

Thermodynamic limit of particle-hole form factors in the massless XXZ Heisenberg chain

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Abstract

We study the thermodynamic limit of the particle-hole form factors of the XXZ Heisenberg chain in the massless regime. We show that, in this limit, such form factors decrease as an explicitly computed power-law in the system-size. Moreover, the corresponding amplitudes can be obtained as a product of a “smooth” and a “discrete” part: the former depends continuously on the rapidities of the particles and holes, whereas the latter has an additional explicit dependence on the set of integer numbers that label each excited state in the associated logarithmic Bethe equations. We also show that special form factors corresponding to zero-energy excitations lying on the Fermi surface decrease as a power-law in the system size with the same critical exponents as in the long-distance asymptotic behavior of the related two-point correlation functions. The methods we develop in this article are rather general and can be applied to other massless integrable models associated to the six-vertex R -matrix and having determinant representations for their form factors.

1 Introduction

This article is a continuation of our study of form factors in massless quantum integrable models. We have recently [1] investigated the thermodynamic limit of a special, Umklapp-type, form factor of the XXZ Heisenberg spin chain [2, 3, 4, 5, 6, 7, 8, 9] starting from its

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determinant representation [10] in the algebraic Bethe Ansatz framework [11, 12, 13]. We now apply this method to general, particle-hole type, form factors. The main goal of our analysis is to pave a way for the calculation of the asymptotic behavior of correlation functions in massless integrable models through their form factor expansion. Our results should also be useful in the numerical computation of dynamical structure factors through their (exact) form factor expressions starting from finite size systems [14, 15, 16, 17, 18] as they allow a precise *a priori* control of the dependence of each form factor in terms of the system size.

For definiteness, we chose to focus on a particular model, the XXZ spin-1/2 Heisenberg chain [2] in the massless regime and in an external magnetic field $h > 0$ for which determinant representations of general form factors were obtained in [10]. However, up to minor modifications specific to the choice of the model, our method and results apply as well to other massless, algebraic Bethe Ansatz-solvable models with known determinant representations of their form factors like the non-linear Schrödinger model [19, 20] or the higher spin XXX [21] and XXZ [22] chains.

The Hamiltonian of the XXZ chain is given by,

$$H = \sum_{k=1}^M (\sigma_k^x \sigma_{k+1}^x + \sigma_k^y \sigma_{k+1}^y + \Delta (\sigma_k^z \sigma_{k+1}^z - 1)) - \frac{h}{2} \sum_{k=1}^M \sigma_k^z, \quad (1.1)$$

where $\sigma_k^{x,y,z}$ are the spin operators (Pauli matrices) acting on the k^{th} site of the chain. The main purpose of this article is to study the asymptotic behavior of the form factors in the thermodynamic limit $M \rightarrow \infty$ of the chain and in the massless regime $|\Delta| < 1$. We will take this limit starting from a chain of finite even size and subject to periodic boundary conditions.

Considering the finite chain allows us to define rigorously the form factors of local spin operators as the normalized matrix elements

$$\mathcal{F}_{\psi \psi'}^{(s)}(m) = \frac{\langle \psi | \sigma_m^s | \psi' \rangle}{\|\psi\| \cdot \|\psi'\|}, \quad s = x, y, z, \quad (1.2)$$

where $|\psi\rangle$ and $|\psi'\rangle$ are two eigenstates of the Hamiltonian (1.1). Such matrix elements can be computed in a systematic way by using the solution to the quantum inverse scattering problem [10, 23] together with the explicit formulae for scalar products [24, 25, 10] in the algebraic Bethe Ansatz framework [11, 12, 13, 26].

Using the closure relation, one can express any zero temperature two-point correlation function of spin operators as a sum over the form factors of the corresponding local operators,

$$\frac{\langle \psi_g | \sigma_m^s \sigma_{m'}^{s'} | \psi_g \rangle}{\langle \psi_g | \psi_g \rangle} = \sum_{|\psi'\rangle} \mathcal{F}_{\psi_g \psi'}^{(s)}(m) \mathcal{F}_{\psi' \psi_g}^{(s')}(m'). \quad (1.3)$$

Here $|\psi_g\rangle$ denotes the ground state of the Hamiltonian (1.1), and the summation is taken with respect to all the eigenstates $|\psi'\rangle$ of (1.1).

One possible way of dealing with (1.3) was proposed in [27, 28], where the sum over the form factors for the finite chain was recast into a multiple contour integral, the so-called master equation. This method then leads to various multiple integral representations for the correlation functions in the thermodynamic limit [27, 28, 29] that are in fact non-trivial summations of

previously obtained multiple integral representations for the correlation functions [30, 31, 32, 33, 34, 35]. Moreover, in [36] we have shown how to derive long-distance asymptotic behavior of certain two-point correlation functions using such master equation representation. It agrees with predictions arising from the Luttinger-liquid and Conformal Field Theories approaches [37, 38, 39, 40, 41, 42, 43, 44]. It is the very remarkable structure of the results obtained in [36] (the amplitudes of the power law decrease of the long distance behavior of the two-point correlation function are related to the modulus squared of some properly normalized form factors) that strongly suggested that another possible way to analyze the asymptotic behavior of the two-point correlation functions would be to take the thermodynamic limit directly in (1.3). It seems indeed quite natural that, in this limit, the main contribution to the sum (1.3) should stem from excitations above the ground state having a finite energy. Such excited states can be characterized in terms of particles, holes and/or string configurations. In this framework, the sum over the complete set of states in (1.3) becomes a sum over all the possible particle-hole-string type excitations above the ground state which, after some possible regularizations, should be replaceable by integrals in the thermodynamic limit. Another important motivation to learn how to deal directly with the form factor expansion of the correlation functions concerns the time dependent case, as in that situation the asymptotic analysis through the dynamical master equation [28] poses yet unsolved problems. The first step to carry out this program is therefore to determine the leading asymptotic behavior of the form factors of the model in the thermodynamic limit. It is the purpose of the present article to solve this problem for the so-called particle/hole type form factors (corresponding to diffusion states). The case of states associated with complex solutions of the Bethe equations such as string type solutions (corresponding to bound states) requires the use of additional techniques and will be considered in a separate publication.

In [1], we have shown that, in the $M \rightarrow \infty$ limit, a special Umklapp-type form factor of the σ^z operator decreases as some negative power of the system size M . The striking feature of this analysis is that this power coincides with one of the critical exponents appearing in the long-distance asymptotic behavior of the zero temperature two-point correlation function $\langle \sigma_1^z \sigma_{m+1}^z \rangle$. In the present article, we will show that general form factors exhibit similar properties: they all decay as some negative power of the size M ; moreover, for special types of form factors corresponding, in the thermodynamic limit, to particle-hole excitations lying on the Fermi surface, these exponents coincide exactly with the critical exponents describing the power-law decay of the long-distance asymptotic behavior of the corresponding two-point correlation functions.

More precisely, in the thermodynamic limit, the product of two form factors appearing in (1.3) can be presented in the following form

$$\mathcal{F}_{\psi_g \psi'}^{(s)}(m') \cdot \mathcal{F}_{\psi' \psi_g}^{(s')}(m) = M^{-\theta_{ss'}} e^{i\mathcal{P}_{ex}(m-m')} \mathcal{S}_{ss'} \mathcal{D}_{ss'}. \quad (1.4)$$

All the dependence on the lattice distance $m - m'$ is contained in an obvious phase factor¹. There \mathcal{P}_{ex} is the excitation momentum. The finite part of the form factors product can be separated into two parts $\mathcal{S}_{ss'}$ and $\mathcal{D}_{ss'}$. We call them smooth and discrete parts respectively.

¹Some form factors (see e.g. (3.1)) may also have an additional factor $(-1)^{m-m'}$, which can be removed by the re-definition of the Hamiltonian (1.1)

We show that the smooth part $\mathcal{S}_{ss'}$ depends continuously on the rapidities of the particles and holes. On the contrary, it is only when the particles (holes) rapidities are separated from the Fermi boundary that the discrete part $\mathcal{D}_{ss'}$ does also depend smoothly on these quantities. As soon as the latter approach the Fermi surface, the discrete structure of the form factors reveals itself in $\mathcal{D}_{ss'}$. This means that a microscopic (of order $1/M$) deviation of a particle (hole)'s rapidity leads to a macroscopic change of $\mathcal{D}_{ss'}$. We believe that one of the consequences of such a structure is the particular role played by the Fermi boundary in bosonization techniques.

The article is organized as follows. In section 2 we give a description of the low-lying excited states of the model. Following the ideas of [1], we consider excitations above the ground state of the twisted transfer matrix. This enables us to formulate precisely our results in section 3, i.e. the structure of the large size asymptotic behavior of general particle-hole form factors in the XXZ spin-1/2 chain. The remaining part of the article is devoted to the proof of this result. In section 4 we show how form factors can be reduced to scalar products of a special type that we can represent in terms of determinants for chains of finite length M . We then calculate the thermodynamic limit of the form factors of the σ^z operator in section 5. In particular, we show that if the rapidities of the particles and holes collapse on the Fermi surface then the form factors have a discrete structure. In section 6 we obtain analogous results for the form factors of the σ^\pm operators². We would like to stress that several methods and results used in the present article are borrowed from our previous work [1]. We conclude by discussing the possibility of applying our results to the calculation of the long-distance asymptotic behavior of the two-point functions at zero temperature. Several auxiliary Lemmas and proofs of technical character are presented in the two Appendices.

2 Space of states of the model

Since our ultimate goal is to analyze the two-point correlation functions at zero temperature through (1.3), the form factors we consider here correspond to matrix elements of a local operator between the ground state and an excited eigenstate of the Hamiltonian (1.1). In this section we recall how such states can be described in the large M limit.

In the algebraic Bethe Ansatz framework [11, 12, 13], the space of states of the model (in finite volume) is constructed by means of the Yang-Baxter algebra realized by the operator entries of the monodromy matrix. In the XXZ case, and more generally for the class of models associated with the six-vertex R-matrix, such monodromy matrices take the form

$$T(\lambda) = \begin{pmatrix} A(\lambda) & B(\lambda) \\ C(\lambda) & D(\lambda) \end{pmatrix}, \quad (2.1)$$

where A, B, C, D are quantum operators depending on some spectral parameter λ . It satisfies Yang-Baxter commutation relations given by the six-vertex R-matrix. In this framework, the eigenstates $|\psi\rangle$ of the Hamiltonian (1.1) coincide with the ones of the transfer matrix $\mathcal{T}(\lambda) = \text{tr} T(\lambda) = A(\lambda) + D(\lambda)$, and can be parameterized as $|\psi\rangle = |\psi(\lambda_1, \dots, \lambda_N)\rangle$, $N = 0, 1, \dots, M/2$,

²Recall that $\sigma^\pm = \frac{1}{2}(\sigma^x \pm i\sigma^y)$

in terms of a set $\{\lambda_j\}_{j=1}^N$ of solutions to the logarithmic Bethe equations

$$Mp_0(\lambda_j) - \sum_{k=1}^N \vartheta(\lambda_j - \lambda_k) = 2\pi n_j, \quad j = 1, \dots, N. \quad (2.2)$$

Here the functions $p_0(\lambda)$ and $\vartheta(\lambda)$ are the bare momentum and phase,

$$p_0(\lambda) = i \log \left(\frac{\sinh(\frac{i\zeta}{2} + \lambda)}{\sinh(\frac{i\zeta}{2} - \lambda)} \right), \quad \vartheta(\lambda) = i \log \left(\frac{\sinh(i\zeta + \lambda)}{\sinh(i\zeta - \lambda)} \right), \quad (2.3)$$

where $0 < \zeta < \pi$ and $\cos \zeta = \Delta$. The numbers n_j , $-M/2 < n_j \leq M/2$, are integers (for N odd) or half-integers (for N even).

2.1 Thermodynamic limit of the ground state

The Bethe roots λ_j , $j = 1, \dots, N$, describing the ground state correspond to the solution of the system of logarithmic Bethe Ansatz equations (2.2) with the special choice $n_j = j - (N + 1)/2$, where N is the number of down spins in the ground state¹ [4, 45, 9, 8]. Thus, for given M and h , these parameters λ_j are fixed quantities. In order to describe how they behave in the thermodynamic limit ($N, M \rightarrow \infty$ such that N/M tends to some fixed average density D), we introduce the ground state counting function,

$$\widehat{\xi}(\omega) = \frac{1}{2\pi} p_0(\omega) - \frac{1}{2\pi M} \sum_{k=1}^N \vartheta(\omega - \lambda_k) + \frac{N+1}{2M}, \quad (2.4)$$

which is build so that $\widehat{\xi}(\lambda_j) = j/M$ for $j = 1, \dots, N$. This function defines the discrete density of the minimal energy state in the N sector by $\widehat{\rho}(\omega) = \widehat{\xi}'(\omega)$. It is possible to argue that, in the thermodynamic limit, the parameters λ_j fill densely a finite interval $[-q, q]$ of the real axis (the Fermi zone), and that the discrete density goes to a smooth function $\rho(\omega)$ that solves the following integral equation

$$\rho(\lambda) + \frac{1}{2\pi} \int_{-q}^q K(\lambda - \mu) \rho(\mu) d\mu = \frac{1}{2\pi} p_0'(\lambda), \quad \text{with } K(\lambda) = \vartheta'(\lambda). \quad (2.5)$$

The value of the endpoint q of the Fermi zone is fixed by requiring that $\int_{-q}^q \rho(\lambda) d\lambda = D$. Note that, since $\lim_{M \rightarrow \infty} \widehat{\xi}(\lambda_1) = 0$, the thermodynamic limit $\xi(\lambda)$ of the counting function is the antiderivative of $\rho(\lambda)$ that vanishes at $-q$. Therefore $\xi(\lambda)$ can be expressed in terms of the dressed momentum $p(\lambda)$, the Fermi momentum being defined by $k_F = p(q)$

$$p(\lambda) = 2\pi \int_0^\lambda \rho(\mu) d\mu, \quad \xi(\lambda) = [p(\lambda) + p(q)]/2\pi, \quad \pi D = p(q) \equiv k_F. \quad (2.6)$$

¹The number N depends on the magnetization of the ground state, which is fixed by the overall magnetic field h . Hereafter, we call N sector the subspace of the space of states having N spins down.

Several other properties of the ground state can be described through the solutions of other linear integral equations. We introduce two such functions that will play an important role in our analysis, namely the dressed charge $Z(\lambda)$ and the dressed phase $\phi(\lambda, \nu)$, which satisfy

$$Z(\lambda) + \frac{1}{2\pi} \int_{-q}^q K(\lambda - \mu) Z(\mu) d\mu = 1, \quad (2.7)$$

and

$$\phi(\lambda, \nu) + \frac{1}{2\pi} \int_{-q}^q K(\lambda - \mu) \phi(\mu, \nu) d\mu = \frac{1}{2\pi} \vartheta(\lambda - \nu). \quad (2.8)$$

In fact, these two functions are not independent. Using that $K(\lambda) = \vartheta'(\lambda)$, one easily obtains that

$$Z(\lambda) = 1 + \phi(\lambda, q) - \phi(\lambda, -q). \quad (2.9)$$

Another non-trivial relationship between Z and ϕ has been established in [46, 47]:

$$1 + \phi(q, q) - \phi(-q, q) = Z^{-1}(q). \quad (2.10)$$

2.2 Thermodynamic limit of the excited states

To describe the other eigenstates of the transfer matrix $\mathcal{T}(\lambda)$, it is convenient for further purposes to consider instead the twisted transfer matrix $\mathcal{T}_\kappa(\lambda) = A(\lambda) + \kappa D(\lambda)$, where κ is some complex (twist) parameter. Hereby the excited states of the Hamiltonian (1.1) are obtained as the $\kappa \rightarrow 1$ limit of the eigenstates of the twisted transfer matrix $\mathcal{T}_\kappa(\lambda)$ [27, 1].

