Bi-partite entanglement entropy in massive QFT with a boundary: the Ising model

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In this paper we give an exact infinite-series expression for the bi-partite entanglement entropy of the quantum Ising model both with a boundary magnetic field and in infinite volume. This generalizes and extends previous results involving the present authors for the bi-partite entanglement entropy of integrable quantum field theories, which exploited the generalization of the form factor program to branch-point twist fields. In the boundary case, we isolate in a universal way the part of the entanglement entropy which is related to the boundary entropy introduced by Affleck and Ludwig, and explain how this relation should hold in more general QFT models. We provide several consistency checks for the validity of our form factor results, notably, the identification of the leading ultraviolet behaviour both of the entanglement entropy and of the two-point function of twist fields in the bulk theory, to a great degree of precision by including up to 500 form factor contributions.

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1 Introduction

Entanglement is a fundamental characteristic of quantum systems, which has great importance, for instance, in the context of quantum computing. Any measure of entanglement is likely to give a good description of the quantum nature of a ground state. Many measures of entanglement have been devised, see e.g. [1]-[5]. However, perhaps due to its geometric character which makes it more theoretically tractable in systems with many degrees of freedom, the entanglement entropy [1] has attracted great interest in theoretical physics. The entanglement entropy can also be argued to be a better measure of fundamental properties of the ground state than correlation functions, as it is not associated to a particular observable, but rather to a sector of mutually local observables. In this paper we continue the research initiated in [6, 7, 8] on the bi-partite entanglement entropy in one-dimensional quantum models with many local degrees of freedom, focusing on the effect of boundaries.

The entanglement entropy is a measure of quantum entanglement between the degrees of freedom of two regions, A and its complement $\bar{A}$, in some quantum state $|\psi\rangle$. Consider a quantum system, with Hilbert space $\mathcal{H} = \mathcal{H}_A \otimes \mathcal{H}_{\bar{A}}$, in a pure state $|\psi\rangle$. The bipartite entanglement entropy S_A is the von Neumann entropy associated to the reduced density matrix ρ_A of the subsystem A,

$$\rho_A = \mathrm{Tr}_{\mathcal{H}_{\bar{A}}}(|\psi\rangle\langle\psi|)\,, \tag{1.1}$$

given by

$$S_A = -\mathrm{Tr}_{\mathcal{H}_A}(\rho_A \log \rho_A) = -\lim_{n\to 1}\frac{d}{dn}\mathrm{Tr}_{\mathcal{H}_A}(\rho_A^n). \tag{1.2}$$

The expression with the n-limit on the right-hand side is often referred to as the replica-trick.

Let us consider now the scaling limit of the quantum system, describing the universal part of the behaviour near a quantum critical point. It is obtained by approaching the critical point while letting the length of the region A go to infinity in a fixed proportion with the correlation lengths. The result is a quantum field theory (QFT) model, which we will take throughout to possess (1 + 1-dimensional) Poincaré invariance. In what follows, we consider only the case where A is a connected region.

In the QFT context, the expression on the right-hand side of the second equation of (1.2) can be understood, for n a natural number, as a normalised partition function for the model on a Riemann surface with two branch points, with n sheets cyclicly connected, or on a surface with two conical singularities of angles $2\pi n$ [9, 10, 11] (see also the explanations in [6, 7]). There is only one way of associating such branch points to well-defined local QFT fields. This was first done in [6] in the case *without boundaries* (with A a region in the bulk). There, it was shown how to relate the entanglement entropy in two-dimensional QFT with a two-point function of certain local fields defined in a model consisting of n copies of the original model, called *branch-point twist fields* (section 2):

$$S_A^{\text{bulk}}(r) = -\lim_{n\to 1}\frac{d}{dn}\mathcal{Z}_n \varepsilon^{4\Delta_n}\langle 0|\tilde{\mathcal{T}}(x_1)\mathcal{T}(x_2)|0\rangle. \tag{1.3}$$

Here A has length $r = |x_1 - x_2|$ and $\langle 0|\cdots|0\rangle$ denote correlation functions in the n-copy model; the state $|0\rangle$ is the vacuum state of the latter. The derivative with respect to n involves an appropriate analytic continuation in n of the correlation function, which is assumed to be in correspondence with the conical-singularity interpretation. We will not discuss further in the present paper the subtleties and assumptions involved in this analytic continuation – see the discussion in [7] for more details. The constant $\mathcal{Z}_n$, with $\mathcal{Z}_1 = 1$, is an n-dependent non-universal constant, ε is a short-distance cut-off which is chosen so that $d\mathcal{Z}_n/dn = 0$ and, finally, Δ_n is the conformal dimension of the counter parts of the fields $\mathcal{T}, \tilde{\mathcal{T}}$ in the underlying n-copy conformal field theory,

$$\Delta_n = \frac{c}{24}\left(n - \frac{1}{n}\right), \tag{1.4}$$

which can be obtained by CFT arguments [11, 6] and where c is the central charge.

In [6, 7], the two-point function $\langle 0|\tilde{\mathcal{T}}(x_1)\mathcal{T}(x_2)|0\rangle$ was studied at large distances r for all 1+1-dimensional integrable QFTs on the line. The main feature of these models is that there is no particle production in any scattering process and the scattering (S) matrix factorizes into products of 2-particle S-matrices which can be calculated exactly (for reviews see e.g. [12]-[16]). Taking the S-matrix as input it is then possible to compute the matrix elements of local operators (also called form factors). This is done by solving a set of consistency equations [17, 18]. This is known as the form factor bootstrap program for integrable QFTs. In [6, 7], this program was used and generalised in order to compute the two-particle approximation of $\langle 0|\tilde{\mathcal{T}}(x_1)\mathcal{T}(x_2)|0\rangle$, and to obtain the leading correction to saturation of the entanglement entropy. This leading correction was observed to be very universal, as it is independent of the scattering matrix. In fact, by similar techniques, this universal correction was also observed to hold outside of integrability [8].

In this paper we generalise the construction above in order to include the presence of one integrable boundary. The study of integrable QFTs with boundaries has attracted a lot of attention in the last two decades (see e.g. [19]-[24]). The present work, will make extensive use of the results of S. Ghoshal and A. B. Zamolodchikov [22], particularly the explicit realization of the boundary which they proposed. Their work provided also a detailed study of the Ising model, for which the integrable boundary conditions were classified and the corresponding reflection amplitudes computed. These reflection amplitudes will provide a crucial input for our entropy computation.

Let us therefore consider a family of integrable boundaries parametrised by the dimensionless constant

$$\kappa = 1 - h^2/(2m) \in (-\infty, 1)\ , \tag{1.5}$$

related to a uniform magnetic field h affecting the boundary Ising spins. We study the entanglement entropy between a region A that extends from the boundary to a distance r, and the rest. For $\kappa \leq 0$, we obtain the full large-distance series expansion; the result depends on the reflection matrix at all orders. It turns out that some of the techniques necessary to obtain this result are also useful in the bulk case, so that as a by-product, we obtain the equivalent expansion in the Ising model without boundaries, extending our previous work [6]. We note that this extension to higher particle contributions involves subtleties that were not present in the two-particle case.

We then evaluate from the form factor expansion the exact universal constant $V(\kappa)$ that relates the large-distance value of the entanglement entropy to the short-distance logarithmic behaviour in the *boundary* case, defined by

$$S_A^{\text{boundary}}(r) = \begin{cases} \frac{c}{6}\log(2r/\varepsilon) + V(\kappa) + o(1) & \varepsilon \ll r \ll m^{-1} \\ -\frac{c}{6}\log(\varepsilon m) + \frac{U}{2} + O((rm)^{-\infty}) & r \gg m^{-1} \end{cases} \tag{1.6}$$

where m is the mass of the particle of the Ising model and $c = 1/2$ is its central charge (and $o(1)$ is in terms of the small combination rm). Note that the corrections to the large-distance saturation are exponential. The constant U is the universal saturation constant that occurs in the bulk case, calculated in the Ising model in [6]:

$$S_A^{\rm bulk}(r) = \left\{ \begin{array}{ll} \frac{c}{3}\log(r/\varepsilon) + o(1) & \varepsilon \ll r \ll m^{-1} \\ -\frac{c}{3}\log(\varepsilon m) + U + O((rm)^{-\infty}) & r \gg m^{-1} \end{array} \right. \tag{1.7}$$

Equations (1.7) and (1.6) provide universal definitions for U and $V(\kappa)$. Note that ε here is in general a different short-distance cut-off in the bulk and boundary cases. The choice of these definitions will become clear later.

Our main findings are 1) the observation of non-monotonicity of the entanglement entropy in the boundary Ising model for boundary magnetic field lower than a critical value, and 2) the relation between the constant $V(\kappa)$ and the boundary degeneracy g of Affleck and Ludwig [25]. Exact re-summations of form factors and CFT arguments strongly suggest the following result:

$$V(\kappa) = \left\{ \begin{array}{ll} \log\sqrt{2} & (\kappa > -\infty) \\ 0 & (\kappa = -\infty). \end{array} \right. \tag{1.8}$$

In more general cases of massive QFT, for h associated to a relevant boundary perturbation, we argue that

$$V(\kappa) = s - \log\mathcal{C}, \tag{1.9}$$

where $s = \log g$ is the boundary entropy in the UV ($\kappa > -\infty$) or infrared ($\kappa = -\infty$), and $\mathcal{C}^2$ is the fraction of the massive ground state degeneracy that is broken by the field h. This provides a way to extract the boundary entropy solely from universal entanglement entropies.

The paper is organised as follows: in section 2 we introduce the bi-partite entanglement entropy of a general massive boundary QFT. We establish a relationship between this quantity and the derivative at $n = 1$ of the boundary one-point function of a twist field associated to the QFT constructed as n non-interacting copies of the original model, similarly as discussed for the bulk case in [6, 7, 8]. We provide a CFT analysis of the constant $V(\kappa)$ introduced above. We then specialize these results to the case of integrable models, introducing the form factor expansion for the boundary entanglement entropy. Finally we introduce the Ising model, for which we review the different kinds of integrable boundary conditions and the associated reflection matrices obtained in [22]. In section 3 we start by reviewing the form factor approach for branch-point twist fields and give a closed expression for all non-vanishing form factors of the Ising model. We proceed to a detailed analysis of the boundary entanglement entropy in the Ising model, giving a closed expression for all form factor contributions. The derivation of these formulae involves a complicated analytic continuation on the variable n, as the derivative is taken, followed by the $n \to 1$ limit. In section 4 a similar analysis is performed for the bulk theory, extending the results of [6]. In section 5 we provide a analytical and numerical study of the ultraviolet behaviour of the entanglement entropy of the bulk and boundary Ising model, and evaluate $V(\kappa)$. In section 6 we provide a discussion of the main results, and in section 7 we summarize our main conclusions and open problems. We provide three appendices: In appendix A we give a proof of several formulae which we have used for the computation of the entanglement entropy. In appendix B we provide alternative formulae for the individual form factor contributions to the bulk and boundary entanglement entropy which are more suitable for numerical computations. In appendix C we provide a detailed analysis of the UV behaviour of the two-point function of the twist fields in the bulk Ising model and extract the coefficient of the logarithmic term with great precision.

