{\kappa V_+(\omega)}{V_-(\omega)} = e^{2\pi i M [\hat{\xi}(\omega) - \hat{\xi}_\kappa(\omega)]}, \tag{5.22}$$

which leads to

$$\prod_{j=1}^{N}\left(\frac{\kappa V_+(\lambda_j)}{V_-(\lambda_j)}-1\right)\left(\frac{V_-(\mu_j)}{\kappa V_+(\mu_j)}-1\right)$$

$$=\prod_{j=1}^{N}\left(e^{2\pi iM[\hat\xi(\lambda_j)-\hat\xi_\kappa(\lambda_j)]}-1\right)\left(e^{-2\pi iM[\hat\xi(\mu_j)-\hat\xi_\kappa(\mu_j)]}-1\right)$$

$$=\prod_{j=1}^{N}\left(e^{2\pi iM[\hat\xi_\kappa(\mu_j)-\hat\xi_\kappa(\lambda_j)]}-1\right)\left(e^{-2\pi iM[\hat\xi(\mu_j)-\hat\xi(\lambda_j)]}-1\right)$$

$$=\prod_{j=1}^{N}\Big[4\sin\big(\pi\hat F_\kappa(\mu_j)\big)\sin\big(\pi\hat F(\lambda_j)\big)\Big]. \tag{5.23}$$

Here we have used that $\hat\xi(\lambda_j)=\hat\xi_\kappa(\mu_j)=j/M$, and the identity

$$\sum_{j=1}^{N}\Big[\hat\xi(\lambda_j)-\hat\xi(\mu_j)+\hat\xi_\kappa(\mu_j)-\hat\xi_\kappa(\lambda_j)\Big]=0 \tag{5.24}$$

which is a consequence of (2.16), (5.1).

The remaining part of the proof is quite trivial. It is based on the expression for the Cauchy determinant in terms of double products

$$\det_N\left(\frac{1}{u_j-v_k}\right)=\frac{\prod\limits_{j>k}^{N}(u_j-u_k)(v_k-v_j)}{\prod\limits_{j,k=1}^{N}(u_j-v_k)}, \tag{5.25}$$

where u_j, v_j are arbitrary complex numbers. Substituting the explicit expressions for all the factors into (5.19), and using again $\hat\xi(\lambda_j)=\hat\xi_\kappa(\mu_j)=j/M$ together with the definition of $\hat F$ and $\hat F_\kappa$ (5.2), one easily reproduces the original representation (4.23) for $D_N^{(\kappa)}$. □

Since the functions $\hat\varphi(\lambda,\mu)$ and $\hat\varphi_\kappa(\lambda,\mu)$ are not singular at $\lambda,\mu\in[-q,q]$, the thermodynamic limits of the last three factors in the r.h.s. of (5.19) can easily be calculated similarly as in the previous subsection. Using (5.6) we find

$$\lim_{N,M\to\infty}\Phi[\hat\varphi]\cdot\Phi[\hat\varphi_\kappa]\cdot\prod_{j=1}^{N}\frac{\hat\varphi(\lambda_j,\lambda_j)\,\hat\varphi_\kappa(\mu_j,\mu_j)}{\hat\varphi(\lambda_j,\mu_j)\,\hat\varphi_\kappa(\mu_j,\lambda_j)}$$

$$=\exp\left\{-\frac{\beta^2}{4\pi^2}\int_{-q}^{q}Z(\lambda)\,Z(\mu)\;\partial_\lambda\partial_\mu\log\varphi(\lambda,\mu)\;\mathrm{d}\lambda\,\mathrm{d}\mu\right\}. \tag{5.26}$$

It remains to compute the limiting values of $H[\hat F]$, $H[-\hat F_\kappa]$. To do this, it is convenient to split $H[\hat F]$ into two factors: $H[\hat F]=H_1[\hat F]\cdot H_2[\hat F]$, with

$$H_1[\hat F]=\exp\left[-\sum_{j=1}^{N}\psi(j)\big[\hat F(\lambda_j)-\hat F(\lambda_{N-j+1})\big]\right]\cdot\prod_{j>k}^{N}\left(1+\frac{\hat F(\lambda_j)-\hat F(\lambda_k)}{j-k}\right), \tag{5.27}$$

$$H_2[\hat{F}] = \exp\left[\sum_{j=1}^{N} \psi(j)\left[\hat{F}(\lambda_j) - \hat{F}(\lambda_{N-j+1})\right]\right] \prod_{\substack{j,k=1\\ j\neq k}}^{N} \left(1 + \frac{\hat{F}(\lambda_j)}{j-k}\right)^{-1} \prod_{j=1}^{N} \frac{\sin[\pi \hat{F}(\lambda_j)]}{\pi \hat{F}(\lambda_j)}, \quad (5.28)$$

$\psi(z)$ being the logarithmic derivative of the Γ-function (*cf* Appendix A.1).