In complete analogy with the standard algebraic Bethe Ansatz considerations, the eigenstates $|\psi_\kappa(\{\mu\})\rangle$ of $\mathcal{T}_\kappa(\lambda)$ can be parameterized by sets of solutions of the twisted Bethe equations

$$Mp_0(\mu_{\ell_j}) - \sum_{k=1}^{N_\kappa} \vartheta(\mu_{\ell_j} - \mu_{\ell_k}) = 2\pi \left(\ell_j - \frac{N_\kappa + 1}{2} \right) + 2\pi\alpha, \quad j = 1, \dots, N_\kappa. \quad (2.11)$$

Such states $|\psi_\kappa(\{\mu\})\rangle$ depend on N_κ parameters $\{\mu_{\ell_k}\}_{k=1}^{N_\kappa}$, where N_κ is the number of spins down and we have set $\kappa = e^{2\pi i\alpha}$. In this article we consider α to be a real number. This restriction $\Im(\alpha) = 0$ is not crucial, but convenient, since then $\langle \psi_\kappa(\{\mu\}) | = (-1)^{N_\kappa} |\psi_\kappa(\{\mu\})\rangle^\dagger$.

Remark 2.1. One could of course from the very beginning set $\alpha = 0$ and deal directly with the standard excited states of the XXZ Hamiltonian (1.1). However, we chose to introduce this extra parameter and keep it throughout our computations since, as we will show later on, an important class of form factors can be obtained by a mere shift of α by some integer value.

In the following, we will consider two cases of interest: $N_\kappa = N$ for form factors of σ^z , and $N_\kappa = N + 1$ for the σ^+ form factors¹. It follows from [8] that the set of real roots of the twisted Bethe equations is completely defined by the choice of the set of integers ℓ_j in the *r.h.s.* of (2.11). Therefore, we have labeled the roots of (2.11) by subscripts ℓ_j .

¹We do not consider the case $N_\kappa = N - 1$ corresponding to form factors of σ^- , since the last ones can be obtained from the form factors of σ^+ .

The state parametrized by the real solutions to (2.11) with $\ell_j = j$, $j = 1, \dots, N_\kappa$, is called α -twisted ground state in the N_κ sector. In the thermodynamic limit, excitations corresponding to real set of solutions to the twisted Bethe equations above this α -twisted ground state can be described in terms of particles and holes. Note that the states associated to complex roots of the Bethe equations (like string solutions) are not considered in the present article. They correspond in particular to form factors of bound states [5, 6, 7, 48] that will be dealt with in a separate publication. All this means that one deals with solutions to the twisted Bethe equations where most of the ℓ_j coincide with their value for the ground state: $\ell_j = j$ except for n integers for which $\ell_j \neq j$, with n remaining finite in the $N_\kappa \rightarrow \infty$ limit. To be more precise, we fix $2n$ distinct integers h_1, \dots, h_n and p_1, \dots, p_n such that $h_k \in \{1, \dots, N_\kappa\}$ and $p_k \notin \{1, \dots, N_\kappa\}$. The integers h_k represent "holes" in respect to the distributions of integers for the ground state in the N_κ sector, whereas the integers p_k represent "particles". In other words, the excited state is described by a set of integers $\{\ell_j\}_{j=1}^{N_\kappa}$ such that $\ell_j = j$ for $j \neq h_1, \dots, h_n$, and $\ell_{h_k} = p_k$.

The terminology of particles and holes takes a clearer interpretation in terms of the counting function $\widehat{\xi}_\kappa$ associated with the N_κ -excited state:

$$\widehat{\xi}_\kappa(\omega) = \frac{1}{2\pi} p_0(\omega) - \frac{1}{2\pi M} \sum_{k=1}^{N_\kappa} \vartheta(\omega - \mu_{\ell_k}) + \frac{N_\kappa + 1}{2M} - \frac{\alpha}{M}. \quad (2.12)$$

One can argue that the counting function is monotonously increasing on the real axis. Thus it is possible to define unambiguously a set of real parameters μ_j as the unique solutions to $\widehat{\xi}_\kappa(\mu_j) = j/M$. One can identify, among this set of parameters, the N_κ solutions of the twisted Bethe equations with integers ℓ_j as being μ_{ℓ_j} as it should be. In this picture, an excited state no-longer corresponds to the set of N_κ consecutive solutions μ_j to the equation $\widehat{\xi}_\kappa(\mu_j) = j/M$, but is rather obtained by removing the solutions $\widehat{\xi}_\kappa(\mu_{h_a}) = h_a/M$ and replacing them by the solutions $\widehat{\xi}_\kappa(\mu_{p_a}) = p_a/M$. It is in this respect that μ_{h_a} stands for the rapidities of the holes and that μ_{p_a} stands for those of the particles. From now on, we agree upon μ_j being the solution to $\widehat{\xi}_\kappa(\mu_j) = j/M$ with $\widehat{\xi}_\kappa$ being given by (2.12).

Similarly as for the ground state in the N sector, one can also define the discrete density of the excited state by $\widehat{\rho}_\kappa(\omega) = \widehat{\xi}'_\kappa(\omega)$. It is easy to see that the thermodynamic limits of this new counting function and its associated density coincide with the limits defined above in (2.5), (2.6).

An excited state is most conveniently characterized in terms of the shift function $\widehat{F}(\omega) = \widehat{F}(\omega|\{\mu_p\}|\{\mu_h\})$ defined by

$$\widehat{F}(\omega) = M(\widehat{\xi}(\omega) - \widehat{\xi}_\kappa(\omega)). \quad (2.13)$$

The shift function describes the spacing between the root λ_j for the ground state in the N sector and the parameters μ_j defined by $\widehat{\xi}_\kappa(\mu_j) = j/M$:

$$\mu_j - \lambda_j = \frac{F(\lambda_j)}{\rho(\lambda_j)M} + O(M^{-2}), \quad (2.14)$$

where $F(\lambda)$ is the thermodynamic limit of the shift function. Recall that we consider the excited states in the N_κ sector with $N_\kappa = N$ (for form factors of σ^z) and $N_\kappa = N + 1$ (for

form factors of σ^+). Respectively we should distinguish between two shift functions $F^{(z)}(\lambda)$ and $F^{(+)}(\lambda)$ corresponding to these two cases. Generically the shift function $F(\lambda)$ satisfies the integral equation

$$F(\lambda) + \int_{-q}^q K(\lambda - \mu) F(\mu) \frac{d\mu}{2\pi} = \alpha + \frac{\delta N}{2} \left[1 - \frac{\vartheta(\lambda - q)}{\pi} \right] + \frac{1}{2\pi} \sum_{k=1}^n [\vartheta(\lambda - \mu_{p_k}) - \vartheta(\lambda - \mu_{h_k})]. \quad (2.15)$$

where $\delta N = N - N_\kappa$. Using (2.7) and (2.8) we conclude that

$$F^{(z)}(\lambda) = \alpha Z(\lambda) + \sum_{k=1}^n \phi(\lambda, \mu_{p_k}) - \sum_{k=1}^n \phi(\lambda, \mu_{h_k}). \quad (2.16)$$

and

$$F^{(+)}(\lambda) = \left(\alpha - \frac{1}{2} \right) Z(\lambda) + \sum_{k=1}^n \phi(\lambda, \mu_{p_k}) - \sum_{k=1}^n \phi(\lambda, \mu_{h_k}) + \phi(\lambda, q). \quad (2.17)$$

3 The main results

We now formulate a precise statement of the results obtained in this article concerning the thermodynamic behavior of form factors. In fact, for later use, we will give this thermodynamic behavior directly for the products of form factors appearing in the spectral expansion of the correlation function (1.3). However, it will be made clear that our method allows also to obtain the behavior of each individual form factor. The proof of the results we present below will be given in the next sections.

We consider the form factors (1.2) of the local spin operators σ_m^s , $s = +, -, z$, between the ground state $|\psi_g\rangle$ and some (different) excited state $|\psi'\rangle$ of the Hamiltonian¹. Here and in the following, we set $|\psi_g\rangle \equiv |\psi(\{\lambda\})\rangle$, $\{\lambda_1, \dots, \lambda_N\}$ being the solution of the Bethe equations (2.2) describing the ground state of the Hamiltonian, and $|\psi'\rangle = \lim_{\kappa \rightarrow 1} |\psi_\kappa(\{\mu\})\rangle$ for $\{\mu_{\ell_1}, \dots, \mu_{\ell_{N_\kappa}}\}$ being a solution of the κ -twisted Bethe equations (2.11) with n particles and n holes. We will be specially interested in the limiting case where, in the thermodynamic limit, all rapidities $\{\mu_{p_j}\}_{j=1}^n$ and $\{\mu_{h_j}\}_{j=1}^n$ of particles and holes condensate on the Fermi boundaries. Such excited states have a zero excitation energy in the thermodynamic limit; we expect that they will produce the main contribution to the asymptotic behavior of correlation functions (this fact is already apparent in the predictions based on the Luttinger liquid theory and Conformal Field Theory for the long-distance asymptotic behavior of two-point functions [37, 38, 39, 40, 41, 42, 43, 44]). We will also consider the opposite limiting case, namely when all particle/hole rapidities remain at finite distance from the Fermi boundaries.

In the thermodynamic limit, up to uniformly $M^{-1} \cdot \log M$ corrections, the products of such form factors behave as

$$\begin{aligned} \mathcal{F}_{\psi_g \psi'}^{(z)}(m') \cdot \mathcal{F}_{\psi' \psi_g}^{(z)}(m) &\sim \delta_{N, N_\kappa} M^{-\theta_{zz}} e^{i\mathcal{P}_{ex}(m-m')} \partial_\alpha^2 \mathcal{S}_{zz} \mathcal{D}_{zz} \Big|_{\alpha=0}, \\ \mathcal{F}_{\psi_g \psi'}^{(+)}(m') \cdot \mathcal{F}_{\psi' \psi_g}^{(-)}(m) &\sim \delta_{N+1, N_\kappa} M^{-\theta_{+-}} (-1)^{m-m'} e^{i\mathcal{P}_{ex}(m-m')} \mathcal{S}_{+-} \mathcal{D}_{+-} \Big|_{\alpha=0}. \end{aligned} \quad (3.1)$$

¹The case when $|\psi'\rangle = |\psi_g\rangle$ is trivial: $\mathcal{F}_{\psi_g \psi_g}^{(\pm)}(m) = 0$, $\mathcal{F}_{\psi_g \psi_g}^{(z)}(m) = 2D - 1$.

Let us explain these formulas. These products decrease as some negative power of the size M of the system, the exponents θ_{zz} , θ_{+-} being specified below. Due to the translation invariance of the model, all the dependence on the lattice spacing $m - m'$ is absorbed into a phase factor, with

$$\mathcal{P}_{ex} = \lim_{M, N \rightarrow +\infty} \left\{ \sum_{j=1}^{N_\kappa} p_0(\mu_{\ell_j}) - \sum_{j=1}^N p_0(\lambda_j) \right\} \quad (3.2)$$

being the momentum of the excited state relative to the ground state. We have split the constant in front of the M and $(m - m')$ dependence in two parts, $\mathcal{S}_{ss'}$ and $\mathcal{D}_{ss'}$, that we call smooth and discrete parts respectively. The reason for this denomination is that the smooth part $\mathcal{S}_{ss'}$ depends continuously on the rapidities μ_{p_j} and μ_{h_j} of the particles and holes, whereas the discrete part $\mathcal{D}_{ss'}$ also depends on the set of integers appearing in the logarithmic Bethe Ansatz equations (2.11) for the excited state. Such a discrete structure can be fairly well approximated by a smooth function of the rapidities μ_{p_j} and μ_{h_j} as long as they are located at a finite distance from the Fermi boundaries. However, as soon as the rapidities of the particles or holes approach the Fermi surface, the discrete structure of the form factors can no longer be neglected: a microscopic (of order $1/M$) deviation of a particle (or hole) rapidity leads to a macroscopic change in $\mathcal{D}_{ss'}$.

3.1 Smooth parts

The smooth parts \mathcal{S}_{zz} and \mathcal{S}_{+-} are decomposed into

$$\mathcal{S}_{zz} = \frac{2}{\pi^2} \sin^2 \left(\frac{\mathcal{P}_{ex}}{2} \right) \cdot \mathcal{A}_n^{(z)} \cdot e^{C_n^{(z)}}, \quad \mathcal{S}_{+-} = \mathcal{A}_n^{(+)} \cdot e^{C_n^{(+)}}. \quad (3.3)$$

Here $C_n^{(z)}$, $\mathcal{A}_n^{(z)}$ are functionals acting on the shift function $F^{(z)}(\lambda)$ given in (2.16), while $C_n^{(+)}$, $\mathcal{A}_n^{(+)}$ are functionals acting on the shift function $F^{(+)}(\lambda)$ given in (2.17). This action is such that the result depends smoothly on the particle/hole rapidities $\{\mu_p\}$ and $\{\mu_h\}$ of the state $|\psi_\kappa(\{\mu\})\rangle$.