2 Entanglement entropy of two-dimensional QFTs with boundaries

2.1 General considerations

We consider here a general massive boundary QFT with one of the particle masses being m, characterising the scale of all other masses, and a boundary parameter h, associated to a relevant perturbation of a conformal boundary condition. More precisely, we may write the action as

$$S = S_{\rm bulk}(m) + h\int dt\,\phi(t), \tag{2.1}$$

where $\phi(t)$ is a boundary field with dimension less than 1 and t is time. For later convenience, we will use $\kappa = 1 - h^2/(2m) \in (-\infty, 1)$.

The main idea of [6] in order to evaluate the entanglement entropy was to use n independent copies of the original model, which preserves integrability. The introduction of extra copies allows for the presence of a $\mathbb{Z}_n$ symmetry, associated to which the branch-point twist fields $\mathcal{T}(x)$ and $\tilde{\mathcal{T}}(x)$ can be defined. It is these twist fields that implement the non-trivial connection between sheets in the Riemann surface with branch points, used to calculate the entanglement entropy. Below we recall some of their main properties, but for more details about branch-point twist fields and the construction in the bulk case, see the discussions in [6, 7].

The branch-point twist fields can be characterized as follows: let $\Psi_1,\ldots,\Psi_n$ be any fields belonging to each copy of the original model*. Then the equal time ($x^0 = y^0$) exchange relations between $\mathcal{T}(x)$ and $\Psi_1(y),\ldots,\Psi_n(y)$ can be written in the following form†:

$$\begin{aligned} \Psi_i(y)\mathcal{T}(x) &= \mathcal{T}(x)\Psi_{i+1}(y) \qquad x^1 > y^1,\\ \Psi_i(y)\mathcal{T}(x) &= \mathcal{T}(x)\Psi_i(y) \qquad x^1 < y^1, \end{aligned} \tag{2.2}$$

for $i = 1,\ldots,n$ and where we identify the indices $n + i \equiv i$ and similarly

$$\begin{aligned} \Psi_i(y)\tilde{\mathcal{T}}(x) &= \tilde{\mathcal{T}}(x)\Psi_{i-1}(y) \qquad x^1 > y^1,\\ \Psi_i(y)\tilde{\mathcal{T}}(x) &= \tilde{\mathcal{T}}(x)\Psi_i(y) \qquad x^1 < y^1, \end{aligned} \tag{2.3}$$

that is $\mathcal{T} = \tilde{\mathcal{T}}^\dagger$. These exchange relations indicate that a branch cut originates from branch-point twist fields in (Euclidean) correlation functions with insertion of fields Ψ_i. The definition of the branch-point twist field is completed by saying that they are spinless, invariant under all symmetries of the original model, and of lowest dimension, and by specifying the CFT normalisation $\tilde{\mathcal{T}}(x)\mathcal{T}(0) \sim |x|^{-4\Delta_n}$ as $|x| \to 0^+$ (space-like), with the conformal dimension given in (1.4). Note that as $n \to 1$, $\mathcal{T} \to \mathbf{1}$.

We now consider the presence of a boundary. We will place the boundary at the origin of space $x^1 = 0$ and therefore have a QFT defined on the (positive) half-line. In order to make a clear connection with the bulk results, we first consider the entanglement entropy $S(r_1, r_2)$ in the case where the region A is a bulk region, extending from $r_1 > 0$ to $r_2 > r_1$, region $\bar{A}$ being the rest, composed of two disconnected components, from 0 to r_1 and from r_2 to ∞. Arguments entirely similar to those of [6, 7] show that the trace in (1.2) becomes a normalised correlation

*The vector space of fields of the multi-copy model contains the n-fold tensor product of the vector space of fields of the original model. Fields belonging to a copy i have the identity field $\mathbf{1}$ for all factors corresponding to copies $j \neq i$.

†Here we employ the standard notation in Minkowski space-time: x^ν with $\nu = 0, 1$, with x^0 being the time coordinate and x^1 being the position coordinate.

function of twist fields as in (1.3), but with the ground state of the model on the half-line, $|0\rangle_B$. Note in particular that the boundary condition is $\mathbb{Z}_n$-invariant, so that the branch cuts originating from the twist fields can be deformed through the boundary.

Then, the entanglement entropy is given by:

$$S_A(r_1, r_2) = -\lim_{n\to 1} \frac{d}{dn} \mathcal{Z}_n \varepsilon^{4\Delta_n} {}_B\langle 0|\tilde{\mathcal{T}}(r_2)\mathcal{T}(r_1)|0\rangle_B \tag{2.4}$$

Again, the non-universal constant $\mathcal{Z}_n$ satisfies $\mathcal{Z}_1 = 1$ and $d\mathcal{Z}_n/dn = 0$, ε is a short-distance cut-off, and Δ_n is given in (1.4). In this equation, we have a vacuum correlation function in the model on the half-line, the twist-fields being at positions r_1 and r_2 on the half-line.

There are two ways to obtain the entanglement entropy S_A for a region A starting from the boundary and ending at r. First, we could consider the limit $r_1 \to 0$ in $S(r_1, r)$, making the bulk region $[r_1, r]$ approach the boundary. As the twist field at r_1 approaches the boundary, the correlation function diverges, because the presence of the boundary changes the regularisation necessary around the branch point. A way to evaluate the divergency is to use boundary conformal field theory, which applies in massive models when a local field is near to a boundary. It tells us that for small r_1 there is a power law determined by the conformal dimension of $\mathcal{T}$: ${}_B\langle 0|\cdots\mathcal{T}(r_1)|0\rangle_B \propto r_1^{-2\Delta_n}$ [26]. We may then define $\mathcal{T}(0)|0\rangle_B$ as $\lim_{r_1\to 0} r_1^{2\Delta_n}\mathcal{T}(r_1)|0\rangle_B$. This appropriately regularised operator $\mathcal{T}(0)$ is simply proportional to the unitary operator performing a $\mathbb{Z}_n$ transformation, since its branch cut, through which $\mathbb{Z}_n$ transformations are performed, now extends through the whole space. But since $|0\rangle_B$ is invariant under such a transformation, we find, with appropriate choice of proportionality constants,

$$S_A^{\text{boundary}}(r) = -\lim_{n\to 1} \frac{d}{dn} \mathcal{Z}_n \varepsilon^{2\Delta_n} {}_B\langle 0|\mathcal{T}(r)|0\rangle_B, \tag{2.5}$$

where we have changed the power of ε in order to keep a scaling dimension of 0 (essentially, this accounts for the change of regularisation necessary around the branch points). We used the fact that the entropy is real in order to change $\tilde{\mathcal{T}} \to \mathcal{T}$ by complex conjugation.

Second, we may take the limit $r_2 \to \infty$ in $S(r, r_2)$. Then, the two-point function in (2.4) reduces to its disconnected part:

$${}_B\langle 0|\tilde{\mathcal{T}}(r_2)\mathcal{T}(r)|0\rangle_B \sim {}_B\langle 0|\tilde{\mathcal{T}}(\infty)|0\rangle_B\, {}_B\langle 0|\mathcal{T}(r)|0\rangle_B \ . \tag{2.6}$$

In the first factor, the twist field does not feel the presence of the boundary, hence this expectation value can be replaced by its expectation value in the model without boundary, $\langle 0|\mathcal{T}|0\rangle$. Dividing out this factor and using the appropriate branch-point regularisation, we find again (2.5).

Some of these considerations are made clearer by using crossing in order to implement the boundary as a state:

$${}_B\langle 0|\tilde{\mathcal{T}}(r_2)\mathcal{T}(r_1)|0\rangle_B = \langle 0|\tilde{\mathcal{T}}(r_2)\mathcal{T}(r_1)|B\rangle. \tag{2.7}$$

The boundary state $|B\rangle$ is in the past at time 0 in the Hilbert space of the model *on the full line*, and the twist fields are placed at *imaginary times* r_1 and r_2. More precisely, the boundary state is the n-fold tensor product of single-copy boundary states. The state $\langle 0|$ is the ground state of the n-copy model on the line, corresponding to asymptotic conditions at positive infinite times. No factor occurs in using crossing symmetry since the branch-point twist fields are spinless. The normalisation of the boundary state $|B\rangle$ is such that $\langle 0|B\rangle = 1$. Using crossing, we get

$$S_A^{\text{boundary}}(r) = -\lim_{n\to 1} \frac{d}{dn} \mathcal{Z}_n \varepsilon^{2\Delta_n} \langle 0|\mathcal{T}(r)|B\rangle. \tag{2.8}$$

It is this approach that we will be exploiting in this paper.

2.2 Large and short distance behaviour

In the calculations above, we did not keep track of the normalisation constants occurring in reaching (2.8). These correspond to an additive constant to the entanglement entropy, which is not universal. However, as mentioned in the introduction, the difference between constants occurring at large and short distances is universal. We now show that the expression (2.8) gives the choice of large distance behaviour (1.6). When r is very large, we may use a decomposition of the identity, between the twist field and the boundary state, in energy eigenstates (see (2.16)). The leading term comes from the ground state, giving

$$S_A^{\rm boundary}(r) \sim -\lim_{n\to 1}\frac{d}{dn}\mathcal{Z}_n\varepsilon^{2\Delta_n}\langle 0|\mathcal{T}|0\rangle \quad (rm\to\infty) \tag{2.9}$$

using $\langle 0|B\rangle = 1$. From [6], this is exactly $-(c/6)\log(\varepsilon m) + U/2$ as defined in (1.7), hence this shows (1.6).