Proposition 5.2. *The thermodynamic limit of the factor* $H_1[\hat{F}]$ (5.27) *is given by*

$$\lim_{N,M\to\infty} \log H_1[\hat{F}] = -\frac{1}{4}\int_{-q}^{q} \left(\frac{F(\lambda) - F(\mu)}{\xi(\lambda) - \xi(\mu)}\right)^2 \rho(\lambda)\,\rho(\mu)\;\mathrm{d}\lambda\,\mathrm{d}\mu. \quad (5.29)$$

Proof — Due to the smoothness of F and ξ, there is an ϵ, $0 < \epsilon < 1$, such that, for M large enough,

$$\left|\frac{\hat{F}(\lambda_j) - \hat{F}(\lambda_k)}{j-k}\right| = \frac{1}{M}\left|\frac{\hat{F}(\lambda_j) - \hat{F}(\lambda_k)}{\hat{\xi}(\lambda_j) - \hat{\xi}(\lambda_k)}\right| < \epsilon\,, \quad \text{uniformy in}\,\lambda_j,\,\lambda_k. \quad (5.30)$$

The logarithm of the double product in the r.h.s. of (5.27) can therefore be expanded into its Taylor integral series of order 2

$$\log \prod_{j>k}^{N}\left(1 + \frac{\hat{F}(\lambda_j) - \hat{F}(\lambda_k)}{j-k}\right) = \sum_{n=1}^{2} \frac{(-1)^{n+1}}{nM^n} \sum_{j>k}^{N} \left(\frac{\hat{F}(\lambda_j) - \hat{F}(\lambda_k)}{\hat{\xi}(\lambda_j) - \hat{\xi}(\lambda_k)}\right)^n$$
$$+ \frac{1}{M^3}\sum_{j>k}^{N} \int_0^1 \mathrm{d}t \frac{(1-t)^2}{\left(1 + \frac{t}{M}\cdot \frac{\hat{F}(\lambda_j)-\hat{F}(\lambda_k)}{\hat{\xi}(\lambda_j)-\hat{\xi}(\lambda_k)}\right)^3} \left(\frac{\hat{F}(\lambda_j) - \hat{F}(\lambda_k)}{\hat{\xi}(\lambda_j) - \hat{\xi}(\lambda_k)}\right)^3. \quad (5.31)$$

The expressions under the double sum over j and k being not singular at $\lambda_j, \lambda_k \in [-q, q]$, the thermodynamic limit of the integral remaining terms in (5.31) vanish due to the M^{-3} pre-factor. The contribution issued from the $n = 1$ term cancels with the pre-factor in (5.27) since

$$\sum_{j>k}^{N} \frac{\hat{F}(\lambda_j) - \hat{F}(\lambda_k)}{j-k} = \sum_{\substack{j,k=1\\ j\neq k}}^{N} \frac{\hat{F}(\lambda_j)}{j-k} = \sum_{j=1}^{N} \psi(j)\left[\hat{F}(\lambda_j) - \hat{F}(\lambda_{N-j+1})\right]. \quad (5.32)$$

Thus, the limit of $\log H_1$ reduces to the one of the term $n = 2$ in the expansion (5.31), which ends the proof. □

Proposition 5.3. *The thermodynamic limit of the factor* $H_2[\hat{F}]$ (5.28) *is given by*

$$\lim_{N,M\to\infty}\left(H_2[\hat{F}]\cdot N^{\frac{F^2(-q)+F^2(q)}{2}}\right) = G\big(1+F(-q)\big)\,G\big(1-F(q)\big)\cdot e^{\frac{F(-q)-F(q)}{2}(1-\log 2\pi)}$$
$$\times \exp\left\{\int_{-q}^{q}\left[\frac{F^2(\lambda) - F^2(q)}{\xi(\lambda) - \xi(q)} - \frac{F^2(\lambda) - F^2(-q)}{\xi(\lambda) - \xi(-q)}\right]\rho(\lambda)\,\mathrm{d}\lambda\right\}, \quad (5.33)$$

where $G(z)$ *is the Barnes function* (A.7).