Before giving explicit expressions for the quantities in (3.3) we introduce the $i\pi$ -periodic Cauchy transform of the shift functions $F^{(z/+)}(\lambda)$ on $[-q, q]$,

$$\mathbf{F}^{(z/+)}(w) = \frac{1}{2\pi i} \int_{-q}^q F^{(z/+)}(\lambda) \coth(\lambda - w) d\lambda. \quad (3.4)$$

Then the coefficient $C_n^{(z)} = C_n^{(z)}(\{\mu_p\}, \{\mu_h\})$ has the form

$$\begin{aligned} C_n^{(z)}[F^{(z)}] &= C_0[F^{(z)}] + 2\pi i \sum_{j=1}^n (\mathbf{F}^{(z)}(\mu_{h_j} - i\zeta) + \mathbf{F}^{(z)}(\mu_{h_j} + i\zeta) - \mathbf{F}^{(z)}(\mu_{p_j} - i\zeta) - \mathbf{F}^{(z)}(\mu_{p_j} + i\zeta)) \\ &\quad + \sum_{j,k=1}^n \log \frac{\sinh(\mu_{h_j} - \mu_{p_k} - i\zeta) \sinh(\mu_{p_k} - \mu_{h_j} - i\zeta)}{\sinh(\mu_{p_j} - \mu_{p_k} - i\zeta) \sinh(\mu_{h_j} - \mu_{h_k} - i\zeta)}, \end{aligned} \quad (3.5)$$

where the functional $C_0[F]$ reads

$$C_0[F] = - \int_{-q}^q \frac{F(\lambda) F(\mu)}{\sinh^2(\lambda - \mu - i\zeta)} d\lambda d\mu. \quad (3.6)$$

The coefficient $C_n^{(+)} = C_n^{(+)}(\{\mu_p\}, \{\mu_h\})$ has similar representation, but it contains several additional terms

$$C_n^{(+)}[F^{(+)}] = C_n^{(z)}[F^{(+)}] - 2\pi i (\mathbf{F}^{(+)}(q + i\zeta) + \mathbf{F}^{(+)}(q - i\zeta)) + \sum_{j=1}^n \log \frac{\sinh(\mu_{h_j} - q - i\zeta) \sinh(\mu_{h_j} - q + i\zeta)}{\sinh(\mu_{p_j} - q - i\zeta) \sinh(\mu_{p_j} - q + i\zeta)}. \quad (3.7)$$

The functional $\mathcal{A}_n^{(z)} = \mathcal{A}_n^{(z)}(\{\mu_p\}, \{\mu_h\})$ has the form

$$\mathcal{A}_n^{(z)}[F^{(z)}] = \left(\frac{\sin \pi \alpha}{\sin \pi F^{(z)}(-q)} \right)^2 \left| e^{-2\pi i \mathbf{F}^{(z)}(-q+i\zeta)} \prod_{k=1}^n \frac{\sinh(q + \mu_{h_k} + i\zeta)}{\sinh(q + \mu_{p_k} + i\zeta)} \right|^2 \times \left| \frac{\det [I + \frac{1}{2\pi i} U^{(z)}(w, w')]}{\det [I + \frac{1}{2\pi} K]} \right|^2. \quad (3.8)$$

The equation (3.8) contains a ratio of Fredholm determinants. The integral operator $I + \frac{1}{2\pi} K$ acts on the interval $[-q, q]$, whereas the integral operators $I + \frac{1}{2\pi i} U^{(z)}$ acts on a counterclockwise oriented contour Γ_q surrounding $[-q, q]$. This contour is such that it contains all the ground state roots and no other singularity of the kernel. The integral kernel is defined by

$$U^{(z)}(w, w') = -\Phi(w) e^{2\pi i (\mathbf{F}^{(z)}(w) - \mathbf{F}^{(z)}(w+i\zeta))} \frac{K_\kappa(w - w') - K_\kappa(-q - w')}{1 - e^{2\pi i F^{(z)}(w)}}, \quad (3.9)$$

with

$$K_\kappa(w) = \coth(w + i\zeta) - \kappa \coth(w - i\zeta), \quad \Phi(w) = \prod_{k=1}^n \frac{\sinh(w - \mu_{p_k}) \sinh(w - \mu_{h_k} + i\zeta)}{\sinh(w - \mu_{h_k}) \sinh(w - \mu_{p_k} + i\zeta)}. \quad (3.10)$$

The coefficient $\mathcal{A}_n^{(+)} = \mathcal{A}_n^{(+)}(\{\mu_p\}, \{\mu_h\})$ also is proportional to a ratio of Fredholm determinants

$$\mathcal{A}_n^{(+)}[F^{(+)}] = \frac{\sin \zeta}{2\pi \kappa} \left| \frac{e^{-2\pi i \mathbf{F}^{(+)}(\frac{i\zeta}{2})}}{\sinh(q - \frac{i\zeta}{2})} \prod_{k=1}^n \frac{\sinh(\mu_{h_k} - \frac{i\zeta}{2})}{\sinh(\mu_{p_k} - \frac{i\zeta}{2})} \cdot \frac{\det [I + \frac{1}{2\pi i} U^{(+)}(w, w')]}{\det [I + \frac{1}{2\pi} K]} \right|^2. \quad (3.11)$$

Similarly to the integral operator defined in (3.9), the operator $I + \frac{1}{2\pi i} U^{(+)}$ acts on the contour Γ_q surrounding $[-q, q]$, with a kernel

$$U^{(+)}[F](w, w') = \Phi(w) \frac{\sinh(w - q)}{\sinh(w - q + i\zeta)} e^{2\pi i (\mathbf{F}^{(+)}(w) - \mathbf{F}^{(+)}(w+i\zeta))} \frac{\mathcal{K}_\kappa(w, w')}{1 - e^{2\pi i F^{(+)}(w)}}, \quad (3.12)$$

where

$$\mathcal{K}_\kappa(w, w') = \frac{\sinh(w' + \frac{3i\zeta}{2})}{\sinh(w' - \frac{i\zeta}{2}) \sinh(w - w' - i\zeta)} - \frac{\kappa \sinh(w' - \frac{3i\zeta}{2})}{\sinh(w' + \frac{i\zeta}{2}) \sinh(w - w' + i\zeta)}, \quad (3.13)$$

and $\Phi(w)$ is given by (3.10).

3.2 Discrete parts and exponents

The values of the discrete parts \mathcal{D}_{zz} and \mathcal{D}_{+-} , as well as of the exponents θ_{zz} and θ_{+-} , depend on whether particles and holes are on the Fermi surface or separated from it. We specify their expressions in the two particular cases we mentioned above: when all particle/hole rapidities remain at finite distance from the Fermi boundaries, or when all particle/hole rapidities collapse on the Fermi boundaries. Other intermediate configurations can be obtained along similar techniques.

3.2.1 Particles and holes away from the Fermi boundaries

In the first case, the exponents in (3.1) giving the algebraic decay of the form factor with the system size read:

$$\begin{aligned}\theta_{zz} &= 2n + \left(F_+^{(z)}\right)^2 + \left(F_-^{(z)}\right)^2, \\ \theta_{+-} &= 2n + 1 + \left(F_+^{(+)}\right)^2 + \left(F_-^{(+)}\right)^2,\end{aligned}\tag{3.14}$$

where $F_{\pm}^{(z/+)} = F^{(z/+)}(\pm q)$ are given in terms of the shift functions defined in (2.16) and (2.17). The discrete part \mathcal{D}_{zz} is given by

$$\begin{aligned}\mathcal{D}_{zz}(\{\mu_p\}, \{\mu_h\}) &= \left[\det_n \frac{1}{\sinh(\mu_{p_j} - \mu_{h_k})} \right]^2 \cdot \mathcal{D}^{(z)}[F^{(z)}] \prod_{k=1}^n \frac{\sin^2(\pi F^{(z)}(\mu_{h_k}))}{\pi^2 \rho(\mu_{h_k}) \rho(\mu_{p_k})} \\ &\quad \times \prod_{k=1}^n \exp \left\{ 2 \int_{-q}^q F^{(z)}(\lambda) [\coth(\lambda - \mu_{p_k}) - \coth(\lambda - \mu_{h_k})] d\lambda \right\},\end{aligned}\tag{3.15}$$

Here a functional $\mathcal{D}^{(z)}[F]$ has the following form:

$$\mathcal{D}^{(z)}[F] = \frac{G^2(1 - F_-) G^2(1 + F_+) (2\pi)^{F_- - F_+}}{[\rho(q) \sinh(2q)]^{(F_-)^2 + (F_+)^2}} e^{C_1[F]}.\tag{3.16}$$

where $G(z)$ is the Barnes function satisfying $G(z + 1) = \Gamma(z)G(z)$, and we have set

$$\begin{aligned}C_1[F] &= \int_{-q}^q \frac{F'(\lambda)F(\mu) - F(\lambda)F'(\mu)}{2 \tanh(\lambda - \mu)} d\lambda d\mu \\ &\quad + F_+ \int_{-q}^q \frac{F_+ - F(\lambda)}{\tanh(q - \lambda)} d\lambda + F_- \int_{-q}^q \frac{F_- - F(\lambda)}{\tanh(q + \lambda)} d\lambda.\end{aligned}\tag{3.17}$$

The discrete part \mathcal{D}_{+-} has the form

$$\begin{aligned}\mathcal{D}_{+-}(\{\mu_p\}, \{\mu_h\}) &= \left[\det_n \frac{1}{\sinh(\mu_{p_j} - \mu_{h_k})} \right]^2 \cdot \mathcal{D}^{(+)}[F^{(+)}] \prod_{k=1}^n \frac{\sin^2(\pi F^{(+)}(\mu_{h_k}))}{\pi^2 \rho(\mu_{h_k}) \rho(\mu_{p_k})} \\ &\quad \times \prod_{k=1}^n \left[\frac{\sinh(\mu_{p_k} - q)}{\sinh(\mu_{h_k} - q)} \right]^2 \exp \left\{ 2 \int_{-q}^q F^{(+)}(\lambda) [\coth(\lambda - \mu_{p_k}) - \coth(\lambda - \mu_{h_k})] d\lambda \right\},\end{aligned}\tag{3.18}$$

where the functional $\mathcal{D}^{(+)}[F]$ reads

$$\mathcal{D}^{(+)}[F] = \mathcal{D}^{(z)}[F] \cdot \frac{\sinh(2q)\Gamma^2(1+F_+)}{[\rho(q)\sinh(2q)]^{1+2F_+}} \exp \left\{ 2 \int_{-q}^q \frac{F_+ - F(\lambda)}{\tanh(q-\lambda)} d\lambda \right\}. \quad (3.19)$$

3.2.2 Particles and holes on the Fermi boundaries

Definition 3.1. *Let an excited state contain n particles and n holes. It is called critical excited state, if all the rapidities $\mu_p, \mu_h = \pm q$ in the thermodynamic limit. We also say that this excited state belongs to the \mathbf{P}_r class if it contains n_p^\pm particles, resp. n_h^\pm holes, with rapidities equal to $\pm q$ such that*

$$n_p^+ - n_h^+ = n_p^- - n_h^- = r, \quad r \in \mathbb{Z}. \quad (3.20)$$

The corresponding form factors are called critical form factors of the \mathbf{P}_r class.

The rapidities of the particles and holes in an excited state belonging to the \mathbf{P}_r class are all located in a close neighborhood of $\pm q$. As a consequence, it is useful to reparametrize the integers describing the position of particles and holes according to

$$\begin{aligned} p_j &= p_j^+ + N_\kappa, & \text{if } \mu_{p_j} &= q, \\ p_j &= 1 - p_j^-, & \text{if } \mu_{p_j} &= -q, \\ h_j &= N_\kappa + 1 - h_j^+, & \text{if } \mu_{h_j} &= q, \\ h_j &= h_j^-, & \text{if } \mu_{h_j} &= -q. \end{aligned} \quad (3.21)$$

All the integers $\{p^\pm\}$ and $\{h^\pm\}$ introduced above are positive and vary in a range such that

$$\lim_{N \rightarrow \infty} \frac{\sum p_j^\pm}{N} = \lim_{N \rightarrow \infty} \frac{\sum h_j^\pm}{N} = 0, \quad (3.22)$$

meaning μ_p and μ_h indeed collapse to the Fermi boundary in the thermodynamic limit.

For σ^z and σ^\pm form factors belonging to the \mathbf{P}_r class, the discrete parts are given by

$$\begin{aligned} \mathcal{D}_{zz} &= \mathcal{D}^{(z)}[F_r^{(z)}] \frac{G^2(1+F_+^{(z)})G^2(1-F_-^{(z)})}{G^2(1+F_{r,+}^{(z)})G^2(1-F_{r,-}^{(z)})} \left(\frac{\sin(\pi F_{r,+}^{(z)})}{\pi} \right)^{2n_h^+} \left(\frac{\sin(\pi F_{r,-}^{(z)})}{\pi} \right)^{2n_h^-} \\ &\quad \times R_{n_p^+, n_h^+}(\{p^+\}, \{h^+\} | F_+^{(z)}) R_{n_p^-, n_h^-}(\{p^-\}, \{h^-\} | -F_-^{(z)}), \end{aligned} \quad (3.23)$$

and

$$\begin{aligned} \mathcal{D}_{+-} &= \mathcal{D}^{(+)}[F_r^{(+)}] \frac{G^2(2+F_+^{(+)})G^2(1-F_-^{(+)})}{G^2(2+F_{r,+}^{(+)})G^2(1-F_{r,-}^{(+)})} \left(\frac{\sin(\pi F_{r,+}^{(+)})}{\pi} \right)^{2n_h^+} \left(\frac{\sin(\pi F_{r,-}^{(+)})}{\pi} \right)^{2n_h^-} \\ &\quad \times R_{n_p^+, n_h^+}(\{p^+\}, \{h^+\} | F_+^{(+)}) R_{n_p^-, n_h^-}(\{p^-\}, \{h^-\} | -F_-^{(+)}). \end{aligned} \quad (3.24)$$

Here we agree upon $F_r^{(z/+)}(\lambda) = F^{(z/+)}(\lambda) + r$ and $F_{r,\pm}^{(z/+)} = F_r^{(z/+)}(\pm q)$. The functionals $\mathcal{D}^{(z)}$ and $\mathcal{D}^{(+)}$ are given respectively in (3.16) and (3.19). The coefficient $R_{n,m}(\{p\}, \{h\} | F)$ is

defined as

$$R_{n,m}(\{p\}, \{h\}|F) = \frac{\prod_{j>k}^n (p_j - p_k)^2 \prod_{j>k}^m (h_j - h_k)^2}{\prod_{j=1}^n \prod_{k=1}^m (p_j + h_k - 1)^2} \Gamma^2 \left(\begin{matrix} \{p_k + F\}, \{h_k - F\} \\ \{p_k\}, \{h_k\} \end{matrix} \right), \quad (3.25)$$

where we have used the standard hypergeometric type notation for ratios of Γ functions:

$$\Gamma \left(\begin{matrix} a_1, \dots, a_\ell \\ b_1, \dots, b_j \end{matrix} \right) = \prod_{k=1}^{\ell} \Gamma(a_k) \cdot \prod_{k=1}^j \Gamma(b_k)^{-1}. \quad (3.26)$$

The exponents θ in this case are

$$\begin{aligned} \theta_{zz}(r) &= \left(F_{r,+}^{(z)} \right)^2 + \left(F_{r,-}^{(z)} \right)^2, \\ \theta_{+-}(r) &= \left(1 + F_{r,+}^{(+)} \right)^2 + \left(F_{r,-}^{(+)} \right)^2. \end{aligned} \quad (3.27)$$

It is crucial to compare the results (3.27) with the critical exponents appearing in the asymptotic behavior of the two-point correlation functions predicted in [37, 38, 39, 40, 41, 42, 43, 44, 49, 50, 36].

In the case of $\theta_{zz}(r)$, it follows from (2.9), (2.16) that $F_r^{(z)}(\lambda) = (\alpha + r)Z(\lambda)$. Therefore, for $\alpha = 0$, we obtain that $\theta_{zz}(r) = 2r^2 Z^2(q)$, $|r| = 1, 2, \dots$. These numbers coincide with the critical exponents appearing in the asymptotic behavior of the $\langle \sigma_1^z \sigma_{m+1}^z \rangle$ correlation function and are associated to the oscillating term with momentum $2rk_F$.