We may give a CFT expression for the short-distance constant $V(\kappa)$. From the general formula for one-point functions in a boundary CFT with boundary state $|B\rangle$ [26], we have

$$\langle 0|\mathcal{T}(r)|B\rangle \sim \langle \mathcal{T}|B\rangle^{CFT}(2r)^{-2\Delta_n} \tag{2.10}$$

as $rm\to 0$. Here, $|\mathcal{T}\rangle$ is the normalised highest weight state corresponding to the primary field $\mathcal{T}$ in CFT. In the cases of finite perturbing boundary parameter h, the state $|B\rangle^{CFT}$ is the UV limit $h\to 0$ of the boundary state $|B\rangle$. In the case where $h\to\infty$ before $rm\to 0$, the state $|B\rangle^{CFT}$ is the corresponding IR limit. Hence from (2.8), we have

$$S_A^{\rm boundary}(r) \sim \frac{c}{6}\log(2r/\varepsilon) - \lim_{n\to 1}\frac{d}{dn}\langle\mathcal{T}|B\rangle^{CFT} + o(1) \quad (rm\to 0) \tag{2.11}$$

which gives

$$V(\kappa) = -\lim_{n\to 1}\frac{d}{dn}\langle\mathcal{T}|B\rangle^{CFT} \tag{2.12}$$

where we recall that $\langle 0|B\rangle^{CFT} = 1$, with $\langle 0|0\rangle = 1$ and $\langle\mathcal{T}|\mathcal{T}\rangle = 1$. We see here that $V(\kappa)$ (with the definition (1.5) for κ) takes only two values, one for κ finite (UV) and one for $\kappa = -\infty$ (IR), in agreement with (1.8). This is the main conclusion that we can derive from (2.12), as it is a non-trivial matter to evaluate this expression, and there may be subtleties associated to massive ground state degeneracies (see section 6).

Note finally that we can write $V(\kappa)$ solely in terms of entanglement entropies:

$$V(\kappa) = \lim_{\eta\to 0}\left(S_A^{\rm boundary}(\eta) - S_A^{\rm boundary}(\eta^{-1}) - \frac{1}{2}S_A^{\rm bulk}(\eta) + \frac{1}{2}S_A^{\rm bulk}(\eta^{-1}) - \frac{c}{6}\log 2\right), \tag{2.13}$$

where boundary and bulk entanglement entropies may be evaluated in different cut-off schemes.

2.3 Integrable models and large-distance expansion

For simplicity, let us consider a model of integrable QFT with a single particle spectrum and no bound states. The asymptotic states forming a basis of the Hilbert space are characterised by a number of particles k and by the rapidities θ_j of these particles. As usual in QFT, two bases can be defined, representing particles coming in (*in*-states) and particles going out (*out*-states). In the n-copy model, we will denote the *in*-states by $|\theta_1,\ldots,\theta_k\rangle_{a_1,\ldots,a_k}$ with $\theta_1 > \ldots > \theta_k$, where a_j are the copy labels; the vacuum will be denoted $|0\rangle$. The scattering matrix describes the linear relations between the two bases. The two-particle scattering matrix of the n-copy model, that depends only on the rapidity difference $\theta = \theta_1 - \theta_2$ by relativistic invariance, is given by

$$S_{ab}(\theta) = S(\theta)^{\delta_{ab}}, \qquad \text{for} \qquad a, b = 1 \ldots n, \tag{2.14}$$

with $S(\theta)$ being the scattering matrix of the original model and a, b the copy labels of the two particles. That is, the different copies of the model do not interact with each other.

As mentioned above, the state $|B\rangle$ is just a tensor product of boundary states in the individual copies. In integrable models, these have an explicit expression as the famous boundary state introduced by Ghoshal and Zamolodchikov [22]. In the case where no boundary bound state can form, we have

$$|B\rangle = \exp\left(\frac{1}{4\pi}\sum_{j=1}^{n}\int_{-\infty}^{\infty} R\left(\frac{i\pi}{2} - \theta\right) Z_j(-\theta)Z_j(\theta)\right)|0\rangle. \tag{2.15}$$

The function $R(\theta)$ is the boundary reflection matrix of the integrable QFT and $Z_j(\theta)$ are the Faddeev-Zamolodchikov operators, which provide a generalization of the creation-anhilation operators for integrable QFTs with non-trivial interactions [13, 27]. Their main properties are

$$\begin{aligned} &Z_{a_1}(\theta_1)\cdots Z_{a_k}(\theta_k)|0\rangle = |\theta_1, \ldots, \theta_k\rangle_{a_1,\ldots,a_k} \text{ for } \theta_1 > \ldots > \theta_k \\ &Z_a(\theta_1)Z_b(\theta_2) = S_{ab}(\theta_1 - \theta_2)Z_b(\theta_2)Z_a(\theta_1). \end{aligned}$$

The tensor-product form of the boundary state indicates that particles living in different copies of the theory do not interact through the presence of the boundary.

One can now expand in (2.8) the boundary operator defined above to obtain a large-r expansion:

$$\langle 0|\mathcal{T}(r)|B\rangle = \langle\mathcal{T}\rangle\sum_{\ell=0}^{\infty} f_\ell(2rm, \kappa), \tag{2.16}$$

where

$$\begin{aligned} \langle\mathcal{T}\rangle f_\ell(t,\kappa) \;&=\; \frac{1}{\ell!(4\pi)^\ell}\sum_{j_1,j_2,\ldots,j_\ell=1}^{n}\left[\prod_{r=1}^{\ell}\int_{-\infty}^{\infty} d\theta_r e^{-t\cosh\theta_r} R\left(\frac{i\pi}{2} - \theta_r\right)\right] \\ &\times\; F_{2\ell}^{\mathcal{T}|j_1 j_1 j_2 j_2 \ldots j_\ell j_\ell}(-\theta_1, \theta_1, \ldots, -\theta_\ell, \theta_\ell), \end{aligned} \tag{2.17}$$

and

$$F_\ell^{\mathcal{T}|j_1\ldots j_\ell}(\theta_1, \ldots, \theta_\ell) = \langle 0|\mathcal{T}(0)Z_{j_1}(\theta_1)\cdots Z_{j_\ell}(\theta_\ell)|0\rangle \tag{2.18}$$

are the ℓ-particle form factors of the operator $\mathcal{T}$ in the n-copy model. For example:

$$f_0(t,\kappa) \;=\; 1, \tag{2.19}$$

$$f_1(t,\kappa) \;=\; \frac{n}{4\pi\langle\mathcal{T}\rangle}\int_{-\infty}^{\infty} d\theta\, R\left(\frac{i\pi}{2} - \theta\right) F_2^{\mathcal{T}|11}(-\theta, \theta)e^{-t\cosh\theta}, \tag{2.20}$$

and so on. This is a useful expansion, because the form factors of branch-point twist fields can be obtained exactly, in principle, by solving a set of consistency equations, first given in [6]. We will calculate these form factors in the next section for the Ising model.

Employing (2.8) and (1.4), the entanglement entropy is given by

$$S_A(rm) = -\frac{c}{6}\log(\varepsilon m) + \frac{U}{2} + \sum_{\ell=1}^{\infty} s_\ell(2rm, \kappa). \tag{2.21}$$

with

$$s_\ell(2rm,\kappa) = -\frac{df_\ell(2rm,\kappa)}{dn}\bigg|_{n=1}, \tag{2.22}$$

and where

$$U = -\frac{d}{dn}[m^{-4\Delta_n}\langle\mathcal{T}\rangle^2]_{n=1} \tag{2.23}$$

is a universal constant, that relates the large-distance saturation to the short-distance logarithmic behaviour in the bulk case. In obtaining the expression (2.21) for the entanglement entropy, we used the fact that $\mathcal{T}$ becomes the identity operator at $n=1$, so that $\langle\mathcal{T}\rangle_{n=1} = 1$ and all its form factors with one or more particles vanish.

It is this form factor expansion that we will use in the sections that follow in order to evaluate the entanglement entropy in the boundary Ising model and in particular the constant $V(\kappa)$.

2.4 Integrable boundaries in the Ising model

The massive Ising model is characterised by the fact that the two-particle scattering matrix, as defined above, is $S(\theta) = -1$ (in the single-copy model): the particles are free Majorana Fermions. The central charge in (2.21) is 1/2 and the constant

$$U = -0.131984... \tag{2.24}$$

was obtained in [6, 28]. Let us now recall the types of integrable boundary conditions that have been found for the Ising model. A family that was studied in much detail in [22] is that corresponding to the presence of a magnetic field that couples to the Ising spin field ($\phi(t)$ in the action (2.1)) on the boundary. To be precise, the spin field is the order parameter, hence we are looking at the scaling limit of the Ising spin chain in a transverse magnetic field whose magnitude is slightly below its critical value, and with a parallel magnetic field on the boundary. The corresponding boundary reflection matrix is given by

$$R(\theta) = -i\tanh\frac{1}{2}\left(\theta - \frac{i\pi}{2}\right)\frac{\kappa - i\sinh\theta}{\kappa + i\sinh\theta}, \tag{2.25}$$

which includes, for special values of the parameter κ, the following physically different types of integrable boundary conditions,

- *Free boundary condition*: $\kappa = 1$,
- *Fixed boundary condition*: $\kappa = -\infty$,
- *Magnetic boundary conditions* (interpolating between the previous two): $\kappa = 1 - \frac{h^2}{2m}$, where h is a boundary magnetic field $0 < h < \infty$. The free boundary condition would then correspond to $h = 0$ whereas the fixed boundary condition is equivalent to having a infinitely large magnetic field fixed at the boundary.

Boundary corrections to the expectation values of the energy and disorder field in the Ising theory were computed using this reflection matrix in [29].

In the cases where $\kappa > 0$, the reflection matrix has a pole on the imaginary line on the physical sheet, $0 < \mathrm{Im}(\theta) \leq i\pi/2$. This implies that the boundary state expression (2.15) is not correct. A modified expression exists [22], but for simplicity, in the present paper we will not analyse this case. Hence, throughout we will consider $\kappa \leq 0$ (except in sub-section 3.2). Note that the case $\kappa = 0$ does not require modifications, since the residue of the R-matrix vanishes at this point. At $\kappa = 0$, the bound state becomes weakly bound, and propagates far into the bulk

The cases $\kappa > -1$, i.e. $h < h_c = 2\sqrt{m}$, are also somewhat special. In these cases, the R-matrix still has a pole on the imaginary θ line, although not on the physical strip when $\kappa \leq 0$. As noted in [22], the case $\kappa = -1$ corresponds to a "critical" value of the magnetic field, h_c, at which the reflection matrix happens to have a third order zero at $\theta = 0$. We will discuss the meaning of this critical point from the viewpoint of the boundary entanglement entropy in section 6.

Finally, we note also that the R matrix at $\kappa = 0$ is just equal to the negative of the fixed-boundary condition R matrix, $\kappa = -\infty$, and that

$$R\left(\frac{i\pi}{2} - \theta\right) \quad = \quad -R\left(\frac{i\pi}{2} + \theta\right). \tag{2.26}$$

3 Form factor expansion for the entanglement entropy in the boundary Ising model

3.1 Higher-particle form factors of Ising branch-point twist fields

In order to evaluate the series (2.17) we need to address first the issue of computing higher-particle form factors of the twist fields in the Ising theory. In [6] the full set of form factor consistency equations was written but only the two-particle form factors were explicitly calculated. However, for the Ising theory, this will be the main piece of information needed, as higher-particle form factors can be obtained out of two-particle ones by using Wick's theorem.