Proof — The product over k in (5.28) can be expressed in terms of Γ-functions as

$$\prod_{\substack{j,k=1\\ j\neq k}}^{N}\left(1+\frac{\hat{F}(\lambda_j)}{j-k}\right)^{-1}\prod_{j=1}^{N}\frac{\sin(\pi\hat{F}(\lambda_j))}{\pi\hat{F}(\lambda_j)}=\prod_{j=1}^{N}\frac{\Gamma^2(j)}{\Gamma\big(j+\hat{F}(\lambda_j)\big)\Gamma\big(j-\hat{F}(\lambda_{N-j+1})\big)}. \tag{5.34}$$

This means that $H_2[\hat{F}]$ can itself be factorized into two factors,

$$H_2[\hat{F}]=H_2^{(1)}[\hat{F}]\cdot H_2^{(2)}[\hat{F}], \tag{5.35}$$

with

$$H_2^{(1)}[\hat{F}]=\prod_{j=1}^{N}\frac{\Gamma(j)}{\Gamma(j+\hat{F}(\lambda_j))}\,e^{\psi(j)\,\hat{F}(\lambda_j)}, \tag{5.36}$$

$H_2^{(2)}[\hat{F}]$ being obtained from (5.36) by the replacement $\hat{F}(\lambda_j)\to-\hat{F}(\lambda_{N-j+1})$.

We first consider $H_2^{(1)}[\hat{F}]$. Let $\hat{F}_-=\hat{F}\big(\hat{\xi}^{-1}(0)\big)$. Evidently, $\hat{F}_-\to F(-q)$ in the thermodynamic limit. We use the fact that the shift function $\hat{F}(\lambda_j)$ is bounded uniformly for any value of N. Thus we can use the following bound $|\hat{F}(\lambda_j)|<n$ for some $n\in\mathbb{N}$ and $j=1,\dots,N$. Then we represent $H_2^{(1)}[\hat{F}]$ as

$$H_2^{(1)}[\hat{F}]=\prod_{j=1}^{N}\frac{\Gamma(j)e^{\psi(j)\hat{F}_-}}{\Gamma(j+\hat{F}_-)}\prod_{j=1}^{n-1}\frac{\Gamma(j+\hat{F}_-)e^{(\hat{F}(\lambda_j)-\hat{F}_-)\psi(j)}}{\Gamma\big(j+\hat{F}(\lambda_j)\big)}\prod_{j=n}^{N}\frac{\Gamma(j+\hat{F}_-)e^{(\hat{F}(\lambda_j)-\hat{F}_-)\psi(j)}}{\Gamma\big(j+\hat{F}(\lambda_j)\big)}. \tag{5.37}$$

Using (A.10), (B.4) we find

$$\prod_{j=1}^{N}\frac{\Gamma(j)e^{\psi(j)\hat{F}_-}}{\Gamma(j+\hat{F}_-)}=\frac{G(N+1)\,G(1+\hat{F}_-)}{G(N+1+\hat{F}_-)}e^{\hat{F}_-(N\psi(N)+1-N)}, \tag{5.38}$$

and thus, applying the asymptotic formulae (A.3), (A.9) we arrive at

$$\lim_{N,M\to\infty}N^{\frac{\hat{F}_-^2}{2}}\prod_{j=1}^{N}\frac{\Gamma(j)e^{\psi(j)\hat{F}_-}}{\Gamma(j+\hat{F}_-)}=G\big(1+F(-q)\big)\cdot e^{\frac{F(-q)}{2}(1-\log 2\pi)}. \tag{5.39}$$