The exponent $\theta_{+-}(r)$ has similar properties. In this case, $F_r^{(+)}(\lambda) = (\alpha + r - 1/2)Z(\lambda) + \phi(\lambda, q)$. It follows from equations (2.9) and (2.10) that

$$\begin{aligned} 1 + \phi(q, q) &= \frac{Z(q) + Z^{-1}(q)}{2}, \\ \phi(-q, q) &= \frac{Z(q) - Z^{-1}(q)}{2}. \end{aligned} \quad (3.28)$$

From this we find

$$\begin{aligned} F_{r,+} + 1 &= (\alpha + r)Z(q) + \frac{Z^{-1}(q)}{2}, \\ F_{r,-} &= (\alpha + r)Z(q) - \frac{Z^{-1}(q)}{2}. \end{aligned} \quad (3.29)$$

Thus, at $\alpha = 0$ we have $\theta_{+-}(r) = Z^{-2}(q)/2 + 2r^2 Z^2(q)$, $|r| = 0, 1, \dots$. Again, these numbers coincide with the critical exponents appearing in the asymptotic behavior of the $\langle \sigma_1^+ \sigma_{m+1}^- \rangle$ correlation function and associated to the oscillating term with momentum $2rk_F$. Thus, we see that the behavior of critical form factors with respect to the size of the system coincides with the asymptotic behavior of two-point correlation functions with respect to the lattice distance.

4 Form factors and scalar products

The solution of the quantum inverse scattering problem enables us to express the local spin operators in terms of the entries of the monodromy matrix [10, 23]:

$$\sigma_m^s = \mathcal{T}^{m-1}(-i\zeta/2) \cdot \text{tr} \left(T(-i\zeta/2) \sigma^s \right) \cdot \mathcal{T}^{-m}(-i\zeta/2). \quad (4.1)$$

In the *l.h.s.* of this expression, the symbol σ_m^s ($s = \pm, z$) denotes the corresponding local spin operator at site m , whereas the symbol σ^s appearing in the *r.h.s.* should be understood as a 2×2 Pauli matrix multiplying the 2×2 monodromy matrix (2.1).

Using (4.1), one can reduce the computation of the form factors of local spin operators in the finite XXZ chain to the one of the scalar products [10]. We have

$$\mathcal{F}_{\psi'\psi_g}^{(z)}(m) = -e^{i(m-1)\sum_{j=1}^N [p_0(\mu_{\ell_j}) - p_0(\lambda_j)]} \left(e^{i\sum_{j=1}^N [p_0(\mu_{\ell_j}) - p_0(\lambda_j)]} - 1 \right) \times \frac{\partial}{\partial \alpha} \frac{\langle \psi_\kappa(\{\mu\}) | \psi(\{\lambda\}) \rangle}{\pi i \|\psi_\kappa(\{\mu\})\| \cdot \|\psi(\{\lambda\})\|} \Big|_{\alpha=0}, \quad (4.2)$$

which is nonzero only if $N_\kappa = N$. The form-factor $\mathcal{F}_{\psi_g\psi'}^{(z)}$ is obtained by complex conjugation $\mathcal{F}_{\psi_g\psi'}^{(z)}(m) = \left(\mathcal{F}_{\psi'\psi_g}^{(z)}(m) \right)^*$. Similarly, one obtains

$$\mathcal{F}_{\psi'\psi_g}^{(-)}(m) = (-1)^{N+m+1} e^{i(m-1)\sum_{j=1}^{N_\kappa} p_0(\mu_{\ell_j}) - im\sum_{j=1}^N p_0(\lambda_j)} \frac{\langle \psi_\kappa(\{\mu\}) | B(-\frac{i\zeta}{2}) | \psi(\{\lambda\}) \rangle}{a(-i\frac{\zeta}{2}) \|\psi_\kappa(\{\mu\})\| \cdot \|\psi(\{\lambda\})\|} \Big|_{\alpha=0}, \quad (4.3)$$

$$\mathcal{F}_{\psi_g\psi'}^{(+)}(m) = (-1)^{N+m} e^{i(m-1)\sum_{j=1}^N p_0(\lambda_j) - im\sum_{j=1}^{N_\kappa} p_0(\mu_{\ell_j})} \frac{\langle \psi(\{\lambda\}) | C(-\frac{i\zeta}{2}) | \psi_\kappa(\{\mu\}) \rangle}{a(-i\frac{\zeta}{2}) \|\psi_\kappa(\{\mu\})\| \cdot \|\psi(\{\lambda\})\|} \Big|_{\alpha=0}, \quad (4.4)$$

which are nonzero only if $N_\kappa = N + 1$. In (4.3) and (4.4), $a(\nu) = \sinh^M(\nu - i\zeta/2)$ denotes the eigenvalue of the operator $A(\nu)$ on the reference state which, in the case of the spin-1/2 chain, is the ferromagnetic state with all spins up. In the following, we will also use the notation $d(\nu) = \sinh^M(\nu + i\zeta/2)$ for the eigenvalue of $D(\nu)$ on this reference state.

Remark 4.1. Although it is possible to set $\alpha = 0$ directly in (4.3) and (4.4), we prefer to take the limit $\alpha = 0$ only in the very end of the calculations to study the properties of the scalar products for general α .

In all the above scalar products, one of the states is an eigenstate of the twisted transfer matrix. There exists an explicit determinant representations for such scalar products and the associated norms:

Proposition 4.1. [24, 25, 10, 36] *Let $\{\lambda\}_1^N$ satisfy the ground state Bethe equations (2.2) and $\{\mu\}_1^{N_\kappa}$ solve the system of α -twisted Bethe Ansatz equations (2.11). Then the following representations for the scalar products hold:*

$$\langle \psi_\kappa(\{\mu\}) | \psi(\{\lambda\}) \rangle = \delta_{N_\kappa, N} \cdot \prod_{a,b=1}^N \frac{\sinh(\mu_{\ell_a} - \lambda_b - i\zeta)}{\sinh(\lambda_a - \mu_{\ell_b})} \cdot \prod_{j=1}^N \left\{ d(\mu_{\ell_j}) d(\lambda_j) \left[e^{2i\pi\widehat{F}(\lambda_j)} - 1 \right] \right\} \times \frac{1 - \kappa}{1 - e^{2\pi i\widehat{F}(-q)}} \cdot \prod_{a=1}^N \frac{\sinh(q + \lambda_a - i\zeta)}{\sinh(q - \mu_{\ell_a} - i\zeta)} \cdot \det_{\Gamma_q} \left[I + \frac{1}{2\pi i} \widehat{U}^{(z)}(w, w') \right], \quad (4.5)$$

$$\begin{aligned}
\langle \psi_\kappa(\{\mu\}) | B(-i\zeta/2) | \psi(\{\lambda\}) \rangle &= \delta_{N_\kappa, N+1} \cdot a(-i\zeta/2) \sinh(-i\zeta) \prod_{j=1}^N \left\{ a(\lambda_j) \left[1 - e^{2i\pi\widehat{F}(\lambda_j)} \right] \right\} \\
&\times \frac{\prod_{b=1}^N \sinh(\lambda_b - i\zeta/2)}{\prod_{b=1}^{N+1} \sinh(\mu_{\ell_b} + i\zeta/2)} \prod_{a=1}^{N+1} \left\{ d(\mu_{\ell_a}) \prod_{b=1}^N \frac{\sinh(\mu_{\ell_a} - \lambda_b - i\zeta)}{\sinh(\mu_{\ell_a} - \lambda_b)} \right\} \cdot \det_{\Gamma_q} \left[I + \frac{1}{2\pi i} \widehat{U}^{(+)}(w, w') \right].
\end{aligned} \tag{4.6}$$

In these expressions $\widehat{F}(\lambda)$ (2.13) depends on whether we consider the N sector or the $(N+1)$ sector (see (2.12)). The integral operators $I + \frac{1}{2\pi i} \widehat{U}^{(z)}$ and $I + \frac{1}{2\pi i} \widehat{U}^{(+)}$ act on a closed anti-clockwise oriented contour Γ_q surrounding the interval $[-q, q]$ where the ground state roots $\{\lambda_a\}_{a=1}^N$ condensate and containing no other singularity of the kernels. The last ones have the form

$$\widehat{U}^{(z)}(w, w') = - \prod_{a=1}^N \frac{\sinh(w - \mu_{\ell_a}) \sinh(w - \lambda_a + i\zeta)}{\sinh(w - \lambda_a) \sinh(w - \mu_{\ell_a} + i\zeta)} \cdot \frac{K_\kappa(w - w') - K_\kappa(-q - w')}{1 - e^{2\pi i \widehat{F}(w)}}, \tag{4.7}$$

$$\widehat{U}^{(+)}(w, w') = \prod_{a=1}^{N+1} \frac{\sinh(w - \mu_{\ell_a})}{\sinh(w - \mu_{\ell_a} + i\zeta)} \prod_{a=1}^N \frac{\sinh(w - \lambda_a + i\zeta)}{\sinh(w - \lambda_a)} \cdot \frac{\mathcal{K}_\kappa(w, w')}{1 - e^{2\pi i \widehat{F}(w)}}, \tag{4.8}$$

where K_κ and \mathcal{K}_κ are given respectively by (3.10) and (3.13).

We also recall the finite size determinant representations for the norms of Bethe states:

Proposition 4.2. [51, 52, 53] Let $\mu_{\ell_1}, \dots, \mu_{\ell_{N_\kappa}}$ satisfy the system (2.12). Then

$$\begin{aligned}
\langle \psi_\kappa(\{\mu\}) | \psi_\kappa(\{\mu\}) \rangle &= (-1)^{N_\kappa} \prod_{j=1}^{N_\kappa} [2\pi i M \widehat{\rho}_\kappa(\mu_{\ell_j}) a(\mu_{\ell_j}) d(\mu_{\ell_j})] \frac{\prod_{a,b=1}^N \sinh(\mu_{\ell_a} - \mu_{\ell_b} - i\zeta)}{\prod_{\substack{a,b=1 \\ a \neq b}}^{N_\kappa} \sinh(\mu_{\ell_a} - \mu_{\ell_b})} \\
&\times \det_{N_\kappa} \Theta_{jk}^{(\mu)}, \tag{4.9}
\end{aligned}$$

where

$$\Theta_{jk}^{(\mu)} = \delta_{jk} + \frac{K(\mu_{\ell_j} - \mu_{\ell_k})}{2\pi M \widehat{\rho}_\kappa(\mu_{\ell_k})}. \tag{4.10}$$

One can see from another representation for the scalar product (B.1) that, when $\Im\alpha = 0$,

$$\langle \psi_\kappa(\{\mu\}) | \psi(\{\lambda\}) \rangle = \left(\langle \psi_\kappa(\{\mu\}) | \psi(\{\lambda\}) \rangle \right)^*, \tag{4.11}$$

and

$$\langle \psi(\{\lambda\}) | C(-\frac{i\zeta}{2}) | \psi_\kappa(\{\mu\}) \rangle = \kappa^{-1} e^{i \sum_{j=1}^{N_\kappa} p_0(\mu_{\ell_j}) + i \sum_{j=1}^N p_0(\lambda_j)} \left(\langle \psi_\kappa(\{\mu\}) | B(-\frac{i\zeta}{2}) | \psi(\{\lambda\}) \rangle \right)^*. \tag{4.12}$$

For the calculation of the two-point correlation functions $\langle \sigma_m^z \sigma_{m'}^z \rangle$ (resp. $\langle \sigma_m^+ \sigma_{m'}^- \rangle$), we need actually to sum up the products $\mathcal{F}_{\psi_g \psi'}^{(z)}(m) \mathcal{F}_{\psi' \psi_g}^{(z)}(m')$ (resp. $\mathcal{F}_{\psi_g \psi'}^{(+)}(m) \mathcal{F}_{\psi' \psi_g}^{(-)}(m')$) over all eigenstates $|\psi'\rangle$. We have the following result:

Proposition 4.3. *The products of two form factors can be written in terms of the former scalar products as*

$$\mathcal{F}_{\psi_g\psi'}^{(z)}(m') \cdot \mathcal{F}_{\psi'\psi_g}^{(z)}(m) = e^{i(m-m')\widehat{\mathcal{P}}_{ex}} \frac{2 \sin^2\left(\frac{\widehat{\mathcal{P}}_{ex}}{2}\right)}{\pi^2} \cdot \frac{\partial^2}{\partial \alpha^2} S_N^z \Big|_{\alpha=0}, \quad (4.13)$$

$$\mathcal{F}_{\psi_g\psi'}^{(+)}(m') \cdot \mathcal{F}_{\psi'\psi_g}^{(-)}(m) = (-1)^{m-m'} e^{i(m-m')\widehat{\mathcal{P}}_{ex}} \cdot S_N^+ \Big|_{\alpha=0}, \quad (4.14)$$

where

$$S_N^z = \left| \frac{\langle \psi_\kappa(\{\mu\}) | \psi(\{\lambda\}) \rangle}{\|\psi_\kappa(\{\mu\})\| \cdot \|\psi(\{\lambda\})\|} \right|^2, \quad (4.15)$$

$$S_N^+ = -\frac{e^{-2\pi i \alpha}}{a^2(-i\zeta/2)} \left| \frac{\langle \psi_\kappa(\{\mu\}) | B(-\frac{i\zeta}{2}) | \psi(\{\lambda\}) \rangle}{\|\psi_\kappa(\{\mu\})\| \cdot \|\psi(\{\lambda\})\|} \right|^2. \quad (4.16)$$

In (4.13) and (4.14), $\widehat{\mathcal{P}}_{ex}$ denotes the relative excitation momentum of the excited states in the N_κ sector in respect to the ground state in the N sector,

$$\widehat{\mathcal{P}}_{ex} = \sum_{j=1}^{N_\kappa} p_0(\mu_{\ell_j}) - \sum_{j=1}^N p_0(\lambda_j). \quad (4.17)$$

Remark 4.2. Here, we did not consider the product $\mathcal{F}_{\psi_g\psi'}^{(-)}(m) \mathcal{F}_{\psi'\psi_g}^{(+)}(m')$, since the equal-time correlation function $\langle \sigma_m^- \sigma_{m'}^+ \rangle$ can be obtained from $\langle \sigma_m^+ \sigma_{m'}^- \rangle$ by the replacement $m \rightarrow m'$.

The calculation of the thermodynamic limit of $\widehat{\mathcal{P}}_{ex}$ is a relatively simple problem. Indeed, it follows from (2.4), (2.12) that

$$\frac{\widehat{\mathcal{P}}_{ex}}{2\pi} = \alpha \frac{N_\kappa}{M} + \sum_{j=1}^{N_\kappa} \hat{\xi}_\kappa(\mu_{\ell_j}) - \sum_{j=1}^N \hat{\xi}(\lambda_j) + \frac{N^2 + N - N_\kappa^2 - N_\kappa}{2M} = \alpha \frac{N_\kappa}{M} + \sum_{k=1}^n (\hat{\xi}_\kappa(\mu_{p_k}) - \hat{\xi}_\kappa(\mu_{h_k})). \quad (4.18)$$

Here we have used the antisymmetry of the bare phase $\vartheta(-\lambda) = -\vartheta(\lambda)$ and $\hat{\xi}_\kappa(\mu_{\ell_j}) = \ell_j/M$, $\hat{\xi}(\lambda_j) = j/M$. Then using (2.6) we obtain

$$\mathcal{P}_{ex} \equiv \lim_{N, M \rightarrow \infty} \widehat{\mathcal{P}}_{ex} = 2\pi D\alpha + \sum_{j=1}^n [p(\mu_{p_j}) - p(\mu_{h_j})]. \quad (4.19)$$

The non-trivial problem is the computation of the thermodynamic limit of the scalar products S_N^z and S_N^+ . This problem will be treated in the remaining part of the article.