Since the branch-point twist field is invariant under the internal $\mathbb{Z}_2$ symmetry of the Ising model, characteristic of the Majorana Fermions, only even-particle form factors will be non-zero. Let us consider some of the consistency equations for the form factors of the twist field $\mathcal{T}$ (with even number of particles k)

$$F_k^{\mathcal{T}|\ldots a_i a_{i+1}\ldots}(\ldots,\theta_i,\theta_{i+1},\ldots) \quad = \quad (-1)^{\delta_{a_i a_{i+1}}} F_k^{\mathcal{T}|\ldots a_{i+1} a_i\ldots}(\ldots,\theta_{i+1},\theta_i,\ldots), \tag{3.1}$$

$$F_k^{\mathcal{T}|a_1\ldots a_k}(\theta_1+2\pi i,\ldots,\theta_k) \quad = \quad F_k^{\mathcal{T}|a_2\ldots a_k(a_1+1)}(\theta_2,\ldots,\theta_k,\theta_1) \tag{3.2}$$

where in we identify the particle types $a+n \equiv a$. Using these relations repeatedly, it is possible to write all form factors in terms of form factors involving only one particle type (say 1). For $1 \leq a_j \leq n$ and with the ordering $a_1 \geq \ldots \geq a_k$, we have

$$F_k^{\mathcal{T}|a_1\ldots a_k}(\theta_1,\ldots,\theta_k) = F_k^{\mathcal{T}|1\ldots 1}(\theta_1+2\pi i(a_1-1),\ldots,\theta_k+2\pi i(a_k-1)), \tag{3.3}$$

and different orderings can be obtained using (3.1), by which extra signs may appear. Using this as a definition for form factors with at least one particle of type different than 1, it is possible to check that equations (3.1) and (3.2) are indeed satisfied, under the condition that (3.1) holds for all particles being of type 1:

$$F_k^{\mathcal{T}|1\ldots 1}(\ldots,\theta_i,\theta_{i+1},\ldots) = -F_k^{\mathcal{T}|1\ldots 1}(\ldots,\theta_{i+1},\theta_i,\ldots) \tag{3.4}$$

and under one additional condition, coming from n applications of (3.2):

$$F_k^{\mathcal{T}|1\ldots 1}(\theta_1+2\pi i n,\ldots,\theta_k) = -F_k^{\mathcal{T}|1\ldots 1}(\theta_1,\ldots,\theta_k) \tag{3.5}$$

where we used the fact that the number of particles is even. That is, the set of equations (3.1) and (3.2) is consistent, and it is sufficient to solve (3.4) and (3.5).

Finally, there are two more conditions on form factors. We will write them in terms of form factors with only particles of type 1. These are the kinematic residue equations:

$$-\,i\mathrm{Res}_{\bar\theta_0=\theta_0}F_{k+2}^{\mathcal{T}|1\ldots1}(\bar\theta_0+i\pi,\theta_0,\theta_1\ldots,\theta_k)=F_k^{\mathcal{T}|1\ldots1}(\theta_1,\ldots,\theta_k), \tag{3.6}$$

$$-\,i\mathrm{Res}_{\bar\theta_0=\theta_0}F_{k+2}^{\mathcal{T}|111\ldots1}(\bar\theta_0+2i\pi n-i\pi,\theta_0,\theta_1\ldots,\theta_k)=-F_k^{\mathcal{T}|1\ldots1}(\theta_1,\ldots,\theta_k). \tag{3.7}$$

Since we are dealing the free Fermion case, it is natural to expect that the form factors of the twist field would admit closed expressions in terms of Pfaffians, as for the order and disorder fields of the Ising theory. This is indeed the case, and it is easy to show that

$$F_k^{\mathcal{T}|11\ldots1}(\theta_1,\ldots,\theta_k)=\langle\mathcal{T}\rangle\mathrm{Pf}(\hat K), \tag{3.8}$$

(recall that the Pfaffian has the property that $\mathrm{Pf}(\hat K)^2=\det(\hat K)$) where $\hat K$ is an anti-symmetric $k\times k$ matrix, k even, with entries

$$\hat K_{ij}=\frac{F_{\min}^{\mathcal{T}|11}(\theta_i-\theta_j)}{F_{\min}^{\mathcal{T}|11}(i\pi)P(\theta_i-\theta_j)}:=K(\theta_i-\theta_j), \tag{3.9}$$

and

$$F_{\min}^{\mathcal{T}|11}(\theta)=-i\sinh\left(\frac{\theta}{2n}\right)\qquad\text{and}\qquad P(\theta)=\frac{2n\sinh\left(\frac{i\pi+\theta}{2n}\right)\sinh\left(\frac{i\pi-\theta}{2n}\right)}{\sin\left(\frac{\pi}{n}\right)}. \tag{3.10}$$

That is, these are the only non-vanishing form factors and are general solutions to (3.4)-(3.7). Note that the Pfaffian expression is nothing else than the application of Wick's theorem on the operators $Z_1(\theta)$ involved in the form factors (2.18) (specialised to all particles being of type 1), a contraction of $Z_1(\theta_1)$ with $Z_1(\theta_2)$ being $K(\theta_1-\theta_2)$. Hereafter the following properties of the function $K(\theta)$ will often be used:

$$K(\theta)=-K(-\theta), \tag{3.11}$$
$$K(\theta)|_{n=1}=0, \tag{3.12}$$
$$(K(\theta+is))^*=-K(\theta-is),\qquad\theta,s\in\mathbb{R}, \tag{3.13}$$

where "*" indicates complex conjugation.

It is easy to prove that (3.9) solves (3.4)-(3.7). Equation (3.4) simply means that if we exchange two lines and the two corresponding (under the transpose) columns of a matrix, its Pfaffian gets a minus sign. Equation (3.5) is a consequence of the property $K(\theta+2i\pi n)=-K(\theta)$ and (3.11), and the fact that if we change the sign of a line and the corresponding column of a matrix, its Pfaffian also gets a minus sign. Finally, the kinematic residue equation (3.6) can also be easily proved from the structure of the Pfaffian, seeing it in terms of Wick's theorem. Looking at the most singular term as $\bar\theta_0\to\theta_0$, using the poles of $K(\theta)$ itself at $\theta=\pm i\pi$ with residues $\pm i$, we obtain (3.6).

3.2 Two- and four-particle boundary corrections to the entanglement entropy

3.2.1 Two-particle correction

Employing (3.8) for the two-particle form factor, it is not difficult to evaluate the first correction to the saturation value of the entanglement entropy (2.21) using (2.22) and (2.20). We find

$$s_1(t,\kappa) = -\frac{1}{8}\int_{-\infty}^{\infty} d\theta \left(\frac{\kappa+\cosh\theta}{\kappa-\cosh\theta}\right)\left(\frac{\cosh\theta-1}{\cosh^2\theta}\right) e^{-t\cosh\theta}, \tag{3.14}$$

since

$$-\frac{d}{dn}\left[nK(-2\theta)\right]_{n=1} = \frac{\left[F_{\min}^{\mathcal{T}|11}(2\theta)\right]_{n=1}}{\left[F_{\min}^{\mathcal{T}|11}(i\pi)\right]_{n=1}} \frac{d}{dn}\left[\frac{n}{P(2\theta)}\right]_{n=1} = \frac{i\pi}{2}\frac{\tanh\theta}{\cosh\theta}. \tag{3.15}$$

The correction $s_1(t,\kappa)$ is finite for all values of t, including $t=0$, as can be seen in figure 1. At this point it is possible to evaluate the integral above explicitly:

$$c_1(\kappa) := s_1(0,\kappa) = \frac{1}{4} - \frac{\pi}{8} + \frac{\pi}{4\kappa} - \frac{\sqrt{1-\kappa}\,\left(\pi + 2\arcsin(\kappa)\right)}{4\kappa\sqrt{1+\kappa}}, \tag{3.16}$$

and in particular

$$c_1(-1) = \frac{10-3\pi}{8} \qquad \text{and} \qquad c_1(0) = \frac{\pi-2}{8}. \tag{3.17}$$

In the case where $\kappa > 0$, as was said in sub-section 2.4, the boundary state expression (2.15) needs modifications due to the presence of a boundary bound state. Following [22], the boundary state in the multi-copy model has the expansion

$$|B\rangle = \left[1 + g_c\sum_{j=1}^{n} Z_j(0) + g_c^2\sum_{j,k=1}^{n} Z_j(0)Z_k(0) + \sum_{j=1}^{n}\int_{-\infty}^{\infty}\frac{d\theta}{4\pi} R\left(\frac{i\pi}{2}-\theta\right) Z_j(-\theta)Z_j(\theta) + \cdots\right]|0\rangle \tag{3.18}$$

where g_c is proportional to the residue of the R-matrix at the bound-state pole. Since the branch-point twist fields have zero one-particle form factors, the only possible modifications to the result for $s_1(t,\kappa)$ above come from the quadratic term $g_c^2\sum_{j,k=1}^{n} Z_j(0)Z_k(0)$. The correction to $s_1(t,\kappa)$ would then be

$$-g_c^2 e^{-t}\frac{d}{dn}\left[\sum_{i,j=1}^{n} F_2^{\mathcal{T}|ij}(0,0)\right]_{n=1} = -g_c^2 e^{-t}\frac{d}{dn}\left[n\sum_{j=0}^{n-1} K(2\pi i j)\right]_{n=1}. \tag{3.19}$$

Using the methods of summation of [6], it is possible to show that this correction vanishes. Hence $s_1(t,\kappa)$ is the correct leading large-distance correction for all $\kappa \leq 1$.