The limit of the second finite product in (5.37) evidently is equal to 1 due to $\hat{F}(\lambda_j)-\hat{F}_-=O(M^{-1})$ for $j=1,\dots,n-1$. Finally, in order to compute the limit of the last product in (5.37) we can use Taylor integral representation for the logarithms of Γ-functions (recall that $|\hat{F}(\lambda_j)|<n\le j$)

$$\begin{aligned}\prod_{j=n}^{N}\frac{\Gamma(j+\hat{F}_-)e^{(\hat{F}(\lambda_j)-\hat{F}_-)\psi(j)}}{\Gamma\big(j+\hat{F}(\lambda_j)\big)}=\exp\Bigg\{&\frac{1}{2}\sum_{j=n}^{N}\psi'(j)\left[\hat{F}_-^2-\hat{F}^2(\lambda_j)\right]\\ &-\frac{1}{2}\sum_{j=n}^{N}\int_0^1 \mathrm{d}t(1-t)^2\left[\psi''\big(\hat{F}(\lambda_j)t+j\big)\,\hat{F}^3(\lambda_j)-\psi''\big(\hat{F}_-t+j\big)\,\hat{F}_-^3\right]\Bigg\}.\end{aligned} \tag{5.40}$$

The limit of the first sum in (5.40) is obtained by applying Lemma B.2 proved in Appendix B. Indeed, as the counting function is invertible and satisfies $\hat{\xi}(\lambda_j) = j/M$, we write $\hat{F}(\lambda_j) = \hat{F}\big(\hat{\xi}^{-1}(\frac{j}{M})\big)$. Then, using (B.9), we find

$$\lim_{N,M\to\infty} \sum_{j=n}^{N} \psi'(j)\,\big[\hat{F}_-^2 - \hat{F}^2(\lambda_j)\big] = -\int_0^D \frac{F^2\big(\xi^{-1}(x)\big) - F^2\big(\xi^{-1}(0)\big)}{x}\,\mathrm{d}x. \tag{5.41}$$

Recall that $D = \lim_{N,M\to\infty} N/M$ is the average density, so that, after the change of variables $\xi^{-1}(x) = \lambda$, we obtain

$$\lim_{N,M\to\infty} \sum_{j=1}^{N} \psi'(j)\,\big[\hat{F}_-^2 - \hat{F}^2(\lambda_j)\big] = -\int_{-q}^{q} \frac{F^2(\lambda) - F^2(-q)}{\xi(\lambda) - \xi(-q)}\rho(\lambda)\,\mathrm{d}\lambda. \tag{5.42}$$

Finally, the same transformation on the function F allows us to apply, uniformly in t, Lemma B.3 to the second sum in (5.40), hence proving that its thermodynamic limit is zero.

Substituting these results into (5.37), we obtain that

$$\lim_{N,M\to\infty} \left(H_2^{(1)}[\hat{F}] \cdot N^{\frac{F^2(-q)}{2}} \right)$$
$$= G\big(1 + F(-q)\big) \cdot \exp\left[\frac{F(-q)}{2}(1 - \log 2\pi) - \frac{1}{2}\int_{-q}^{q} \frac{F^2(\lambda) - F^2(-q)}{\xi(\lambda) - \xi(-q)}\,\rho(\lambda)\,\mathrm{d}\lambda \right]. \tag{5.43}$$

The thermodynamic limit of $H_2^{(2)}[\hat{F}]$ can be deduced from the previous calculation due to the fact that $\hat{F}(\lambda_{N-j+1}) = \hat{F}\big(\hat{\xi}^{-1}(\frac{N+1}{M} - \frac{j}{M})\big)$. □

The limit of $H[-\hat{F}_\kappa]$ is obtained in the same spirit as above. Since the limits of $\hat{F}$, $\hat{\rho}$ and $\hat{\xi}$ coincide with those of their κ-deformed analogs, the result is given by (5.29) and (5.33) provided that one makes the replacement $F \to -F$.