5 Thermodynamic limit of S_N^z

In the paper [1] we studied the thermodynamic limit of the scalar product S_N^z in the particular case where the state $|\psi_\kappa(\{\mu\})\rangle$ was the α -twisted ground state in the N sector. In the general case, when the excited state contains n particles and n holes, the result also depends on their rapidities $\{\mu_p\}$ and $\{\mu_h\}$. As we have already announced, such dependence is not sufficient to characterize completely the thermodynamic limit of the form factor. Indeed, the latter

decomposes into a product of a smooth and a discrete part. The smooth part can actually be completely described in terms of the rapidities of the particles and holes. However, for the description of the discrete part one should use also the integer numbers $\{p_a\}$ and $\{h_a\}$.

In the first part of this section, we explicitly factorize S_N^z into the aforementioned product. Then, we investigate the thermodynamic limit of the smooth part, postponing the more complicated analysis of the discrete part until subsection 5.3.

Note that in this section we deal only with the excited states in the N sector. Therefore the thermodynamic limit of the shift function $\widehat{F}(\lambda)$ is equal to $F^{(z)}(\lambda)$ given by (2.16). However, in order to lighten notations we omit the superscript (z) throughout this section, denoting the limiting value of the shift function simply by $F(\lambda)$.

5.1 Representation of the scalar product S_N^z

Assume that the excited state $|\psi_\kappa(\{\mu\})\rangle$ is an excited state in the N sector containing n particles with rapidities $\{\mu_{p_a}\}_{a=1}^n$ and n holes with rapidities $\{\mu_{h_a}\}_{a=1}^n$. One can fairly expect that the limiting value of S_N^z depends on the thermodynamic limit of these rapidities $\{\mu_p\}$ and $\{\mu_h\}$, *i.e.* $\lim S_N^z = S_n^z(\{\mu_p\}, \{\mu_h\})$.

Using Propositions 4.1 and 4.2 as well as (4.15), it is readily seen that S_N^z has the following representation:

$$S_N^z(\{\mu_p\}, \{\mu_h\}) = \mathcal{A}_N^{(z)}(\{\mu_p\}, \{\mu_h\}) \cdot D_N^{(z)}(\{\mu_p\}, \{\mu_h\}) \cdot \exp \left\{ C_N^{(z)}(\{\mu_p\}, \{\mu_h\}) \right\}, \quad (5.1)$$

where

$$C_N^{(z)}(\{\mu_p\}, \{\mu_h\}) = \sum_{a,b=1}^N \log \frac{\sinh(\lambda_a - \mu_{\ell_b} - i\zeta) \sinh(\mu_{\ell_b} - \lambda_a - i\zeta)}{\sinh(\lambda_a - \lambda_b - i\zeta) \sinh(\mu_{\ell_a} - \mu_{\ell_b} - i\zeta)}, \quad (5.2)$$

$$D_N^{(z)}(\{\mu_p\}, \{\mu_h\}) = \left(\det_N \frac{1}{\sinh(\mu_{\ell_j} - \lambda_k)} \right)^2 \cdot \prod_{j=1}^N \frac{\sin^2 \pi \widehat{F}(\lambda_j)}{\pi^2 M^2 \widehat{\rho}(\lambda_j) \widehat{\rho}_\kappa(\mu_{\ell_j})}, \quad (5.3)$$

and

$$\mathcal{A}_N^{(z)}(\{\mu_p\}, \{\mu_h\}) = \left| \frac{\sin \pi \alpha}{\sin \pi \widehat{F}(-q)} \prod_{a=1}^N \frac{\sinh(q + \lambda_a - i\zeta)}{\sinh(q - \mu_{\ell_a} - i\zeta)} \right|^2 \frac{\left| \det_{\Gamma_q} \left[I + \frac{1}{2\pi i} \widehat{U}^{(z)}(w, w') \right] \right|^2}{\det_N \Theta_{jk}^{(\lambda)} \cdot \det_N \Theta_{jk}^{(\mu)}}. \quad (5.4)$$

We remind here that $\widehat{U}^{(z)}$ has been defined in (4.7) and that the $N \times N$ matrices $\Theta_{jk}^{(\lambda)}$ and $\Theta_{jk}^{(\mu)}$ are

$$\Theta_{jk}^{(\lambda)} = \delta_{jk} + \frac{K(\lambda_j - \lambda_k)}{2\pi M \widehat{\rho}(\lambda_k)}, \quad \Theta_{jk}^{(\mu)} = \delta_{jk} + \frac{K(\mu_{\ell_j} - \mu_{\ell_k})}{2\pi M \widehat{\rho}_\kappa(\mu_{\ell_k})}. \quad (5.5)$$

5.2 Thermodynamic limit of the smooth part

The smooth part of the scalar product consists of factors $\mathcal{A}_N^{(z)}$ and $C_N^{(z)}$. Their limits can be computed exactly in the same manner as in [1]. We set

$$\begin{aligned} C_n^{(z)}(\{\mu_p\}, \{\mu_h\}) &= \lim_{N, M \rightarrow \infty} C_N^{(z)}(\{\mu_p\}, \{\mu_h\}), \\ \mathcal{A}_n^{(z)}(\{\mu_p\}, \{\mu_h\}) &= \lim_{N, M \rightarrow \infty} \mathcal{A}_N^{(z)}(\{\mu_p\}, \{\mu_h\}). \end{aligned} \quad (5.6)$$

We illustrate the main idea behind the calculation of $C_n^{(z)}$ and $\mathcal{A}_n^{(z)}$ on the following toy-example. Assume that $f(\lambda) \in C^1(\mathbb{R})$, and consider the computation of the thermodynamic limit of the sum

$$S_f = \sum_{j=1}^N [f(\mu_{\ell_j}) - f(\lambda_j)]. \quad (5.7)$$

To compute this limit one can decompose the sum as follows

$$S_f = \sum_{j=1}^N [f(\mu_j) - f(\lambda_j)] + \sum_{j=1}^n [f(\mu_{p_j}) - f(\mu_{h_j})] \rightarrow \sum_{j=1}^n [f(\mu_{p_j}) - f(\mu_{h_j})] + \int_{-q}^q F(\lambda) f'(\lambda) d\lambda. \quad (5.8)$$

There we have used the leading behavior in M^{-1} (2.14) for the spacing between μ_j and λ_j . It is convenient to introduce a modified shift function by

$$F_{mod}(\lambda) = F(\lambda) \chi_{[-q,q]}(\lambda) + \sum_{j=1}^n \left(\chi_{[-\infty, \mu_{p_j}]}(\lambda) - \chi_{[-\infty, \mu_{h_j}]}(\lambda) \right), \quad (5.9)$$

where $\chi_{[a,b]}$ is the characteristic function of the interval $[a, b]$. Then equation (5.8) can be recast simply as

$$S_f \rightarrow \int_{-\infty}^{\infty} F_{mod}(\lambda) f'(\lambda) d\lambda. \quad (5.10)$$

Therefore, provided that one extends the integration contours to the whole real axis and replaces F with F_{mod} , one formally reduces the computations to the case considered in [1] where one was dealing with an excited state $|\psi_\kappa(\{\mu\})\rangle$ having no particles or holes. From this observation, the results of section 3 follow straightforwardly (by a mere replacement of the shift function by F_{mod}) from those of [1]. In this way, starting from the equations (5.2), (5.4) we arrive at (3.5), (3.8).

Thus, the limits $\mathcal{A}_n^{(z)}$ and $C_n^{(z)}$ are well defined for arbitrary positions of particles and holes. They depend on $\{\mu_p\}$ and $\{\mu_h\}$ only. In particular, they do not depend on the underlying integer numbers.

At this stage it is interesting to consider the limiting case where, in the thermodynamic limit, all rapidities of particles and holes condensate on the Fermi boundaries.

Corollary 5.1. *Let $|\psi_\kappa(\{\mu\})\rangle$ belongs to the \mathbf{P}_r class as in (3.20), and denote*

$$\begin{aligned} C_{n,r}^{(z)} &= C_n^{(z)}(\{+q\}_{n_p^+} \cup \{-q\}_{n_p^-}, \{+q\}_{n_h^+} \cup \{-q\}_{n_h^-}), \\ \mathcal{A}_{n,r}^{(z)} &= \mathcal{A}_n^{(z)}(\{+q\}_{n_p^+} \cup \{-q\}_{n_p^-}, \{+q\}_{n_h^+} \cup \{-q\}_{n_h^-}), \end{aligned} \quad (5.11)$$

where subscripts show the number of elements in the corresponding subsets. Let $F_r(\lambda) = F(\lambda) + r$ and $\mathbf{F}_r(w)$ be the $i\pi$ -periodic Cauchy transform of $F_r(\lambda)$. Then the coefficient $C_{n,r}^{(z)}$ takes the form

$$C_{n,r}^{(z)} = C_0[F_r], \quad (5.12)$$

where the functional $C_0[F]$ is defined in (3.6). The coefficient $\mathcal{A}_{n,r}^{(z)}$ becomes

$$\mathcal{A}_{n,r}^{(z)} = \left(\frac{\sin \pi \alpha}{\sin \pi F(-q)} \right)^2 \left| e^{-2\pi i \mathbf{F}_r(-q+i\zeta)} \right|^2 \left| \frac{\det [I + \frac{1}{2\pi i} U_r^{(z)}(w, w')]}{\det [I + \frac{1}{2\pi} K]} \right|^2, \quad (5.13)$$

where

$$U_r^{(z)}(w, w') = -e^{2\pi i(\mathbf{F}_r(w) - \mathbf{F}_r(w+i\zeta))} \frac{K_\kappa(w - w') - K_\kappa(-q - w')}{1 - e^{2\pi i F(w)}}, \quad (5.14)$$

Proof. This follows straightforwardly from $F_{mod}(\lambda) = F_r(\lambda) \chi_{[-q, q]}(\lambda)$. \square

Using (2.9), (2.16) we find that

$$F_r(\lambda) = (r + \alpha) Z(\lambda), \quad (5.15)$$

and we see that up to a replacement $\alpha + r \rightarrow \alpha$ our results coincide with the ones obtained in [1]. This coincidence is not accidental.

In the thermodynamic limit, the class \mathbf{P}_r contains an infinite number of states. Indeed, knowing that a particle or hole's rapidity equals to $\pm q$ in this limit does not allow to fix the corresponding integers p (resp. h) unambiguously. For instance, knowing that $\mu_p = q$ only allows one to say that $p/M \rightarrow D$. The latter is satisfied as long as one chooses $p = N + u_M$ with $u_M = o(M)$, but arbitrary otherwise.

It is clear that quantities having well defined thermodynamic limits (such as $C_{n,r}^{(z)}$ and $\mathcal{A}_{n,r}^{(z)}$), must only depend on the macroscopic realization $\{\mu_p\}$ and $\{\mu_h\}$ of the excited state and not on the microscopic quantum numbers $\{p\}$ and $\{h\}$ leading to such a macroscopic configuration of the rapidities. Therefore, the calculation of their thermodynamic limit in the case of an excited state belonging to the \mathbf{P}_r class can be done by choosing any of its representative. One of these representatives is given by the $(\alpha + r)$ -twisted ground state. Indeed, set $n_p^- = n_h^+ = 0$ and choose the integers describing the holes and particles according to

$$h_k = k, \quad p_k = N + k, \quad k = 1, \dots, r. \quad (5.16)$$

The excited state is thus described by the set of integers,

$$\ell_j = j \quad \text{for } j = r + 1, \dots, N, \quad \text{and } \ell_j = N + j \quad \text{for } j = 1, \dots, r. \quad (5.17)$$

Observe now that if we replace α by $\alpha + r$ in the *r.h.s.* of (2.11), then up to a re-ordering of the equations, we obtain the same set of integers (5.17). Thus, the above representative of the class \mathbf{P}_r coincides with the $(\alpha + r)$ -twisted ground state. Therefore the smooth part of all the critical form factors belonging to the \mathbf{P}_r class coincides with the one of the form factor of the σ^z operator taken between the ground state and the $(\alpha + r)$ -twisted ground state.

5.3 Thermodynamic limit of the discrete part

As we have seen, the modified shift function (5.9) can be used for the calculation of the thermodynamic limits of sums (products, determinants) in the case when we deal with smooth functions of the rapidities of the excited state. One cannot apply this method in the case of the factor $D_N^{(z)}(\{\mu_p\}, \{\lambda_h\})$ as it depends on the Cauchy determinant of $\{\lambda\}$ and $\{\mu\}$. In the thermodynamic limit, certain entries of this matrix become divergent and more care is needed for the calculation of this limit.