3.2.2 Four-particle correction

Let us consider now the four-particle boundary correction. From (2.17) and (2.22) we find

$$s_2(t,\kappa) = -\frac{1}{2}\left[\prod_{k=1}^{2}\int_{-\infty}^{\infty}\frac{d\theta_k}{4\pi} R\left(\frac{i\pi}{2}-\theta_k\right) e^{-t\cosh\theta_k}\right]\frac{d}{dn}\left[\sum_{i,j=1}^{n}\frac{1}{\langle\mathcal{T}\rangle} F_4^{\mathcal{T}|iijj}(-\theta_1,\theta_1,-\theta_2,\theta_2)\right]_{n=1}, \tag{3.20}$$

where

$$\sum_{i,j=1}^{n} F_4^{\mathcal{T}|iijj}(-\theta_1,\theta_1,-\theta_2,\theta_2) = n\sum_{j=1}^{n} F_4^{\mathcal{T}|11jj}(-\theta_1,\theta_1,-\theta_2,\theta_2)$$
$$= n\sum_{j=0}^{n-1} F_4^{\mathcal{T}|1111}(-\theta_1,\theta_1,-\theta_2+2\pi ij,\theta_2+2\pi ij). \quad (3.21)$$

Here we have used (3.1) and (3.3). Employing (3.8) we find

$$\frac{n}{\langle\mathcal{T}\rangle}\sum_{j=0}^{n-1} F_4^{\mathcal{T}|1111}(-\theta_1,\theta_1,-\theta_2+2\pi ij,\theta_2+2\pi ij) \quad (3.22)$$
$$= n\sum_{a=0}^{n-1}\Big(K(2\theta_1)K(2\theta_2)+K(\theta_{12}-2\pi ia)K(\theta_{12}+2\pi ia)+K(\hat{\theta}_{12}-2\pi ia)K(-\hat{\theta}_{12}-2\pi ia)\Big)$$
$$= n^2K(2\theta_1)K(2\theta_2)+n\sum_{a=0}^{n-1}\Big(K(\theta_{12}-2\pi ia)K(\theta_{12}+2\pi ia)-K(\hat{\theta}_{12}-2\pi ia)K(\hat{\theta}_{12}+2\pi ia)\Big).$$

Here and below we use $\theta_{ij}=\theta_i-\theta_j$ and $\hat{\theta}_{ij}=\theta_i+\theta_j$. It is simple to show that the $n^2K(2\theta_1)K(2\theta_2)$ term will give no contribution to the derivative at $n=1$ (this is due to property (3.12)) so that only the terms in the sum remain. These terms will give a contribution, since, employing (3.13), they can actually be rewritten as

$$-n\sum_{a=0}^{n-1}\left[|K(\theta_{12}-2\pi ia)|^2-|K(\hat{\theta}_{12}-2\pi ia)|^2\right]. \quad (3.23)$$

Writing things in this way is useful as we can employ one of our main results in [6], namely that

$$\frac{d}{dn}\left[n\sum_{a=1}^{n-1}|K(\theta-2\pi ia)|^2\right]_{n=1}=\frac{\pi^2}{2}\delta(\theta). \quad (3.24)$$

Under integration in (3.20), the term with $\hat{\theta}_{12}$ can be changed into θ_{12}, and the change of variable required inverts the sign of $R(i\pi/2-\theta_2)$ using property (2.26). Hence both terms give the same contribution. Thus we find that the four-particle correction to the saturation value of the Ising entanglement entropy is given by

$$s_2(t,\kappa) = \frac{1}{32}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} d\theta_1 d\theta_2 R\left(\frac{i\pi}{2}-\theta_1\right)R\left(\frac{i\pi}{2}-\theta_2\right)\delta(\theta_{12})e^{-2t\cosh\frac{\theta_{12}}{2}\cosh\frac{\hat{\theta}_{12}}{2}}, \quad (3.25)$$
$$= \frac{1}{32}\int_{-\infty}^{\infty} d\theta R\left(\frac{i\pi}{2}-\theta\right)^2 e^{-2t\cosh\theta} = \frac{1}{32}\int_{-\infty}^{\infty} d\theta\left(\frac{\kappa+\cosh\theta}{\kappa-\cosh\theta}\right)^2\frac{1-\cosh\theta}{1+\cosh\theta}e^{-2t\cosh\theta}.$$

Contrarily to the two-particle correction, we find that the four-particle contribution is divergent as $t\to 0$. Technically, the reason for this is that the integrand of (3.25) is a function that tends to the value -1 as $\theta\to\infty$ when $t=0$. Therefore the integral at $t=0$ is divergent. In order to find the precise behaviour of the correction as t approaches 0, one can rewrite the integral above as:

$$s_2(t,\kappa)=\frac{1}{32}\int_{-\infty}^{\infty} d\theta\left[\left(\frac{\kappa+\cosh\theta}{\kappa-\cosh\theta}\right)^2\frac{1-\cosh\theta}{1+\cosh\theta}+1\right]e^{-2t\cosh\theta}-\frac{1}{16}K_0(2t). \quad (3.26)$$

The behaviour of the Bessel function as t goes to zero is well-known,

$$K_0(2t) = -\gamma - \log(t) + O(t^2 \log t), \tag{3.27}$$

where $\gamma = 0.577216...$ is the Euler-Mascheroni constant. Written in this form, the integral part is now a finite constant at $t = 0$, and we may define

$$\begin{aligned} c_2(\kappa) &= \frac{1}{16} \int_0^\infty d\theta \left[\left(\frac{\kappa + \cosh\theta}{\kappa - \cosh\theta} \right)^2 \frac{1 - \cosh\theta}{1 + \cosh\theta} + 1 \right] \\ &= -\frac{1}{8(1+\kappa)^2} \left[2\kappa - 3\kappa^2 - 1 + \frac{\kappa\,(2\kappa - 1)\,(\pi + 2\arcsin\kappa)}{\sqrt{1-\kappa^2}} \right], \end{aligned} \tag{3.28}$$

with in particular

$$c_2(-1) = \frac{23}{120}. \tag{3.29}$$

The constant $c_2(\kappa)$ is an increasing function of the magnetic field (i.e. a decreasing function of κ). Therefore we have

$$s_2(t,\kappa) = \frac{1}{16}\log(t) + \frac{\gamma}{16} + c_2(\kappa) + O(t) \tag{3.30}$$

(the order $O(t)$ comes from the next correction to the integral part of (3.26)). Note that in view of the short-distance behaviour of the entanglement entropy (1.6), we expect that the coefficients of the logarithmic divergencies at small rm will add up to the finite number 1/12 when all corrections are considered. This will be proven in section 5. Also, the constant $c_2(\kappa)$, like $c_1(\kappa)$ above, is a part of the constant $V(\kappa)$ in (1.6); again, in principle one should add up all such constants, for all corrections, in order to obtain $V(\kappa)$. This will be discussed also in section 5.

An interesting mathematical phenomenon can be observed: although the integral in (3.26) has the same value for $\kappa = -\infty$ as for $\kappa = 0$ for any $t > 0$, we have $c_2(-\infty) = 3/8$ different from $c_2(0) = 1/8$. The explanation is that the limit $t \to 0$ of the integral in (3.26) as a function of κ is not uniform. For all values of $t > 0$ we have $s_2(t, -\infty) = s_2(t, 0)$, and there is a maximum for $\kappa \in (-\infty, 1)$ at a unique value $\kappa = \kappa_0$. But as t becomes smaller, the position of this maximum shifts towards more negative values, until it reaches $-\infty$ at $t = 0$. There, if we take away the constant (as function of κ) term $\frac{1}{16}\log(t)$ in order to make the limit finite, the value of the maximum itself reaches $c_2(-\infty)$. It is also possible to observe in the integral in (3.28) that the symmetry between $\kappa = -\infty$ and $\kappa = 0$ is broken. Indeed, if κ is very negative, the term in parenthesis can be approximated by 1 except for values of θ where $\kappa + \cosh\theta \approx 0$. These are very large values of θ, but they are not damped by any other factor, hence the mistake in approximating by 1 is non-negligible for any κ.

This means that formally, the expansion (3.30) is valid only for $\kappa > -\infty$. For the case $\kappa = -\infty$, that is, the fixed boundary condition, we have to consider the other order of the limits: first $\kappa \to -\infty$, then $t \to 0$. By the symmetry between $\kappa = -\infty$ and $\kappa = 0$, we define

$$c_2(-\infty) =: c_2(0) = \frac{1}{8} \tag{3.31}$$

so that (3.30) still holds in the case of a fixed boundary condition, $\kappa = -\infty$.

In fact, it is instructive to obtain a more general small-t expansion, where we take simultaneously $\kappa \to -\infty$. Let us consider $t \to 0$ with $-\kappa t = a$ fixed. We may use the change of variable

$s = \cosh\theta - 1$ and write $s_2(t,\kappa)$ as

$$\frac{1}{16}\int_0^\infty ds \left(\frac{k+1+s}{k-1-s}\right)^2 \left(-\frac{\sqrt{s}}{(s+2)^{3/2}} + \frac{1}{s+1}\right) e^{-2t(s+1)} - \frac{1}{16}\int_0^\infty ds \left(\frac{k+1+s}{k-1-s}\right)^2 \frac{e^{-2t(s+1)}}{s+1}. \tag{3.32}$$

The first integral as a function of κ has a uniform limit as $t \to 0$ on $\kappa \in [-\infty, 0)$, so that we can directly take $\kappa = -\infty$ and $t = 0$; this gives $(2 - \log 2)/16$. The second integral does not have a uniform limit, but it can be evaluated explicitly:

$$\frac{1}{16(a+t)}\left(4ae^{-2t} - (a+t)\Gamma(0,2t)e^{2t} - 8a(a+t)e^{2(a+t)}\Gamma(0,2(a+t))\right)$$

where $\Gamma(z,u)$ is the incomplete Gamma function, $\int_u^\infty v^{z-1}e^{-v}dv$. The small-$t$ limit can then easily be taken:

$$s_2(t,-a/t) = \frac{1}{16}\log(t) + \frac{\gamma}{16} + c_2^\natural(a) + O(t). \tag{3.33}$$

where

$$c_2^\natural(a) = \frac{3}{8} - \frac{1}{2}ae^{2a}\Gamma(0,2a). \tag{3.34}$$

It is easy to see that $c_2^\natural(a)$ interpolates between $\lim_{\kappa\to-\infty} c_2(\kappa)$ at $a = 0$ to $c_2(-\infty)$ at $a = \infty$.

We expect this phenomenon of non-commutativity of the limits to be generic: it should occur at all orders, except, as we have seen, for the very first two-particle correction. Its meaning will be explained in section 6. We also refer the reader to section 6 for an analysis of the large-distance corrections found here.

3.3 Higher particle boundary corrections to the entanglement entropy

As one would expect, the form factor expressions which are obtained from (3.8) become more and more involved as the number of particles is increased. In particular, it is easy to see that the 2ℓ-particle form factor of $\mathcal{T}$ is made out of the sum of

$$1 \times 3 \times 5 \times \ldots \times (2\ell - 1) = \frac{(2\ell-1)!}{2^{\ell-1}(\ell-1)!}, \tag{3.35}$$

terms. This number grows faster than exponentially with ℓ. However, as we have already seen for the 4-particle corrections, not all of these terms contribute to the derivative at $n = 1$ and those that contribute give in many cases the same contribution due to the fact that they are identical when integrated over. For example, the two contributions in (3.23) are actually equivalent when integrated over θ_1 and θ_2. The combination of these two factors, that is, terms whose derivative vanishes at $n = 1$ and terms that can be grouped together, allows us to reduce very dramatically the amount of non-vanishing contributions to the derivative that we obtain from higher particle form factors.