This enables us to obtain the thermodynamic limit of $D_N^{(\kappa)}$:

Proposition 5.4. *The product $D_N^{(\kappa)}$ admits the following thermodynamic limit:*

$$\lim_{N,M\to\infty} \left(D_N^{(\kappa)}\, M^{-\frac{\beta^2 \mathcal{Z}^2}{2\pi^2}} \right) = G^2\big(1, \tfrac{\beta\mathcal{Z}}{2\pi i}\big)\,\big[\rho(q)\,\sinh 2q\big]^{\frac{\beta^2\mathcal{Z}^2}{2\pi^2}}\, e^{-\frac{\beta^2}{4\pi^2}C_1}, \tag{5.44}$$

where C_1 is given by (3.5). *We remind that $G(a,z) = G(a-z)G(a+z)$ and $\mathcal{Z} = Z(q)$.*

Proof — Using the expression (5.5) of F and the symmetry properties of Z, ρ and ξ,

$$Z(\lambda) = Z(-\lambda), \quad \rho(\lambda) = \rho(-\lambda), \quad \text{and} \quad \xi(\lambda) = D - \xi(-\lambda),$$

we obtain from Propositions 5.2, 5.3 that

$$\lim_{N,M\to\infty} \left(D_N^{(\kappa)}\, N^{-\frac{\beta^2\mathcal{Z}^2}{2\pi^2}} \right) = G^2\big(1, \tfrac{\beta\mathcal{Z}}{2\pi i}\big)\, \exp\left[\frac{\beta^2}{8\pi^2} \int_{-q}^{q} \left(\frac{Z(\lambda) - Z(\mu)}{\xi(\lambda) - \xi(\mu)} \right)^2 \rho(\lambda)\,\rho(\mu)\,\mathrm{d}\lambda\,\mathrm{d}\mu \right]$$
$$\times \exp\left[-\frac{\beta^2}{4\pi^2} \int_{-q}^{q} Z(\lambda)Z(\mu)\,\partial_\lambda\partial_\mu \log\varphi(\lambda,\mu)\,\mathrm{d}\lambda\,\mathrm{d}\mu - \frac{\beta^2}{2\pi^2} \int_{-q}^{q} \frac{Z^2(\lambda) - \mathcal{Z}^2}{\xi(\lambda) - \xi(q)}\rho(\lambda)\,\mathrm{d}\lambda \right]. \tag{5.45}$$

After some simple algebra the combination of integrals in (5.45) can be reduced to the constant C_1 (3.5), and the result takes the announced form. $\square$

5.4 Results for the normalized scalar product and special form factor

Putting together the individual limits (5.44), (5.9) and (5.15) yields

$$\lim_{N,M\to\infty}\left(S_N^{(\kappa)}\cdot M^{-\frac{\beta^2\mathcal{Z}^2}{2\pi^2}}\right)=\left[\frac{2\sinh\frac{\beta}{2}}{\beta\mathcal{Z}}\,G\big(2,\tfrac{\beta\mathcal{Z}}{2\pi i}\big)\right]^2\,\big[\rho(q)\,\sinh 2q\big]^{\frac{\beta^2\mathcal{Z}^2}{2\pi^2}}\,e^{-\frac{\beta^2}{4\pi^2}(C_1-C_0)}\,\widetilde{\mathcal{A}}(\beta). \tag{5.46}$$

The limits being uniform in β and its derivatives, we take the second β derivative at $\beta=2\pi i$ and obtain

$$\lim_{N,M\to\infty}\left(-\,\partial_\beta^2 S_N^{(\kappa)}\Big|_{\beta=2\pi i}\cdot M^{2\mathcal{Z}^2}\right)=\frac{1}{2}\left(\frac{G(2,\mathcal{Z})}{\pi\mathcal{Z}}\right)^2\frac{e^{C_1-C_0}\,\widetilde{\mathcal{A}}(\beta)}{\big[\rho(q)\,\sinh 2q\big]^{2\mathcal{Z}^2}}\Big|_{\beta=2\pi i}. \tag{5.47}$$

We still need to compute the excitation momentum $\mathcal{P}_{ex}$ in (4.9) to finish our proof. We have

$$\lim_{N,M\to\infty}\mathcal{P}_{ex}=\lim_{N,M\to\infty}\sum_{j=1}^{N}\big[p_0(\mu_j)-p_0(\lambda_j)\big]=\int_{-q}^{q}p_0'(\lambda)\,Z(\lambda)\,\mathrm{d}\lambda. \tag{5.48}$$

The integral equations (2.20), (2.25) for the density and the dressed charge then lead to

$$\int_{-q}^{q}p_0'(\lambda)\,Z(\lambda)\,\mathrm{d}\lambda=2\pi\int_{-q}^{q}\rho(\lambda)\,\mathrm{d}\lambda=2p_{F}, \tag{5.49}$$

due to (2.24). Substituting (5.49) and (5.47) into (4.9) and comparing the result with the amplitude (3.3), we finally arrive at (3.2).