Proposition 5.1. *The discrete part $D_N^{(z)}$ behaves in the thermodynamic as*

$$D_N^{(z)}(\{\mu_p\}, \{\mu_h\}) = M^{-F_+^2 - F_-^2} \cdot E_0(\{\mu_h, \mu_p\}; \{h_a, p_a\}) \cdot \prod_{k=1}^n H_N(\mu_{h_k}, h_k) \\ \times \prod_{k=1}^n P_N(\mu_{p_k}, p_k) \cdot \mathcal{D}^{(z)}[F] \cdot \left(1 + \mathcal{O}\left(\frac{\log M}{M}\right)\right). \quad (5.18)$$

The factor E_0 depends explicitly on the integers $\{h_a\}$ and $\{p_a\}$ which are the quantum numbers defining the excited state

$$E_0 = \frac{\prod_{\substack{j,k=1 \\ j \neq k}}^n (h_j - h_k)(p_j - p_k) \varphi(\mu_{h_j}, \mu_{h_k}) \varphi(\mu_{p_j}, \mu_{p_k})}{\prod_{j,k=1}^n (p_j - h_k)^2 \varphi^2(\mu_{p_j}, \mu_{h_k})}, \quad (5.19)$$

where $\varphi(\lambda, \mu) = (2\pi \sinh(\lambda - \mu)) / (p(\lambda) - p(\mu))$ and $p(\lambda)$ is the dressed momentum (2.6). The factors P_N and H_N also depend on the quantum numbers defining the holes and the particles

$$P_N(\mu_{p_k}, p_k) = \frac{e^{J[F^{(z)}](\mu_{p_k})}}{\rho(\mu_{p_k})} \Gamma^2 \left(\begin{matrix} p_k, p_k - N + F(\mu_{p_k}) \\ p_k + F(\mu_{p_k}), p_k - N \end{matrix} \right), \quad (5.20)$$

$$H_N(\mu_{h_k}, h_k) = \frac{\sin^2(\pi F(\mu_{h_k}))}{e^{J[F^{(z)}](\mu_{h_k})} \pi^2 \rho(\mu_{h_k})} \Gamma^2 \left(\begin{matrix} h_k + F(\mu_{h_k}), N + 1 - h_k - F(\mu_{h_k}) \\ h_k, N + 1 - h_k \end{matrix} \right). \quad (5.21)$$

There we have introduced the functional J which is defined in terms of the dressed momentum $p(\lambda)$ and acts on the shift function F :

$$J[F](\omega) = 2 \int_{-q}^q \left\{ F(\lambda) \partial_\lambda \log \varphi(\lambda, \omega) + \frac{F(\lambda) - F(\omega)}{p(\lambda) - p(\omega)} p'(\lambda) \right\} d\lambda. \quad (5.22)$$

Finally, we remind that the functional $\mathcal{D}^{(z)}$ is given in (3.16)

Remark 5.1. The definition of $P_N(\mu_{p_k}, p_k)$ is given in the case where the rapidities of all particles are to the right of the Fermi zone (ie $p_k > N$). If some particles have their rapidities to the left of the Fermi zone ($p_k \leq 0$), then the corresponding arguments of the Γ -functions in (5.20) become negative integers. The aforementioned formula remains however valid provided that the arguments of these Γ -function are understood as limits

$$\frac{\Gamma(p_k)}{\Gamma(p_k - N)} = \lim_{\varepsilon \rightarrow 0} \frac{\Gamma(p_k + \varepsilon)}{\Gamma(p_k - N + \varepsilon)} = (-1)^N \frac{\Gamma(N + 1 - p_k)}{\Gamma(1 - p_k)}. \quad (5.23)$$

Proof. Following the strategy applied in [1], we multiply and divide the original Cauchy determinant by the Cauchy determinant of the counting functions $\widehat{\xi}_\kappa(\lambda)$. Let

$$\widehat{\varphi}(\lambda, \mu) = \frac{\sinh(\lambda - \mu)}{\widehat{\xi}(\lambda) - \widehat{\xi}(\mu)}, \quad \widehat{\varphi}_\kappa(\lambda, \mu) = \frac{\sinh(\lambda - \mu)}{\widehat{\xi}_\kappa(\lambda) - \widehat{\xi}_\kappa(\mu)}. \quad (5.24)$$

After some algebra, we recast $D_N^{(z)}(\{\mu_p\}, \{\lambda_h\})$ into the following product:

$$D_N^{(z)}(\{\mu_p\}, \{\lambda_h\}) = \widehat{E}_0 \cdot \prod_{k=1}^n \widehat{H}_k \cdot \prod_{k=1}^n \widehat{P}_k \cdot D_{N,0}. \quad (5.25)$$

Here \widehat{E}_0 depends only on the particle/hole rapidities and the corresponding integers:

$$\widehat{E}_0 = \frac{\prod_{\substack{j,k=1 \\ j \neq k}}^n (h_j - h_k)(p_j - p_k) \widehat{\varphi}_\kappa(\mu_{h_j}, \mu_{h_k}) \widehat{\varphi}_\kappa(\mu_{p_j}, \mu_{p_k})}{\prod_{j,k=1}^n (p_j - h_k)^2 \widehat{\varphi}_\kappa^2(\mu_{p_j}, \mu_{h_k})}. \quad (5.26)$$

The factors \widehat{P}_k depend on the rapidities μ_{p_k} , integers p_k , the ground state parameters $\{\lambda\}$, and the roots μ_j such that $\widehat{\xi}_\kappa(\mu_j) = j/M$, $j = 1, \dots, N$. Their explicit representations are

$$\widehat{P}_k = \frac{1}{\widehat{\rho}_\kappa(\mu_{p_k})} \prod_{j=1}^N \left\{ \frac{j - p_k - \widehat{F}(\mu_{p_k})}{j - p_k - \widehat{F}(\lambda_j)} \cdot \frac{\widehat{\varphi}_\kappa(\mu_{p_k}, \mu_j)}{\widehat{\varphi}_\kappa(\mu_{p_k}, \lambda_j)} \right\}^2 \Gamma^2 \left(\begin{matrix} p_k, p_k - N + \widehat{F}(\mu_{p_k}) \\ p_k + \widehat{F}(\mu_{p_k}), p_k - N \end{matrix} \right). \quad (5.27)$$

The representations for \widehat{H}_k are similar to (5.27), but they depend on μ_{h_k} and h_k :

$$\widehat{H}_k = \frac{\sin^2(\pi \widehat{F}(\mu_{h_k}))}{\pi^2 \widehat{\rho}_\kappa(\mu_{h_k})} \prod_{j=1}^N \left\{ \frac{j - h_k - \widehat{F}(\lambda_j)}{j - h_k - \widehat{F}(\mu_{h_k})} \cdot \frac{\widehat{\varphi}_\kappa(\mu_{h_k}, \lambda_j)}{\widehat{\varphi}_\kappa(\mu_{h_k}, \mu_j)} \right\}^2 \times \Gamma^2 \left(\begin{matrix} h_k + \widehat{F}(\mu_{h_k}), N + 1 - h_k - \widehat{F}(\mu_{h_k}) \\ h_k, N + 1 - h_k \end{matrix} \right). \quad (5.28)$$

Finally, $D_{N,0}$ does not depend on the particle/hole rapidities and the corresponding integers

$$D_{N,0} = \prod_{j=1}^N \frac{\widehat{\rho}_\kappa(\lambda_j)}{\widehat{\rho}(\lambda_j)} \prod_{j,k=1}^N \frac{\widehat{\varphi}_\kappa(\lambda_j, \lambda_k) \widehat{\varphi}_\kappa(\mu_j, \mu_k)}{\widehat{\varphi}_\kappa^2(\mu_j, \lambda_k)} \times \prod_{j>k}^N \left(1 - \frac{\widehat{F}(\lambda_j) - \widehat{F}(\lambda_k)}{j - k} \right)^2 \prod_{\substack{j,k=1 \\ j \neq k}}^N \left(1 - \frac{\widehat{F}(\lambda_j)}{j - k} \right)^{-2} \prod_{j=1}^N \left\{ \frac{\sin(\pi \widehat{F}(\lambda_j))}{\pi \widehat{F}(\lambda_j)} \right\}^2. \quad (5.29)$$

The fact that $\widehat{E}_0 \rightarrow E_0$ follows from $\widehat{\varphi}_\kappa \rightarrow \varphi$. The calculation of the limit of the first product in (5.29) is based on the definition of the shift function (2.13):

$$\begin{aligned} \prod_{j=1}^N \frac{\widehat{\rho}_\kappa(\lambda_j)}{\widehat{\rho}(\lambda_j)} &= \prod_{j=1}^N \left(1 + \frac{(\widehat{\xi}'_\kappa(\lambda_j) - \widehat{\xi}'(\lambda_j))}{\widehat{\rho}(\lambda_j)} \right) \\ &= \prod_{j=1}^N \left(1 - \frac{\widehat{F}'(\lambda_j)}{M \widehat{\rho}(\lambda_j)} \right) \rightarrow \exp \left(- \int_{-q}^q F'(\lambda) d\lambda \right) = e^{F_- - F_+}. \end{aligned} \quad (5.30)$$

The limit of the remaining part of $D_{N,0}$ was computed in [1], what gives us

$$D_{N,0} = M^{-F_+^2 - F_-^2} \cdot \mathcal{D}^{(z)}[F] \cdot \left(1 + \mathcal{O} \left(\frac{\log M}{M} \right) \right). \quad (5.31)$$

Finally, the limits $\widehat{P}_k \rightarrow P_N(\mu_{p_k}, p_k)$ and $\widehat{H}_k \rightarrow H_N(\mu_{h_k}, h_k)$ follow from

$$\lim_{N, M \rightarrow \infty} \prod_{j=1}^N \left\{ \frac{j - k - \widehat{F}(\mu_k) \widehat{\varphi}_\kappa(\mu_k, \mu_j)}{j - k - \widehat{F}(\lambda_j) \widehat{\varphi}_\kappa(\mu_k, \lambda_j)} \right\}^2 = e^{J[F](\mu_k)}. \quad (5.32)$$

This formula is proved in appendix A (see (A.9)). \square

Assuming general positions of the particles and holes, we can not make further simplifications in the formula for $D_N^{(z)}$. Therefore we now study two limiting cases of interest, exactly as we did for the smooth parts: first when all particles and holes are separated from the Fermi boundaries, and then when all particles and holes are in the vicinity of the Fermi zone (critical form factor in the class \mathbf{P}_r).

Corollary 5.2. *Suppose that, in the thermodynamic limit, particles and holes are separated from the Fermi boundaries: $\mu_{p_a} \neq \pm q$ and $\mu_{h_a} \neq \pm q$. Then the thermodynamic limit of the factor $D_N^{(z)}$ becomes a smooth function of the rapidities $\{\mu_p\}$ and $\{\mu_h\}$:*

$$D_N^{(z)} = M^{-2n - F_-^2 - F_+^2} \cdot D_n^{(z)}(\{\mu_p\}, \{\mu_h\}) \cdot \left(1 + \mathcal{O}\left(\frac{\log M}{M}\right) \right), \quad (5.33)$$

where $D_n^{(z)}(\{\mu_p\}, \{\mu_h\})$ is given by the expression (3.15) for \mathcal{D}_{zz} .

Proof. If the rapidities of particles and holes are separated from the Fermi boundaries, then all the arguments of the Γ -functions in (5.20) and (5.21) are large and we can apply the Stirling formula for their simplification. Then

$$\begin{aligned} \lim_{N, M \rightarrow \infty} \Gamma^2 \left(\begin{array}{c} p_k, p_k - N + \widehat{F}(\mu_{p_k}), N + 1 - h_k - \widehat{F}(\mu_{h_k}), h_k + \widehat{F}(\mu_{h_k}) \\ p_k - N, p_k + \widehat{F}(\mu_{p_k}), N + 1 - h_k, h_k \end{array} \right) \\ = \lim_{N, M \rightarrow \infty} \left(\frac{p_k - N}{p_k} \right)^{2F(\mu_{p_k})} \left(\frac{N - h_k}{h_k} \right)^{-2F(\mu_{h_k})} \\ = \left(\frac{p(\mu_{p_k}) - p(q)}{p(\mu_{p_k}) - p(-q)} \right)^{2F(\mu_{p_k})} \left(\frac{p(q) - p(\mu_{h_k})}{p(\mu_{h_k}) - p(-q)} \right)^{-2F(\mu_{h_k})}, \end{aligned} \quad (5.34)$$

where we have used (2.6). Combining (5.34) with the explicit form (5.22) of $J(\omega)$, we arrive at

$$\begin{aligned} P_N(\mu_{p_k}, p_k) H_N(\mu_{h_k}, h_k) &= \frac{\sin^2(\pi F(\mu_{h_k}))}{\pi^2 \rho(\mu_{h_k}) \rho(\mu_{p_k})} \\ &\times \exp \left\{ 2 \int_{-q}^q F(\lambda) (\coth(\lambda - \mu_{p_k}) - \coth(\lambda - \mu_{h_k})) d\lambda \right\}. \end{aligned} \quad (5.35)$$

The limit of \widehat{E}_0 is almost trivial:

$$\lim_{N, M \rightarrow \infty} \widehat{E}_0 M^{2n} = \left(\det_n \frac{1}{\sinh(\mu_{p_j} - \mu_{h_k})} \right)^2. \quad (5.36)$$

Gathering all these results, we get the claim. \square

Hence, in the limit when the rapidities of particles and holes remain at finite distance from the Fermi boundaries, the discrete part $D_N^{(z)}$, up to an M -dependent normalization, can be approximated by a smooth function of these rapidities. However, as soon as some rapidities go to $\pm q$, then certain integrals in the second line of (3.15) become ill-defined. There can also appear singularities in the Cauchy determinants present in the first line of (3.15). Therefore, the discrete structure of $D_N^{(z)}$ manifests itself when particles and holes condensate on the Fermi boundaries.

We now describe the asymptotic behavior of an excited state $|\psi_\kappa(\{\mu_{\ell_j}\})\rangle$ belonging to the \mathbf{P}_r class. This means that the rapidities of all particles and holes are located in vicinities of the Fermi boundaries with the condition (3.20). Any such state, can be parameterized by a set of integers as given in (3.21).

Corollary 5.3. *The asymptotic behavior of $D_N^{(z)}$ for an excited state in the \mathbf{P}_r class parameterized as in (3.21) reads*

$$D_N^{(z)}(\{+q\}_{n_p^+} \cup \{-q\}_{n_p^-}, \{+q\}_{n_h^+} \cup \{-q\}_{n_h^-}) = M^{-F_{r,+}^2 - F_{r,-}^2} D_{n,r}^{(z)} \left(1 + O\left(\frac{\log M}{M}\right) \right), \quad (5.37)$$

where $D_{n,r}^{(z)}$ is given by the expression (3.23) for \mathcal{D}_{zz} .

Remark 5.2. Thence, when particles and holes are in the vicinity of the Fermi boundaries, the behavior of $D_N^{(z)}$ cannot be called a thermodynamic limit. Indeed, the factors $R_{n_p^+, n_h^+}$ and $R_{n_p^-, n_h^-}$, and thus the form factor, depend explicitly on the microscopic characteristics p^\pm and h^\pm of the excited state.

Proof. In this case, the limits E_0 , $P_N(\mu_{p_k}, p_k)$ and $H_N(\mu_{h_k}, h_k)$ should be re-calculated.