The 2ℓ-particle form factors contributing to the entanglement entropy (see (2.22) and (2.17)) occur in a sum of the form

$$\begin{aligned}&\sum_{j_1,\ldots,j_\ell=0}^{n} F_{2\ell}^{\mathcal{T}|j_1 j_1\ldots j_\ell j_\ell}(-\theta_1,\theta_1,-\theta_2,\theta_2,\ldots,-\theta_\ell,\theta_\ell)\\ &= n\sum_{j_1,\ldots,j_{\ell-1}=0}^{n-1} F_{2\ell}^{\mathcal{T}|1\ldots1}(-\theta_1,\theta_1,(-\theta_2)^{j_1},\theta_2^{j_1},\ldots,(-\theta_\ell)^{j_{\ell-1}},\theta_\ell^{j_{\ell-1}}),\end{aligned} \tag{3.36}$$

where

$$\theta_a^b = \theta_a + 2\pi i b. \tag{3.37}$$

Here, we used (3.3) and (3.1), along with the fact that every copy number occurs in pairs, so that no sign remains. From Wick's theorem, one of the terms contributing to this sum will be the following contraction:

$$F_{2\ell}^{\mathcal{T}|1\ldots1}(-\theta_1, \theta_1, (-\theta_2)^{j_1}, \theta_2^{j_1}, (-\theta_3)^{j_2}, \ldots, \theta_{\ell-2}^{j_{\ell-3}}, (-\theta_{\ell-1})^{j_{\ell-2}}, \theta_{\ell-1}^{j_{\ell-2}}, (-\theta_\ell)^{j_{\ell-1}}, \theta_\ell^{j_{\ell-1}}), \tag{3.38}$$

which corresponds to

$$\sum_{j_1,\ldots,j_{\ell-1}=0}^{n-1} K((-\hat{\theta}_{12})^{j_1}) K(\hat{\theta}_{23}^{j_1-j_2}) K(\hat{\theta}_{34}^{j_2-j_3}) \ldots K(\hat{\theta}_{\ell-1\,\ell}^{j_{\ell-2}-j_{\ell-1}}) K(\hat{\theta}_{\ell 1}^{j_{\ell-1}}). \tag{3.39}$$

We will call such a term "fully connected", which denotes any contraction where the sums over j's cannot be factorised into a product of sums.

Thanks to (3.12), any fully connected term vanishes as $n \to 1$. Below we will show that the derivative with respect to n is not zero as $n \to 1$, but converges to a distribution in the rapidities, generalising the main result (3.24) of [6]. This means that the product of two or more fully connected term has a vanishing derivative as $n \to 1$, so that the only terms that will contribute to (3.36) are the fully connected Wick contractions. We will further show below that all fully connected terms can be brought to the form (3.38).

3.3.1 Explicit evaluation of fully connected terms

The sum (3.39) can be obtained in a systematic way by exploiting a result which was first obtained in appendix 3 of [6]. The result derived there was a special case of the sum

$$\sum_{a=0}^{n-1} K((-x)^a) K(y^a) = -\frac{i \sinh\left(\frac{y+x}{2}\right)}{2\cosh\frac{x}{2}\cosh\frac{y}{2}} \left(K(x+y-i\pi) + K(x+y+i\pi)\right), \tag{3.40}$$

which can be computed in exactly the same manner. The sum (3.39) can be evaluated by simply using (3.40) recursively. When doing so one realizes the need to distinguish two special cases, depending on whether ℓ is even or odd in (3.39). The final expressions are,

$$\sum_{j_1,\ldots,j_{2\ell-1}=0}^{n-1} K((-x_1)^{j_1}) K(x_2^{j_1-j_2}) \ldots K(x_{2\ell-1}^{j_{2\ell-2}-j_{2\ell-1}}) K(x_{2\ell}^{j_{2\ell-1}}) = \frac{(-1)^\ell 2i \sinh(\frac{\sum_{i=1}^{2\ell} x_i}{2})}{\prod_{i=1}^{2\ell} 2\cosh\frac{x_i}{2}}$$
$$\times \sum_{j=1}^{\ell} \begin{pmatrix} 2\ell-1 \\ \ell-j \end{pmatrix} \left[K(\sum_{i=1}^{2\ell} x_i + (2j-1)\pi i) + K(\sum_{i=1}^{2\ell} x_i - (2j-1)\pi i)\right], \tag{3.41}$$

and

$$\sum_{j_1,\ldots,j_{2\ell}=0}^{n-1} K((-x_1)^{j_1}) K(x_2^{j_1-j_2}) \ldots K(x_{2\ell}^{j_{2\ell-1}-j_{2\ell}}) K(x_{2\ell+1}^{j_{2\ell}}) = \frac{(-1)^{\ell+1} 2\cosh(\frac{\sum_{i=1}^{2\ell+1} x_i}{2})}{\prod_{i=1}^{2\ell+1} 2\cosh\frac{x_i}{2}}$$
$$\times \left[\begin{pmatrix} 2\ell \\ \ell \end{pmatrix} K(\sum_{i=1}^{2\ell+1} x_i) + \sum_{j=1}^{\ell} \begin{pmatrix} 2\ell \\ \ell-j \end{pmatrix} \left[K(\sum_{i=1}^{2\ell+1} x_i + 2\pi i j) + K(\sum_{i=1}^{2\ell+1} x_i - 2\pi i j)\right]\right] \tag{3.42}$$

A proof by induction of these identities is provided in appendix A.

3.3.2 Analytic continuation in n and computation of the derivative at $n = 1$ of fully connected terms

Let us start by considering the analytic continuation and evaluating the derivative at $n = 1$ of (3.41). This summation formula already provides an analytic continuation in n of the multiple sum over j's for any fix x's. Naturally, such an analytic continuation is not unique. Additionally, this formula itself gives many more analytic continuations when taken under integration over the x variables. Indeed, for integer n, all poles of the functions K involved are exactly cancelled by the zeros of $\sinh(\frac{\sum_{i=1}^{2\ell} x_i}{2})$, hence the integration contours can be moved away from the real x-axis without any change to the answer. But for non-integer n, poles and zeros generically are at different points, except for the poles of K at values of its argument $\pm i\pi$. Hence, different integration contours give different analytic continuations of the integrals.

Below we suggest that the formula (3.41) is the correct one, but that the contours need to be taken differently. Let us consider the rapidity variables θ_i, with $x_i = \hat{\theta}_{i,i+1}$ (and $x_{2\ell} = \theta_{2\ell,1}$). For n large enough, all the poles of K are beyond the integration contour of the variable

$$\theta = \sum_i \theta_i = \frac{1}{2}\sum_i x_i \tag{3.43}$$

for all j's in (3.41). However, as n decreases, poles cross the θ integration contour. At the points where these poles cross, there is a zero provided by the hyperbolic sine function, so that no discontinuity occurs. Yet as function of n, the result is not smooth, since there is a discontinuity in the *derivative* with respect to n. This is because as n approaches an integer value where a pole crosses the integration contour, the right-hand side of (3.41) is not uniformly convergent as function of θ, and develops an infinitely thin peak of finite height at $\theta = 0$. There is no natural way of modifying (3.41) in order to avoid this phenomenon. Indeed, it is related to the fact that for integer values of n, the unambiguous value of the sum in (3.41) at $\theta = 0$ varies with n up to $n = \ell + 1$, but from $n = \ell + 1$ up to infinity it takes the same values. Hence, any analytic continuation will have to reproduce this unnatural behaviour. We note that this phenomenon is a generalisation of that observed in [6] in the two-particle approximation of the bulk two-point function (and above in the four-particle boundary case): there the value of the sum at $\theta = 0$ at $n = 2, 3, 4, \ldots$ is constant and non-zero, while the value at $n = 1$ is zero. The resulting non-uniform convergence was at the basis of the calculation of the derivative with respect to n at $n = 1$.

In order to recover a smooth function of n up to $n = 1$, we then need to move the θ integration contour towards values where the argument of K is just $\theta \pm i\pi$ in (3.41), for all j's. It is convenient to still avoid poles of the hyperbolic cosine factors in the denominator. Hence, we consider shifting all θ_i by $\mp\frac{j-1}{2\ell}\pi i$, so that we get the following summation formula, valid under integration:

$$\sum_{j_1,\ldots,j_{2\ell-1}=0}^{n-1} K((-\hat{\theta}_{12})^{j_1})K(\hat{\theta}_{23}^{j_1-j_2})\ldots K(\hat{\theta}_{2\ell,1}^{j_{2\ell-1}}) \stackrel{\int}{=} 2i\sinh\theta$$
$$\times \sum_{j=1}^{\ell}\sum_{q=\pm}(-1)^{\ell+j-1}\binom{2\ell-1}{\ell-j}\frac{K(2\theta+q\pi i)\prod_{i=1}^{2\ell}\text{shift}_{\theta_i\to\theta_i-q\frac{j-1}{2\ell}\pi i}}{\prod_{i=1}^{2\ell}2\cosh\left(\frac{\hat{\theta}_{i,i+1}}{2}-q\frac{j-1}{2\ell}\pi i\right)}. \tag{3.44}$$

Here, $\text{shift}_{\theta_i\to\theta_i-\frac{j-1}{2\ell}\pi i}$ is an operator acting on all other functions in the integrand (that is, those not appearing here), indicating that their arguments must be modified as written. More precisely, this indicates a shift of contour, and if the other functions in the integrand have poles that are crossed by this shift, then the residues must be taken. It is important, of course, that the integrals over rapidities stay convergent at all stages of the shifts.

The strongest evidence for the validity of this formula is provided by the fact that in the bulk case, the scaling dimension of the twist fields can be reproduced by re-summing the form factor expansion, for any real $n > 1$. In appendix C we provide very convincing numerics for this scaling dimension.