Conclusion

In the present article, we have initiated the development of a method to study form factors in the massless regime of the XXZ Heisenberg spin chain. In particular we have given explicitly the thermodynamic limit of a special form factor in the XXZ chain. This form factor corresponds to the matrix element of the operator σ^z between the ground state and an excited state containing one particle and one hole on the different ends of the Fermi zone. It is clear however that our method can be applied to other form factors as well, where excited states contain arbitrary number of particles and holes in arbitrary positions. This method can also be applied to other integrable models, for example to the system of one-dimensional bosons.

One of the unsolved problems is to prove that at zero magnetic field our result coincides with the amplitude predicted in [30, 31]. The limit $h\to 0$ corresponds to the limit $q\to\infty$ in (5.46). It is easy to see that the constants C_0, C_1, $\widetilde{\mathcal{A}}$, $\rho(q)\sinh 2q$, being finite for finite q, become divergent at $q\to\infty$. We were able to prove that the total combination giving F_σ remains finite for $h=0$, but we did not obtain a simple expression for its value in this limit. We succeeded nevertheless to compute explicitly this quantity in the vicinity of the free fermion point ($\zeta=\frac{\pi}{2}$) up to the second order in $\epsilon=\frac{\zeta}{\pi}-\frac{1}{2}$. Our computation confirms the result [30, 31] up to that order.

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A ψ-function and Barnes function

We recall in this appendix the definitions of the ψ-function and the Barnes function, as well as several standard formulae that are useful for our study.

A.1 The ψ-function and its derivatives

The ψ-function is defined as the logarithmic derivative $\psi(z) = \frac{\mathrm{d}}{\mathrm{d}z}\log\Gamma(z)$ of the Γ-function. The multiplication property of the Γ-function implies that,

$$\psi^{(n)}(z+1) - \psi^{(n)}(z) = \frac{(-1)^n n!}{z^{n+1}}. \tag{A.1}$$

It follows from (A.1) that

$$\sum_{k=0}^{N-1} \frac{1}{(k+a)^{n+1}} = \frac{(-1)^n}{n!}\Big(\psi^{(n)}(N+a) - \psi^{(n)}(a)\Big). \tag{A.2}$$

When $z \to \infty$ with $-\pi < \arg(z) < \pi$, one has

$$\psi(z) = \log z - \frac{1}{2z} + O\left(\frac{1}{z^2}\right), \qquad \psi^{(n)}(z) = \frac{(-1)^{n-1}(n-1)!}{z^n} + O\left(\frac{1}{z^{n+1}}\right). \tag{A.3}$$

For $n \geq 1$, the n^{th}-derivative of the ψ-function admits the following integral representation:

$$\psi^{(n)}(z) = -\int_0^1 \frac{x^{z-1}\log^n x}{1-x}\,\mathrm{d}x. \tag{A.4}$$

The latter implies in particular that, for $z > 0$,

$$(-1)^{n-1}\psi^{(n)}(z) > 0, \qquad n \geq 1. \tag{A.5}$$

It is also easy to see that

$$\psi'(z) - \frac{1}{z} = \int_0^1 x^{z-1}\left(\frac{\log x}{x-1} - 1\right)\mathrm{d}x > 0, \qquad z > 0. \tag{A.6}$$

A.2 The Barnes function

The Barnes function $G(z)$ is the unique solution of

$$G(1+z)=\Gamma(z)\,G(z),\quad \text{with}\quad G(1)=1\quad \text{and}\quad \frac{\mathrm{d}^3}{\mathrm{d}z^3}\log G(z)\geq 0,\quad z>0. \tag{A.7}$$

It has the following integral representation

$$\log G(1+z)=\frac{z(1-z)}{2}+\frac{z}{2}\log 2\pi+\int_0^z x\,\psi(x)\,\mathrm{d}x,\qquad \Re(z)>-1. \tag{A.8}$$

The Barnes function has the following asymptotic behavior when $z\to\infty$, $-\pi<\arg(z)<\pi$:

$$\log G(1+z)=\Big(\frac{z^2}{2}-\frac{1}{12}\Big)\log z-\frac{3z^2}{4}+\frac{z}{2}\log 2\pi+\zeta'(-1)+O\Big(\frac{1}{z}\Big), \tag{A.9}$$

Due to (A.7), one has

$$\sum_{k=0}^{N-1}\log\Gamma(k+a)=\log G(N+a)-\log G(a). \tag{A.10}$$

B Sums with logarithmic derivatives of Γ-function

In this appendix, we explain how to compute the thermodynamic limit of some sums involving the ψ-function and its derivatives.