Let us first consider the coefficient \widehat{E}_0 . Using that $\varphi(q, q) = \varphi(-q, -q) = \rho^{-1}(q)$ and $\varphi(q, -q) = \varphi(-q, q) = \sinh(2q)/D$, we get

$$\lim_{N, M \rightarrow \infty} \widehat{E}_0 = \left(\frac{D}{\rho(q) \sinh(2q)} \right)^{2r^2} \rho^{2n}(q) \lim_{N, M \rightarrow \infty} \left(\det_n \frac{1}{p_j - h_k} \right)^2. \quad (5.38)$$

Using the specific parametrization (3.21) of the integers belonging to the \mathbf{P}_r class we see that the thermodynamic limit of the Cauchy determinant in (5.38) can be factorized in two parts:

$$\left(\det_n \frac{1}{p_j - h_k} \right)^2 \rightarrow N^{-2r^2} L_{n_p^+, n_h^+}(\{p^+\}, \{h^+\}) L_{n_p^-, n_h^-}(\{p^-\}, \{h^-\}), \quad (5.39)$$

with

$$L_{n,m}(\{p\}, \{h\}) = \frac{\prod_{j>k}^n (p_j - p_k)^2 \prod_{j>k}^m (h_j - h_k)^2}{\prod_{j=1}^n \prod_{k=1}^m (p_j + h_k - 1)^2}. \quad (5.40)$$

This leads eventually to the following estimate

$$\lim_{N, M \rightarrow \infty} \widehat{E}_0 (M \rho(q) \sinh(2q))^{2r^2} = \rho^{2n}(q) L_{n_p^+, n_h^+}(\{p^+\}, \{h^+\}) L_{n_p^-, n_h^-}(\{p^-\}, \{h^-\}). \quad (5.41)$$

When computing the limits of \widehat{P}_k and \widehat{H}_k , some of the arguments of the Γ -functions are not large anymore. Therefore, we can only use Stirling formula partly. We have

$$\prod_{k=1}^n \Gamma^2 \left(\begin{array}{c} p_k, p_k - N + \widehat{F}(\mu_{p_k}), N + 1 - h_k - \widehat{F}(\mu_{h_k}), h_k + \widehat{F}(\mu_{h_k}) \\ p_k - N, p_k + \widehat{F}(\mu_{p_k}), N + 1 - h_k, h_k \end{array} \right) \\ \sim N^{-2r(F_+ + F_-)} \Gamma^2 \left(\begin{array}{c} \{p^+ + F_+\}, \{h^+ - F_+\}, \{h^- + F_-\}, \{p^- - F_-\} \\ \{p^+\}, \{h^+\}, \{h^-\}, \{p^-\} \end{array} \right). \quad (5.42)$$

We precise that the notation $\{p^+ + F_+\}$ means $\{p_j^+ + F_+\}_{j=1}^{n_p^+}$ and similarly for other sets of parameters in (5.42). Combining all these results we obtain

$$\lim_{N, M \rightarrow \infty} \widehat{E}_0 (M \rho(q) \sinh(2q))^{2r^2 + 2r(F_+ + F_-)} \prod_{k=1}^n \widehat{P}_k \widehat{H}_k = \\ \left(\frac{\sin(\pi F_+)}{\pi} \right)^{2n_h^+} \left(\frac{\sin(\pi F_-)}{\pi} \right)^{2n_h^-} R_{n_p^+, n_h^+}(\{p^+\}, \{h^+\} | F_+) R_{n_p^-, n_h^-}(\{p^-\}, \{h^-\} | -F_-) \\ \times \exp \left\{ 2r \int_{-q}^q \frac{F_+ - F(\lambda)}{\tanh(q - \lambda)} d\lambda + 2r \int_{-q}^q \frac{F_- - F(\lambda)}{\tanh(q + \lambda)} d\lambda \right\}. \quad (5.43)$$

After some simple algebra we get the claim. \square

To conclude this section we would like to stress that the evaluation of the S_N^z thermodynamic limit was done without using the explicit form of the shift function $F(\lambda)$ (2.16). We have used this representation only in (5.15) in order to relate the smooth part of the critical form factors of \mathbf{P}_r class with the one corresponding to the $(\alpha + r)$ -twisted ground state. However in all other respects $F(\lambda)$ played the role of a free functional parameter.

6 The scalar product S_N^+

We now study the scalar product S_N^+ for $|\psi_\kappa(\{\mu\})\rangle$ being an α -twisted excited state with n particles and n holes in the $N + 1$ sector (*i.e.* $N_\kappa = N + 1$). As previously, $\{\mu_{p_a}\}_{a=1}^n$ and $\{\mu_{h_a}\}_{a=1}^n$ denote the rapidities of the particles and holes respectively. The notation $\widehat{F}(\lambda)$ now means the shift function in the $N + 1$ sector, whose thermodynamic limit $F^{(+)}(\lambda)$ is given by (2.17). However, like in the previous section, we omit the superscript $(+)$ in order to lighten the notations.

6.1 Representation for the scalar product S_N^+

In comparison with the S_N^z case, the excited state now depends on $N + 1$ parameters μ . Using the determinant representation given in Proposition 4.1 as well as the norm formula of Proposition 4.2, we get the following representation for S_N^+ (4.16):

$$S_N^+(\{\mu_p\}, \{\mu_h\}) = \mathcal{A}_N^{(+)}(\{\mu_p\}, \{\mu_h\}) \cdot \exp \left\{ C_N^{(+)}(\{\mu_p\}, \{\mu_h\}) \right\} \cdot D_N^{(+)}(\{\mu_p\}, \{\mu_h\}). \quad (6.1)$$

Here

$$D_N^{(+)}(\{\mu_p\}, \{\mu_h\}) = \frac{M\pi^2 \widehat{\rho}(\lambda_{N+1})}{\sin^2 \pi \widehat{F}(\lambda_{N+1})} \frac{\prod_{a=1}^{N+1} \sinh^2(\lambda_{N+1} - \mu_{\ell_a})}{\prod_{a=1}^N \sinh^2(\lambda_{N+1} - \lambda_a)} \cdot D_{N+1}^{(z)}(\{\mu_p\}, \{\mu_h\}), \quad (6.2)$$

where $D_{N+1}^{(z)}$ is given by (5.3) with N replaced by $N+1$. It is expressed in terms of the $N+1$ parameters μ_{ℓ_a} as well as the $N+1$ parameters λ_j defined by $\widehat{\xi}(\lambda_j) = j/M$, $\widehat{\xi}(\lambda)$ being the counting function (2.4) for the ground state. In other words λ_j , $j = 1, \dots, N$, are Bethe roots for the ground state, whereas λ_{N+1} is the point where $M\widehat{\xi}(\lambda)$ takes its next integer value, ie $M\widehat{\xi}(\lambda_{N+1}) = N+1$.

The coefficient $C_N^{(+)}$ is now modified according to

$$\exp \left[C_N^{(+)}(\{\mu_p\}, \{\mu_h\}) \right] = \prod_{a=1}^{N+1} \left| \frac{\sinh(\lambda_a - \lambda_{N+1} - i\zeta)}{\sinh(\mu_{\ell_a} - \lambda_{N+1} - i\zeta)} \right|^2 \cdot \exp \left[C_{N+1}^{(z)}(\{\mu_p\}, \{\mu_h\}) \right], \quad (6.3)$$

where, up to the evident modifications stemming from $N \rightarrow N+1$, $C_{N+1}^{(z)}$ is given by (5.2). Finally the factor $\mathcal{A}_N^{(+)}$ has the following form:

$$\mathcal{A}_N^{(+)}(\{\mu_p\}, \{\mu_h\}) = \frac{\sin \zeta}{2\pi\kappa} \left| \frac{\prod_{a=1}^N \sinh(\lambda_a - \frac{i\zeta}{2})}{\prod_{a=1}^{N+1} \sinh(\mu_{\ell_a} - \frac{i\zeta}{2})} \right|^2 \cdot \frac{\left| \det \left[I + \frac{1}{2\pi i} \widehat{U}^{(+)}(w, w') \right] \right|^2}{\det_{N+1} \Theta_{jk}^{(\mu)} \cdot \det_N \Theta_{jk}^{(\lambda)}}, \quad (6.4)$$

and we refer to (4.8) for the definition of the kernel $\widehat{U}^{(+)}(w, w')$.

6.2 Thermodynamic limit of the smooth part

The smooth part of S_N^+ consists of the coefficients $\mathcal{A}_N^{(+)}$ and $\exp C_N^{(+)}$. The computation of their thermodynamic limits $C_n^{(+)}$ and $\mathcal{A}_n^{(+)}$ does not contain any subtleties comparing with the derivation described in section 5.2. The use of the modified shift function (5.9) formally reduces the computations to the case where the excited state does not contain particles and holes. In this way, starting from the representations (6.3), (6.4) we arrive at the equations (3.7), (3.11). One can easily see that the coefficients $C_n^{(+)}$ and $\mathcal{A}_n^{(+)}$ are well defined for general positions of particles and holes. In particular, for the critical form factors of the \mathbf{P}_r class the smooth part effectively depends on the shift function $F_r(\lambda) = F(\lambda) + r$.

6.3 Thermodynamic limit of the discrete part

Proposition 6.1. *The discrete part $D_N^{(+)}$ behaves in the thermodynamic as*

$$D_N^{(+)}(\{\mu_p\}, \{\mu_h\}) = M^{-F_-^2 - (F_+ + 1)^2} E_0(\{\mu_h, \mu_p\}, \{h_a, p_a\}) \cdot \prod_{k=1}^n H_{N+1}(\mu_{h_k}, h_k) \\ \times \prod_{k=1}^n P_{N+1}(\mu_{p_k}, p_k) \cdot \prod_{a=1}^n \left(\frac{\sinh(\mu_{p_a} - q)}{\sinh(\mu_{h_a} - q)} \right)^2 \cdot \mathcal{D}^{(+)}[F] \cdot \left(1 + \mathcal{O}\left(\frac{\log M}{M}\right) \right), \quad (6.5)$$

where E_0 , H_{N+1} and P_{N+1} are defined as in Proposition 5.1, but with N replaced by $N + 1$. Finally, we remind that the functional $\mathcal{D}^{(+)}$ is given in (3.19).

Proof. As the limit of $D_{N+1}^{(z)}$ is already known, it remains to evaluate the limit of the product

$$P = \frac{\prod_{a=1}^{N+1} \sinh^2(\lambda_{N+1} - \mu_{\ell_a})}{\prod_{a=1}^N \sinh^2(\lambda_{N+1} - \lambda_a)}. \quad (6.6)$$

Harping on the steps in the analysis of $D_N^{(z)}$, we multiply and divide by the counting function $\widehat{\xi}(\lambda)$ (2.4). We obtain

$$P = \frac{\prod_{a=1}^{N+1} \left(N + 1 - \ell_a - \widehat{F}(\mu_{\ell_a}) \right)^2}{M^2 \prod_{a=1}^N (N + 1 - a)^2} \cdot \frac{\prod_{a=1}^{N+1} \widehat{\varphi}^2(\lambda_{N+1}, \mu_{\ell_a})}{\prod_{a=1}^N \widehat{\varphi}^2(\lambda_{N+1}, \lambda_a)}, \quad (6.7)$$

where $\varphi(\lambda, \mu)$ was introduced in (5.24). Then using Corollary A.2 we obtain that, in the thermodynamic limit, the product P behaves as

$$P \rightarrow \frac{e^{J[F](q)}}{M^2 \rho^2(q)} \Gamma^2 \left(\begin{matrix} N + 1 - F_+ \\ N + 1, -F_+ \end{matrix} \right) \cdot \prod_{k=1}^n \left(\frac{\sinh(q - \mu_{p_k})}{\sinh(q - \mu_{h_k})} \right)^2, \quad (6.8)$$

with $J[F](q)$ defined as in (5.22). Using now that N is large, we have

$$e^{J[F](q)} \Gamma^2 \left(\begin{matrix} N + 1 - F_+ \\ N + 1, -F_+ \end{matrix} \right) \rightarrow \frac{\Gamma^2(1 + F_+) \sin^2 \pi F_+}{\pi^2 (\rho(q) \sinh(2q) M)^{2F_+}} \exp \left\{ 2 \int_{-q}^q \frac{F(\lambda) - F_+}{\tanh(\lambda - q)} \right\}, \quad (6.9)$$

It remains to combine the obtained result with the known limit of $D_{N+1}^{(z)}$ and to substitute it into (6.2). A few algebraic manipulations lead then to the claim. \square

We now particularize this result to the two limiting cases we considered previously, namely when all particles and holes are separated from the Fermi boundaries, or when all particles and holes are on the Fermi boundaries. The proofs go along the same lines as in the previous section and we omit them here.

Corollary 6.1. *Suppose that, in the thermodynamic limit, particles and holes are separated from the Fermi boundaries: $\mu_{p_a} \neq \pm q$ and $\mu_{h_a} \neq \pm q$. Then the thermodynamic limit of $D_N^{(+)}$ becomes a smooth function of the rapidities $\{\mu_p\}$ and $\{\mu_h\}$:*

$$D_N^{(+)} = M^{-2n - F_+^2 - (F_+ + 1)^2} \cdot D_n^{(+)}(\{\mu_p\}, \{\mu_h\}) \cdot \left(1 + \mathcal{O} \left(\frac{\log M}{M} \right) \right), \quad (6.10)$$

where $D_n^{(+)}(\{\mu_p\}, \{\mu_h\})$ is given by the expression (3.18) for \mathcal{D}_{+-} .

Corollary 6.2. *The asymptotic behavior of $D_N^{(z)}$ for an excited state in the \mathbf{P}_r class parameterized as in (3.21) reads*

$$D_N^{(+)}(\{+q\}_{n_p^+} \cup \{-q\}_{n_p^-}, \{+q\}_{n_h^+} \cup \{-q\}_{n_h^-}) = M^{-(F_{r,+}+1)^2 - F_{r,-}^2} D_{n,r}^{(+)} \left(1 + O\left(\frac{\log M}{M}\right) \right), \quad (6.11)$$

where $D_{n,r}^{(+)}$ is given by the expression (3.24) for \mathcal{D}_{+-} .

Conclusion

In this article we have provided the first steps towards the study of correlation functions *via* the form factor approach. For this purpose we have calculated the thermodynamic limits of the so-called particle/hole form factors. Although we have considered the specific case of the XXZ chain, our method is straightforwardly applicable to other massless integrable models solvable by means of the algebraic Bethe Ansatz and having determinant representations of their form factors. In particular, one can use it for the calculation of the thermodynamic limit of form factors in the model of one-dimensional bosons. Determinant representations for the form factors of this model in the finite volume were given in [19, 20]. Their thermodynamic limit can be directly obtained from the results given in the present article.

Our results show that the idea to replace, in the thermodynamic limit, the sum over excited states by an integration with respect to particles and holes should be essentially modified. In particular, a formal replacement of the discrete sums over n -particle/hole excited states $|\psi'(\{\mu_p\}, \{\mu_h\})\rangle$ by integrals as

$$\sum_{|\psi'(\{\mu_p\}, \{\mu_h\})\rangle} \mathcal{F}_{\psi_g \psi'}^{(s)}(m) \mathcal{F}_{\psi' \psi_g}^{(s')}(m') \rightarrow M^{2n} \int \mathcal{F}_{\psi_g \psi'}^{(s)}(m) \mathcal{F}_{\psi' \psi_g}^{(s')}(m') \prod_{j=1}^n \rho(\mu_{p_j}) \rho(\mu_{h_j}) d\mu_{p_j} d\mu_{h_j}, \quad (6.12)$$

leads to senseless results. First of all, even in the region where the form factors depend smoothly on $\{\mu_p\}$ and $\{\mu_h\}$, the coefficient M^{2n} does not compensate the factors $M^{-\theta_{ss'}}$, therefore in the above expression, the *r.h.s.* vanishes. On the other hand, the corresponding integral becomes divergent when the rapidities of particles and holes approach the Fermi boundaries (see (3.15), (3.18)). Lastly, due to the discrete structure of the form factors when some rapidities agglomerate on the Fermi boundaries, one cannot replace the sum over the excited states in the \mathbf{P}_r class by an integral. For such excited states, one has to take the microscopic structure of the excited state into account and perform the discrete sums over the parameters p^\pm , h^\pm (3.21).