We can now evaluate the derivative with respect to n at $n = 1$ of this. For generic θ, the function on the right-hand side of (3.44) is zero at $n = 1$, but at $\theta = 0$, it is non-zero. Hence, we need to properly take the limit $n \to 1$ of the derivative of the right-hand side of (3.44) as a distribution. We have

$$-\frac{d}{dn}\left[\sinh\theta\, K(2\theta \pm \pi i)\right]_{n=1} = \mp\frac{\pi}{2}\frac{\cosh\theta}{\sinh\theta}, \tag{3.45}$$

but this has a pole at $\theta = 0$, coming from the kinematic pole of K at $\pm(2n-1)\pi i$. It can be resolved by noticing that for $\theta \to 0$ and $n \to 1$, we have

$$-\frac{d}{dn}\left[\sinh\theta\, K(2\theta \pm \pi i)\right] \sim \mp\frac{\pi}{2}\frac{1}{\theta \mp (n-1)\pi i}. \tag{3.46}$$

Hence, as a distribution,

$$-\frac{d}{dn}\left[\sinh\theta\, K(2\theta \pm \pi i)\right]_{n=1} = \mp\frac{\pi}{2}\frac{\cosh\theta}{\sinh(\theta \mp i0^+)} \tag{3.47}$$

and this gives

$$-\frac{d}{dn}\left[\sum_{j_1,\ldots,j_{2\ell-1}=0}^{n-1} K((-\hat\theta_{12})^{j_1})K(\hat\theta_{23}^{j_1-j_2})\ldots K(\hat\theta_{2\ell,1}^{j_{2\ell-1}})\right]_{n=1} \stackrel{\int}{=} \pi i\cosh\theta$$
$$\times\sum_{j=1}^{\ell}\sum_{q=\pm}(-1)^{\ell+j}q\begin{pmatrix}2\ell-1\\ \ell-j\end{pmatrix}\frac{\operatorname{csch}(\theta - qi0^+)\prod_{i=1}^{2\ell}\mathrm{shift}_{\theta_i\to\theta_i-q\frac{j-1}{2\ell}\pi i}}{\prod_{i=1}^{2\ell}2\cosh\left(\frac{\hat\theta_{i,i+1}}{2}-q\frac{j-1}{2\ell}\pi i\right)}. \tag{3.48}$$

Finally, we may simplify this formula by shifting back the contours towards their initial positions. Doing so, the integrand will be zero, and the only contributions will be poles taken on the way. The final result is

$$-\frac{d}{dn}\left[\sum_{j_1,\ldots,j_{2\ell-1}=0}^{n-1} K((-\hat\theta_{12})^{j_1})K(\hat\theta_{23}^{j_1-j_2})\ldots K(\hat\theta_{2\ell,1}^{j_{2\ell-1}})\right]_{n=1} \stackrel{\int}{=} \tag{3.49}$$
$$-2\pi^2\sum_{j=1}^{\ell}\sum_{k=1}^{j}\sum_{q=\pm}(-1)^{\ell+j}\left\{\begin{array}{ll}1/2 & (k=j)\\ 1 & (k<j)\end{array}\right\}\begin{pmatrix}2\ell-1\\ \ell-j\end{pmatrix}\frac{\prod_{i=1}^{2\ell}\mathrm{shift}_{\theta_i\to\theta_i+q\frac{j-k}{2\ell}\pi i}}{\prod_{i=1}^{2\ell}2\cosh\left(\frac{\hat\theta_{i,i+1}}{2}+q\frac{j-k}{2\ell}\pi i\right)}\delta(\theta).$$

The case $k = j$ in this formula can be simplified using

$$-\frac{2\pi^2\delta(\theta)\sum_{j=1}^{\ell}\begin{pmatrix}2\ell-1\\ \ell-j\end{pmatrix}(-1)^{j+\ell}}{\prod_{j=1}^{2\ell}2\cosh\frac{\hat\theta_{jj+1}}{2}} = \frac{\begin{pmatrix}2\ell-2\\ \ell-1\end{pmatrix}(-1)^{\ell}2\pi^2\delta(\theta)}{\prod_{j=1}^{2\ell}2\cosh\frac{\hat\theta_{jj+1}}{2}}, \tag{3.50}$$

so that we obtain

$$-\frac{d}{dn}\left[\sum_{j_1,\ldots,j_{2\ell-1}=0}^{n-1} K((-\hat\theta_{12})^{j_1})K(\hat\theta_{23}^{j_1-j_2})\ldots K(\hat\theta_{2\ell,1}^{j_{2\ell-1}})\right]_{n=1} \stackrel{\int}{=} \tag{3.51}$$

$$(-1)^\ell 2\pi^2\delta(\theta)\left[\frac{\begin{pmatrix}2\ell-2\\ \ell-1\end{pmatrix}}{\prod_{j=1}^{2\ell} 2\cosh\frac{\hat\theta_{jj+1}}{2}} - \sum_{j=1}^{\ell}\sum_{k=1}^{j-1}\sum_{q=\pm}\frac{\begin{pmatrix}2\ell-1\\ \ell-j\end{pmatrix}(-1)^j\prod_{i=1}^{2\ell}\mathrm{shift}_{\theta_i\to\theta_i+q\frac{j-k}{2\ell}\pi i}}{\prod_{i=1}^{2\ell}2\cosh\left(\frac{\hat\theta_{i,i+1}}{2}+q\frac{j-k}{2\ell}\pi i\right)}\right].$$

Note that the first term inside the square brackets on the right-hand side is what is obtained by directly using (3.41), without contour shifts; it is a direct generalisation of the four-particle case. The other terms are corrections, characteristic of higher-particle contributions only.

A similar analysis can be made for the odd case, (3.42). The result is

$$-\frac{d}{dn}\left[\sum_{j_1,\ldots,j_{2\ell}=0}^{n-1} K((-\hat\theta_{12})^{j_1})K(\hat\theta_{23}^{j_1-j_2})\ldots K(\hat\theta_{2\ell+1,1}^{j_{2\ell}})\right]_{n=1} \stackrel{\int}{=} \tag{3.52}$$

$$(-1)^\ell 2\pi^2\delta(\theta)\sum_{j=1}^{\ell}\sum_{k=1}^{j}\sum_{q=\pm}\frac{\begin{pmatrix}2\ell\\ \ell-j\end{pmatrix}(-1)^j q\prod_{i=1}^{2\ell+1}\mathrm{shift}_{\theta_i\to\theta_i+q\frac{j-k+1/2}{2\ell+1}\pi i}}{\prod_{i=1}^{2\ell+1}2\cosh\left(\frac{\hat\theta_{i,i+1}}{2}+q\frac{j-k+1/2}{2\ell+1}\pi i\right)}.$$

Note that in this case, we get "pure correction terms", as directly taking the derivative with respect to n at $n=1$ of (3.42), without contour shifts, gives zero.

The final results as written in (3.51) and (3.52) hold only if the other functions of the integrand do not have poles on the region covered by the shifts; then the shift operators are just shift of arguments. The contributions of poles may be evaluated in a similar way, but below we will avoid these complications. Also, these formulae are valid for $\ell = 1, 2, 3, \ldots$ only, that is, excluding $\ell = 0$.

3.3.3 Putting everything together

The final step in order to evaluate $s_\ell(t,\kappa)$ is to work out the "multiplicity" of (3.39) for a fixed particle number. This can be easily done by exploiting the Wick contraction picture introduced in (3.38). Let us pick the first rapidity $-\theta_1$. There are $2(\ell-1)$ possible contractions that could be performed as a contraction with θ_1 is not allowed (that would produce a non-fully connected term). Let us assume that $-\theta_1$ is connected to θ_i^j for some fixed i, j. Then, if we now pick the next rapidity, that is θ_1, it can be connected to almost any term, except for $-\theta_i^j$ (that would again be non-fully connected) and the two that are already connected. That gives us $2(\ell-2)$ possibilities. We carry on this argument by connecting θ_i^j to some $\theta_{-i'}^{j'}$, then $\theta_{i'}^{j'}$ to some $\theta_{-i''}^{j''}$, etc., until no rapidities are left. Hence we find that the total number of fully connected terms is $(\ell-1)!2^{\ell-1}$. All these terms are identical when integrated in all rapidities because they can all be brought to the form (3.39) by a series of two types of operation. First, we may change the sign of a rapidity, getting a minus sign from the R matrix thanks to property (2.26), then change the order of the two Z operators associated to this rapidity, which cancels this minus sign. Second, we may move pairs of Z operators associated to a given rapidity without getting any sign.

In order to be able to use formulae (3.51) and (3.52), we must make sure that no poles occur in the regions covered by the shifts, for any ℓ. This imposes that the other functions in the integrand should not have poles for $\mathrm{Im}(\theta_i) \in (-\pi/2, \pi/2)$. Since factors $R(i\pi/2 - \theta_i)$ occur in the integrand, we must take

$$\kappa \leq 0. \tag{3.53}$$

With this restriction, we obtain

$$\begin{aligned} s_{2\ell}(t,\kappa) &= \frac{(2\ell-1)!2^{2\ell-1}}{(2\ell)!(4\pi)^{2\ell}} \left[\prod_{k=1}^{2\ell} \int_{-\infty}^{\infty} d\theta_k e^{-t\cosh\theta_k} R\left(\frac{i\pi}{2} - \theta_k\right)\right] \\ & \times \left(-\frac{d}{dn}\right) \left[\sum_{j_1,\ldots,j_{2\ell-1}=0}^{n-1} K(-\hat{\theta}_{12}^{j_1}) K(\hat{\theta}_{23}^{j_1-j_2}) \ldots K(\hat{\theta}_{2\ell,1}^{j_{2\ell-1}})\right]_{n=1} \\ &= \frac{\pi^2(-1)^\ell}{2\ell} \left[\prod_{k=1}^{2\ell} \int_{-\infty}^{\infty} \frac{d\theta_k}{4\pi}\right] \delta(\theta) \left[\begin{pmatrix} 2\ell-2 \\ \ell-1 \end{pmatrix} \prod_{j=1}^{2\ell} \frac{e^{-t\cosh\theta_j} R\left(\frac{i\pi}{2} - \theta_j\right)}{\cosh\frac{\hat{\theta}_{jj+1}}{2}}\right. \\ & \left. - \sum_{j=1}^{\ell} \sum_{k=1}^{j-1} \sum_{q=\pm} \begin{pmatrix} 2\ell-1 \\ \ell-j \end{pmatrix} (-1)^j \prod_{i=1}^{2\ell} \frac{e^{-t\cosh(\theta_i + q\frac{j-k}{2\ell}\pi i)} R\left(\frac{i\pi}{2} - (\theta_i + q\frac{j-k}{2\ell}\pi i)\right)}{\cosh\left(\frac{\hat{\theta}_{i,i+1}}{2} + q\frac{j-k}{2\ell}\pi i\right)}\right] \end{aligned} \tag{3.54}$$

and similarly

$$\begin{aligned} s_{2\ell+1}(t,\kappa) &= \frac{\pi^2(-1)^\ell}{2\ell+1} \left[\prod_{k=1}^{2\ell+1} \int_{-\infty}^{\infty} \frac{d\theta_k}{4\pi}\right] \delta(\theta) \\ & \times \sum_{j=1}^{\ell} \sum_{k=1}^{j} \sum_{q=\pm} \begin{pmatrix} 2\ell \\ \ell-j \end{pmatrix} (-1)^j q \prod_{i=1}^{2\ell+1} \frac{e^{-t\cosh(\theta_i + q\frac{j-k+1/2}{2\ell+1}\pi i)} R\left(\frac{i\pi}{2} - (\theta_i + q\frac{j-k+1/2}{2\ell+1}\pi i)\right)}{\cosh\left(\frac{\hat{\theta}_{i,i+1}}{2} + q\frac{j-k+1/2}{2\ell+1}\pi i\right)}, \end{aligned} \tag{3.55}$$

both formulae hold for $\ell = 1, 2, 3, \ldots$. All integrals involved are absolutely convergent, and it is easy to see that this holds throughout all shifts required. Notice that for $\ell = 1$ in (3.54) we recover the result (3.25) as it should be. Setting $\ell = 0$ in (3.55) does not give (3.14), since $\ell = 0$ is out of the range of applicability of these formulae; the two-particle case $s_1(t,\kappa)$ is a special case.