B.1 Finite sums involving ψ-function

Lemma B.1. *For $n\geq 0$, $a\neq -1,-2,\dots$, and an arbitrary complex α, one has the following identity*

$$\sum_{k=1}^{N}\psi^{(n)}(k+a)e^{\alpha k}=\frac{1}{e^{\alpha}-1}\cdot\left[\psi^{(n)}(N+a)e^{\alpha(N+1)}-\psi^{(n)}(a)e^{\alpha}-(-1)^n n!\sum_{k=1}^{N-1}\frac{e^{\alpha(k+1)}}{(k+a)^{n+1}}\right]. \tag{B.1}$$

Proof — Denote the l.h.s. of (B.1) as $f(\alpha)$,

$$f(\alpha)=\sum_{k=1}^{N}\psi^{(n)}(k+a)\,e^{\alpha k}. \tag{B.2}$$

Shifting k by $k+1$ and using (A.1), we obtain

$$\begin{aligned} f(\alpha)&=e^{\alpha}\sum_{k=0}^{N-1}\psi^{(n)}(k+a+1)\,e^{\alpha k}\\ &=e^{\alpha}\sum_{k=0}^{N-1}\psi^{(n)}(k+a)\,e^{\alpha k}+(-1)^n n!\sum_{k=0}^{N-1}\frac{e^{\alpha(k+1)}}{(k+a)^{n+1}}\\ &=e^{\alpha}f(\alpha)+e^{\alpha}\psi^{(n)}(a)-e^{\alpha(N+1)}\psi^{(n)}(N+a)+(-1)^n n!\sum_{k=0}^{N-1}\frac{e^{\alpha(k+1)}}{(k+a)^{n+1}}. \end{aligned} \tag{B.3}$$

Then (B.1) follows immediately. □

Taking derivatives of (B.1) with respect to α at $\alpha = 0$ one obtains formulae for the sums of the type $\psi^{(n)}(k+a)k^p$. Let us give explicitly several of them.

One has for $p = 0$, $n = 0$,

$$\sum_{k=1}^{N} \psi(k+a) = (N+a)\psi(N+a) - a\psi(a) - N, \tag{B.4}$$

and for $p = 0$, $n \geq 1$,

$$\sum_{k=1}^{N} \psi^{(n)}(k+a) = (N+a)\psi^{(n)}(N+a) - a\psi^{(n)}(a+1) + n\Big(\psi^{(n-1)}(N+a) - \psi^{(n-1)}(a+1)\Big). \tag{B.5}$$

One also has for $p = 1$, $n = 1$,

$$\begin{aligned}\sum_{k=1}^{N} k\psi'(k+a) = \frac{(N+a)(N+1-a)}{2}\psi'(N+a) + \frac{a(a-1)}{2}\psi^{(n)}(a+1) \\ - \frac{2a-1}{2}\Big(\psi(N+a) - \psi(a+1)\Big) + \frac{N-1}{2},\end{aligned} \tag{B.6}$$

and for $p = 1$, $n \geq 2$,

$$\begin{aligned}\sum_{k=1}^{N} k\psi^{(n)}(k+a) = \frac{(N+a)(N+1-a)}{2}\psi^{(n)}(N+a) + \frac{a(a-1)}{2}\psi^{(n)}(a+1) \\ - \frac{n(2a-1)}{2}\Big(\psi^{(n-1)}(N+a) - \psi^{(n-1)}(a+1)\Big) - \frac{n(n-1)}{2}\Big(\psi^{(n-2)}(N+a) - \psi^{(n-2)}(a+1)\Big).\end{aligned} \tag{B.7}$$

B.2 More complicated sums

We now consider sums involving in addition some regular function(s).