In a forthcoming publication [54], we will describe a way to overcome these difficulties. We will show that in the asymptotic regime (large lattice distances m between local spin operators) only particles and holes having their rapidities close to the Fermi boundaries contribute to the form factor sums. In such a limit, one can send the rapidities of the particles and holes to $\pm q$ in the smooth part of the form factor. Hence, it becomes a constant that only depends on the \mathbf{P}_r class $\mathcal{S}_{ss'} = \mathcal{S}_{ss'}^{(r)}(\{\pm q\}, \{\pm q\})$. In its turn the summation over the integers $\{p\}$ and $\{h\}$ present in the discrete part of the form factors leads to the natural re-scaling $M \rightarrow 2\pi m$ of the system

size M into the distance m between the operators. This mechanism explains the appearance of the critical exponents $\theta_{ss'}$ in the asymptotic behavior of the correlation functions.

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A Summation identities

Lemma A.1. *Let $f \in C^1([0, a])$ for some $a > D$. Then, in the limit $N, M \rightarrow +\infty$, $N/M \rightarrow D$, the following sums vanish:*

$$\lim_{N, M \rightarrow \infty} \sum_{k=1}^N \frac{f\left(\frac{k}{M}\right) - f(0)}{k^n} = 0, \quad n \geq 2. \quad (\text{A.1})$$

Proof. Let $n = 2$. Then

$$\sum_{k=1}^N \frac{f\left(\frac{k}{M}\right) - f(0)}{k^2} = \frac{1}{M^2} \sum_{k=1}^N \frac{f\left(\frac{k}{M}\right) - f(0) - \frac{k}{M}f'(0)}{\left(\frac{k}{M}\right)^2} + \frac{f'(0)}{M} \sum_{k=1}^N \frac{1}{k}. \quad (\text{A.2})$$

The second term vanishes in the limit, as it is of order $\frac{\log N}{M}$. The first term vanishes due to the Euler–Maclaurin summation formula:

$$\lim_{\substack{N, M \rightarrow \infty \\ N/M \rightarrow D}} \frac{1}{M^2} \sum_{k=1}^N \frac{f\left(\frac{k}{M}\right) - f(0) - \frac{k}{M}f'(0)}{\left(\frac{k}{M}\right)^2} = \lim_{\substack{N, M \rightarrow \infty \\ N/M \rightarrow D}} \frac{1}{M} \int_0^D \frac{f(x) - f(0) - xf'(0)}{x^2} dx = 0. \quad (\text{A.3})$$

For $n > 2$, we have

$$\left| \sum_{k=1}^N \frac{f\left(\frac{k}{M}\right) - f(0)}{k^n} \right| = \left| \sum_{k=1}^N \frac{1}{k^{n-2}} \cdot \frac{f\left(\frac{k}{M}\right) - f(0)}{k^2} \right| \leq \left| \sum_{k=1}^N \frac{f\left(\frac{k}{M}\right) - f(0)}{k^2} \right| \rightarrow 0, \quad (\text{A.4})$$

which ends the proof. \square

Lemma A.2. *Let $f(x) \in C^1([0, a])$ for some $a > D$. Let $n_0 \in \mathbb{N}$ be such that $\sup_{z \in [0, D]} |f(x)| < n_0$. Then*

$$S_{n_0; N}(f) = \sum_{k=n_0}^N \left[\log\left(k + f\left(\frac{k}{M}\right)\right) - \log\left(k + f(0)\right) \right] \xrightarrow[\substack{N, M \rightarrow \infty \\ N/M \rightarrow D}]{} \int_0^D \frac{f(x) - f(0)}{x} dx. \quad (\text{A.5})$$

Proof. Expanding the logarithms into their Taylor series we obtain

$$S_{n_0;N}(f) = \sum_{k=n_0}^N \sum_{r=1}^{\infty} \frac{(-1)^{r+1}}{r} \cdot \frac{f^r\left(\frac{k}{M}\right) - f^r(0)}{k^r}. \quad (\text{A.6})$$

The result of Lemma A.1 shows that only the terms corresponding to $r = 1$ give non-vanishing contributions. These are computed as a Riemann sum:

$$\lim_{\substack{N, M \rightarrow \infty \\ N/M \rightarrow D}} S_{n_0;N}(f) = \lim_{\substack{N, M \rightarrow \infty \\ N/M \rightarrow D}} \frac{1}{M} \sum_{k=1}^N \frac{f\left(\frac{k}{M}\right) - f(0)}{\frac{k}{M}} = \int_0^D \frac{f(x) - f(0)}{x} dx. \quad (\text{A.7})$$

□

Corollary A.1. *Let $f(x)$ satisfy the conditions of Lemma A.2. Let also $0 < N' < N$ and $D' = N'/M$. Then*

$$S_{n_0;N'}(f) = \sum_{k=n_0}^{N'} \left[\log\left(k + f\left(\frac{k}{M}\right)\right) - \log\left(k + f(0)\right) \right] \xrightarrow[\substack{N, M \rightarrow \infty \\ N/M \rightarrow D}]{\longrightarrow} \int_0^{D'} \frac{f(x) - f(0)}{x} dx. \quad (\text{A.8})$$

Corollary A.2. *Let $\xi(\lambda)$ be a strictly monotonous smooth function on \mathbb{R} such that $\xi^{-1}(0) = -q$ and $\xi(D) = q$. Define $\lambda_k = \xi^{-1}(k/M)$, $k \in \mathbb{Z}$ and $\rho(\lambda) = \xi'(\lambda)$. Then, independently whether the thermodynamic limit of λ_h belongs or not to the interval $[-q, q]$, one has*

$$\lim_{\substack{N, M \rightarrow \infty \\ N/M \rightarrow D}} \prod_{k=1}^N \frac{k - h + f(\lambda_k)}{k - h + f(\lambda_h)} = \exp \left\{ \int_{-q}^q \frac{f(\lambda) - f(\lambda_h)}{\xi(\lambda) - \xi(\lambda_h)} \rho(\lambda) d\lambda \right\}. \quad (\text{A.9})$$

Proof. Assume that $h \in \{1, \dots, N\}$ and set $\tilde{f} = f \circ \xi^{-1}$. Choose $n_0 > \sup_{z \in [0, D]} |\tilde{f}(x)|$ and decompose the original product into

$$\prod_{k=1}^N \frac{k - h + f(\lambda_k)}{k - h + f(\lambda_h)} = \prod_{|k-h| < n_0} \frac{k - h + \tilde{f}\left(\frac{k}{M}\right)}{k - h + \tilde{f}\left(\frac{h}{M}\right)} \prod_{|k-h| \geq n_0} \frac{k - h + \tilde{f}\left(\frac{k}{M}\right)}{k - h + \tilde{f}\left(\frac{h}{M}\right)}. \quad (\text{A.10})$$

The first product contains a fixed finite number of factors. Each of them goes to 1 in the limit considered. Hence, the first product goes to 1. The second can be calculated by using Lemma A.1. We obtain

$$\lim_{\substack{N, M \rightarrow \infty \\ N/M \rightarrow D}} \prod_{k=1}^N \frac{k - h + f(\lambda_k)}{k - h + f(\lambda_h)} = \exp \left\{ \int_0^D \frac{\tilde{f}(x) - \tilde{f}(x_h)}{x - x_h} dx \right\}, \quad (\text{A.11})$$

where $x_h = \lim_{N, M \rightarrow +\infty} h/M$. Equation (A.9) follows from (A.11) after the change of variable $\lambda = \xi^{-1}(x)$. The case of $h \notin \{1, \dots, N\}$ is proven along the same lines. □

B The Fredholm determinant representations for the scalar products

The Fredholm determinant representation for the scalar product (4.5) has been proven in [36]. The proof is based on the extraction of a Cauchy determinant from the original determinant defining the scalar product, an idea which was first introduced in [55, 56]. Here, we only sketch the proof of the second determinant identity (4.6).

The proof is based on the following representation for a scalar product [24, 25, 10], valid whenever $\mu_{\ell_1}, \dots, \mu_{\ell_{N_\kappa}}$ satisfy the system (2.12) and $\nu_1, \dots, \nu_{N_\kappa}$ are generic complex numbers:

$$\langle \psi_\kappa(\{\mu\}) | \psi(\{\nu\}) \rangle = \frac{\prod_{a=1}^{N_\kappa} d(\mu_{\ell_a})}{\prod_{a>b}^{N_\kappa} \sinh(\mu_{\ell_a} - \mu_{\ell_b}) \sinh(\nu_b - \nu_a)} \cdot \det_{N_\kappa} \Omega_\kappa(\{\mu\}, \{\nu\} | \{\mu\}). \quad (\text{B.1})$$

The $N_\kappa \times N_\kappa$ matrix $\Omega_\kappa(\{\mu\}, \{\nu\} | \{\mu\})$ is defined as

$$\begin{aligned} (\Omega_\kappa)_{jk}(\{\mu\}, \{\nu\} | \{\mu\}) &= a(\nu_j) t(\mu_{\ell_k}, \nu_j) \prod_{a=1}^{N_\kappa} \sinh(\mu_{\ell_a} - \nu_j - i\zeta) \\ &\quad - \kappa d(\nu_j) t(\nu_j, \mu_{\ell_k}) \prod_{a=1}^{N_\kappa} \sinh(\mu_{\ell_a} - \nu_j + i\zeta), \end{aligned} \quad (\text{B.2})$$

with

$$t(\mu, \nu) = \frac{-i \sin \zeta}{\sinh(\mu - \nu) \sinh(\mu - \nu - i\zeta)} \quad \text{and} \quad \begin{cases} a(\mu) = \sinh^M(\mu - i\zeta/2) \\ d(\mu) = \sinh^M(\mu + i\zeta/2) \end{cases}. \quad (\text{B.3})$$

Following [36], we consider the matrix $\Omega_\kappa(\{z\}, \{\nu\} | \{z\})$ for two sets of $N_\kappa = N + 1$ generic parameters $\{z\}$ and $\{\nu\}$. In this case we write

$$\det_{N+1} [\Omega_\kappa] = \frac{\det_{N+1}(\Omega_\kappa A)}{\det_{N+1} A} \quad \text{with} \quad A_{jk} = \frac{\prod_{a=1}^{N+1} \sinh(z_j - \nu_a)}{\prod_{\substack{a=1 \\ a \neq j}}^{N+1} \sinh(z_j - z_a)} \times \begin{cases} \coth(z_j - \nu_k) & \text{for } k \leq N, \\ 1 & \text{for } k = N + 1. \end{cases} \quad (\text{B.4})$$

The effect of multiplication by the matrix A is computed similarly to the method presented in [36]. We get

$$\det_{N+1} [\Omega_\kappa(\{z\}, \{\nu\} | \{z\})] = \det_{N+1} \left[\frac{1}{\sinh(z_k - \nu_j)} \right] \cdot \det_{N+1} S_{jk}, \quad (\text{B.5})$$

where

$$S_{jk} = \delta_{jk} \mathcal{Y}_\kappa(\nu_k | \{z\}) + \frac{\prod_{a=1}^{N+1} \sinh(\nu_j - z_a)}{\prod_{\substack{a=1 \\ a \neq j}}^{N+1} \sinh(\nu_j - \nu_a)} \cdot \frac{\partial}{\partial y_j} \mathcal{Y}_\kappa(\nu_k | \{y\}) \Big|_{\{y\}=\{\nu\}}, \quad k \leq N, \quad (\text{B.6})$$

$$S_{j,N+1} = \mathcal{Y}_\kappa(\nu_j | \{\nu\}), \quad (\text{B.7})$$

and we have set for arbitrary complex y_1, \dots, y_{N+1}

$$\mathcal{Y}_\kappa(\nu | \{y\}) = a(\nu) \prod_{k=1}^{N+1} \sinh(y_k - \nu - i\zeta) + \kappa d(\nu) \prod_{k=1}^{N+1} \sinh(y_k - \nu + i\zeta). \quad (\text{B.8})$$

Finally we reduce the size of $\det_{N+1} S$ by one by performing linear combinations of the lines

$$\det_{N+1} [S_{jk}] = S_{N+1,N+1} \det_N \left[S_{jk} - S_{j,N+1} \frac{S_{N+1,k}}{S_{N+1,N+1}} \right]. \quad (\text{B.9})$$

Thus, we arrive at the following representation for $\det_{N+1} \Omega_\kappa$ depending on generic complex z_1, \dots, z_{N+1} and ν_1, \dots, ν_{N+1} :

$$\det_{N+1} [\Omega_\kappa(\{z\}, \{\nu\} | \{z\})] = S_{N+1,N+1} \det_{N+1} \left[\frac{1}{\sinh(z_k - \nu_j)} \right] \det_N \left[S_{jk} - S_{j,N+1} \frac{S_{N+1,k}}{S_{N+1,N+1}} \right], \quad (\text{B.10})$$

where S_{jk} are given by (B.6), (B.7).

Now we set $z_a = \{\mu_{\ell_a}\}$ for $a = 1, \dots, N+1$, $\nu_k = \lambda_k$ for $k = 1, \dots, N$ and $\nu_{N+1} = -i\zeta/2$. We assume that the parameters $\{\mu_{\ell_a}\}$ satisfy the system (2.11), while the parameters $\{\lambda_k\}$ satisfy the system (2.2). Then we obtain for $j \leq N$,

$$\begin{aligned} \frac{\mathcal{Y}_\kappa(\nu_j | \{\nu\})}{a(\lambda_j) \prod_{b=1}^N \sinh(\lambda_b - \lambda_j - i\zeta)} &= \kappa \sinh(\lambda_j - \frac{i\zeta}{2}) - \sinh(\lambda_j + \frac{3i\zeta}{2}), \\ \frac{\partial \mathcal{Y}_\kappa(\nu_j | \{y\}) / \partial y_k}{a(\lambda_j) \prod_{b=1}^N \sinh(\lambda_b - \lambda_j - i\zeta)} \Big|_{\{y\}=\{\nu\}} &= \kappa \frac{\sinh(\lambda_j - \frac{i\zeta}{2})}{\tanh(\lambda_k - \lambda_j + i\zeta)} - \frac{\sinh(\lambda_j + \frac{3i\zeta}{2})}{\tanh(\lambda_k - \lambda_j - i\zeta)}, \end{aligned} \quad (\text{B.11})$$

and for $j = N+1$,

$$\begin{aligned} \mathcal{Y}_\kappa(\nu_{N+1} | \{\nu\}) &= a(-i\zeta/2) \sinh(-i\zeta) \prod_{b=1}^N \sinh(\lambda_b - \frac{i\zeta}{2}), \\ \partial \mathcal{Y}_\kappa(\nu_j | \{y\}) / \partial y_k \Big|_{\{y\}=\{\nu\}} &= a(-i\zeta/2) \sinh(-i\zeta) \coth(\lambda_k - \frac{i\zeta}{2}) \prod_{b=1}^N \sinh(\lambda_b - \frac{i\zeta}{2}), \end{aligned} \quad (\text{B.12})$$

It also follows from (2.4), (2.12) and the definition of the shift function (2.13) that

$$\kappa \prod_{a=1}^{N+1} \frac{\sinh(\mu_{\ell_a} - w + i\zeta)}{\sinh(\mu_{\ell_a} - w - i\zeta)} \prod_{a=1}^N \frac{\sinh(\lambda_a - w - i\zeta)}{\sinh(\lambda_a - w + i\zeta)} = e^{2\pi i \widehat{F}(w)}. \quad (\text{B.13})$$

Substituting all these formulae into (B.10) we arrive at (4.6). \square

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