Lemma B.2. *Let $f \in C^1([0,a])$ for $a > 0$. Let us consider the sum*

$$S_1^{(N,M)}[f] = \sum_{k=1}^{N} \left[f\left(\tfrac{k}{M}\right) - f(0)\right]\psi'(k). \tag{B.8}$$

In the limit $N, M \to \infty$, $N/M \to D$ with $D \in [0, a[$, it tends to

$$S_1^{(N,M)}[f] \to \int_0^D \frac{f(t) - f(0)}{t}\,\mathrm{d}t. \tag{B.9}$$

Proof — We have

$$S_1^{(N,M)}[f] = \sum_{k=1}^{N}\left(\psi'(k) - \frac{1}{k}\right)\frac{k}{M}\int_0^1 f'\left(\frac{kt}{M}\right)\mathrm{d}t + \sum_{k=1}^{N}\frac{1}{M}\int_0^1 f'\left(\frac{kt}{M}\right)\mathrm{d}t. \tag{B.10}$$

It is easy to see that the first sum vanishes in the limit considered. Indeed, setting $\|f\| = \sup_{[0,a]}|f|$, we get using (B.6), (A.6) and (A.3),

$$\begin{aligned}\left|\sum_{k=1}^{N}\left(\psi'(k)-\frac{1}{k}\right)\frac{k}{M}\int_0^1 f'\left(\frac{kt}{M}\right)\mathrm{d}t\right| &\le \frac{\|f'\|}{M}\sum_{k=1}^{N}\big(k\psi'(k)-1\big)\\ &= \frac{\|f'\|}{2M}\left[N(N+1)\psi'(N)+\psi(N)-\psi(1)-N-1\right] = \frac{\|f'\|}{2M}\left[\log N + O(1)\right]. \quad \text{(B.11)}\end{aligned}$$

Thus, the limit of $S_1^{(N,M)}[f]$ reduces to one of the second term in (B.10), which is quite straightforward due to Euler–Maclaurin summation formula

$$\lim_{N,M\to\infty} S_1^{(N,M)}[f] = \lim_{N,M\to\infty}\sum_{k=1}^{N}\frac{1}{M}\int_0^1 f'\left(\frac{kt}{M}\right)\mathrm{d}t = \int_0^D \mathrm{d}y\int_0^1 f'(yt)\mathrm{d}t = \int_0^D \frac{f(y)-f(0)}{y}\mathrm{d}y, \tag{B.12}$$

and Lemma B.2 is proved. □

Lemma B.3. *Let $F, f \in C^1([0,a])$, with $a>0$. Let $n \in \mathbb{N}$ be such that $\|F\| = \sup_{[0,a]}|F| < n$. Then, for $m>1$, the sum*

$$\widetilde{S}_m^{(N,M)}[f,F] = \sum_{k=n}^{N}\left[f\left(\frac{k}{M}\right)\psi^{(m)}\left(F\left(\frac{k}{M}\right)+k\right) - f(0)\,\psi^{(m)}\big(F(0)+k\big)\right] \tag{B.13}$$

vanishes in the limit $N, M\to\infty$, $N/M\to D$ with $D\in[0,a]$.

Proof — We have

$$\begin{aligned}\widetilde{S}_m^{(N,M)}[f,F] = \sum_{k=n}^{N}\frac{k}{M}\int_0^1 \mathrm{d}t\Bigg[& f'\left(\frac{tk}{M}\right)\psi^{(m)}\left(F\left(\frac{tk}{M}\right)+k\right)\\ &+ f\left(\frac{tk}{M}\right)F'\left(\frac{tk}{M}\right)\psi^{(m+1)}\left(F\left(\frac{tk}{M}\right)+k\right)\Bigg]. \quad \text{(B.14)}\end{aligned}$$

Due to (A.5), (A.6) $(-1)^{m-1}\psi^{(m)}(z)$ is positive monotonically decreasing function for $z>0$. Then one has the following estimate

$$|\widetilde{S}_m^{(N,M)}[f,F]| \le \frac{\|F'\|\,\|f\| + \|f'\|}{M}\sum_{k=n}^{N} k\left[(-1)^m\,\psi^{(m+1)}(k-\|F\|) + (-1)^{m-1}\,\psi^{(m)}(k-\|F\|)\right]. \tag{B.15}$$

The last sum is readily computed by (B.7). It is easy to see that it is a $O(\log N)$ at most. □

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