Hence, we have for the entanglement entropy in the boundary case

$$S_A^{\text{boundary}}(rm) = -\frac{1}{12}\log(\varepsilon m) + \frac{U}{2} + \sum_{\ell=1}^{\infty} s_\ell(2rm, \kappa) \tag{3.56}$$

with (3.14), (3.54) and (3.55).

Formulae (3.54) and (3.55) are quite lengthy, but can be written in a more symmetric way, more appropriate for numerical calculations. We present such alternative expressions in appendix B.

4 Form factor expansion for the bulk entanglement entropy

We have studied the entropy of the Ising model in the presence of a boundary. However the form factor approach employed so far has first been used for bulk theories in [6] where the entropy was obtained in the two-particle approximation. We should mention here that the entanglement entropy of free theories was obtained by a different method in [30, 31]. There it was shown how it is connected to Painlevé transcendents. The analysis of the previous sections can be easily adapted now to find closed expressions for all entropy contributions in the bulk case. Employing a form factor expansion for the two-point functions of the twist fields in the bulk theory we can write

$$\langle \mathcal{T}(r)\tilde{\mathcal{T}}(0)\rangle - \langle \mathcal{T}\rangle^2 = \sum_{\ell=1}^{\infty}\frac{1}{(2\ell)!}\sum_{j_1,\ldots,j_{2\ell}=1}^{n}\left[\prod_{j=1}^{2\ell}\int_{-\infty}^{\infty}\frac{d\theta_j}{2\pi}\,e^{-rm\cosh\theta_j}\right]\left|F_{2\ell}^{\mathcal{T}|j_1j_2\ldots j_{2\ell}}(\theta_1,\ldots,\theta_{2\ell})\right|^2$$

$$= \sum_{\ell=1}^{\infty}\frac{n}{(2\ell)!}\sum_{j_1,\ldots,j_{2\ell-1}=0}^{n-1}\left[\prod_{j=1}^{2\ell}\int_{-\infty}^{\infty}\frac{d\theta_j}{2\pi}\,e^{-rm\cosh\theta_j}\right]\left|F_{2\ell}^{\mathcal{T}|1\ldots1}(\theta_1,\theta_2^{j_1},\ldots,\theta_{2\ell}^{j_{2\ell-1}})\right|^2. \tag{4.1}$$

Since we want to compute the derivative at $n=1$ of the above, we need to evaluate

$$-\frac{d}{dn}\left[n\sum_{j_1,\ldots,j_{2\ell-1}=0}^{n-1}\left|F_{2\ell}^{\mathcal{T}|1\ldots1}(\theta_1,\theta_2^{j_1},\ldots,\theta_{2\ell}^{j_{2\ell-1}})\right|^2\right]_{n=1}. \tag{4.2}$$

Notice that, for the free Fermion theory

$$\left|F_{2\ell}^{\mathcal{T}|1\ldots1}(\theta_1,\theta_2^{j_1},\ldots,\theta_{2\ell}^{j_{2\ell-1}})\right|^2 = (-1)^{\ell}F_{2\ell}^{\mathcal{T}|1\ldots1}(\theta_1,\theta_2^{j_1},\ldots,\theta_{2\ell}^{j_{2\ell-1}})F_{2\ell}^{\mathcal{T}|1\ldots1}(\theta_1,\theta_2^{-j_1},\ldots,\theta_{2\ell}^{-j_{2\ell-1}}), \tag{4.3}$$

where we used (3.13).

The only contribution to the derivative (4.2) will again come from the fully connected terms for similar reasons as in the boundary case. In fact, it is not difficult to convince oneself that the non-vanishing contributions coming from the 2ℓ-particle form factor will be completely analogous to the non-vanishing contributions coming from the 4ℓ-particle form factor in the boundary case, the only difference being the presence of the reflection matrices in the latter case and the amount of terms that contribute. Let us consider a very particular fully connected term, corresponding to the Wick contractions

$$F_{2\ell}^{\mathcal{T}|1\ldots1}(\theta_1,\theta_2^{j_1},\theta_3^{j_2},\theta_4^{j_3},\ldots,\theta_{2\ell-1}^{j_{2\ell-2}},\theta_{2\ell}^{j_{2\ell-1}})F_{2\ell}^{\mathcal{T}|1\ldots1}(\theta_1,\theta_2^{-j_1},\theta_3^{-j_2},\ldots,\theta_{2\ell-2}^{-j_{2\ell-3}},\theta_{2\ell-1}^{-j_{2\ell-2}},\theta_{2\ell}^{-j_{2\ell-1}}). \tag{4.4}$$

The contribution of this term to (4.2) is

$$-\frac{d}{dn}\left[n(-1)^{\ell}\sum_{j_1,\ldots,j_{2\ell-1}}\left(K(\theta_{12}^{-j_1})\prod_{k=1}^{\ell-1}K(\theta_{2k+1,2k+2}^{j_{2k}-j_{2k+1}})\right)\left(K(\theta_{1,2\ell}^{j_{2\ell-1}})\prod_{k=1}^{\ell-1}K(\theta_{2k,2k+1}^{-j_{2k-1}+j_{2k}})\right)\right]_{n=1}$$

$$= -\frac{d}{dn}\left[n\sum_{j_1,\ldots,j_{2\ell-1}}\left(K((-\theta_{12})^{j_1})K(\theta_{1,2\ell}^{j_{2\ell-1}})\prod_{k=1}^{\ell-1}K(\theta_{2k+1,2k+2}^{j_{2k}-j_{2k+1}})K((-\theta_{2k,2k+1})^{j_{2k-1}-j_{2k}})\right)\right]_{n=1}.$$

By changing the sign of rapidities with odd index, which does not change the result under integration in (4.1), we obtain exactly (3.51).

As for the boundary case, it is possible to argue that all fully connected terms are identical to the one above when integrated in all rapidities. The number of such terms can easily be evaluated by the following argument: Let us consider the first form factor in the product (3.35) and pick one of the rapidity variables on which it depends, say θ_i^j for some fixed i, j. It can be connected to any other rapidity in the same form factor, say $\theta_{i'}^{j'}$, and therefore there are $2\ell - 1$ possibilities. Now we can look at the second form factor, picking $\theta_{i'}^{-j'}$. There are $2\ell - 2$ possible connections, since it cannot be connected to θ_i^{-j} as this would produce a factorisable term. Suppose it is connected to $\theta_{i''}^{-j''}$. We now come back to the first form factor, looking at $\theta_{i''}^{j''}$. It can be connected to any other available rapidities, so there are $2\ell - 3$. Continuing, we find that there are $(2\ell - 1)!$ fully connected terms. Under the integral all these terms are equivalent, because exchanging two rapidities in both factors simultaneously does not bring out any sign. Therefore,

$$-\frac{d}{dn}\left[\langle \mathcal{T}(r)\tilde{\mathcal{T}}(0)\rangle - \langle \mathcal{T}\rangle^2\right] = \sum_{\ell=1}^{\infty} e_\ell(rm) \tag{4.5}$$

with

$$e_\ell(rm) = \frac{\pi^2(-1)^\ell}{\ell}\left[\prod_{k=1}^{2\ell}\int_{-\infty}^{\infty}\frac{d\theta_k}{4\pi}\right]\delta(\theta) \tag{4.6}$$

$$\times\left[\begin{pmatrix} 2\ell-2 \\ \ell-1 \end{pmatrix}\prod_{j=1}^{2\ell}\frac{e^{-rm\cosh\theta_j}}{\cosh\frac{\hat\theta_{jj+1}}{2}} - \sum_{j=1}^{\ell}\sum_{k=1}^{j-1}\sum_{q=\pm}\begin{pmatrix} 2\ell-1 \\ \ell-j \end{pmatrix}(-1)^j\prod_{i=1}^{2\ell}\frac{e^{-rm\cosh(\theta_i + q\frac{j-k}{2\ell}\pi i)}}{\cosh\left(\frac{\hat\theta_{i,i+1}}{2} + q\frac{j-k}{2\ell}\pi i\right)}\right]$$

so that

$$S_A^{\text{bulk}}(rm) = -\frac{1}{6}\log(\varepsilon m) + U + \sum_{\ell=1}^{\infty} e_\ell(rm). \tag{4.7}$$

Again, see appendix B for an alternative expression of $e_\ell(rm)$. In particular, the $\ell = 1$ contribution is given by

$$e_1(rm) = -\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\frac{d\theta_1 d\theta_2}{16}\, e^{-rm(\cosh\theta_1+\cosh\theta_2)}\frac{\delta(\hat\theta_{12})}{\cosh^2\frac{\hat\theta_{12}}{2}} = -\int_{-\infty}^{\infty}\frac{d\theta}{16}\, e^{-2rm\cosh\theta} = -\frac{K_0(2rm)}{8}, \tag{4.8}$$

which is one of the main results obtained in [6].

5 Exact UV behaviour of the entanglement entropy in the boundary Ising model

5.1 Exact logarithmic behaviour

Let us start by extracting the exact small-rm logarithmic behaviour of the bulk entanglement entropy from the full form factor expansion (4.7). For this purpose, after integrating $\theta_{2\ell}$ using the delta-function, it is convenient to change variables to the set $x_i = \hat\theta_{i,i+1}$ for $i = 1, \ldots, 2\ell - 2$, and $\theta_{2\ell-1}$. Then, we have

$$\theta_i = \sum_{j=i}^{2\ell-2}(-1)^{j-i}x_j + (-1)^{1+i}\theta_{2\ell-1} \tag{5.1}$$

and in particular,

$$\sum_{i=1}^{2\ell-1}\theta_i = \sum_{j=1}^{\ell-1}x_{2j-1} + \theta_{2\ell-1}, \quad \sum_{i=1}^{2\ell-2}\theta_i = \sum_{j=1}^{\ell-1}x_{2j-1}, \quad \sum_{i=2}^{2\ell-1}\theta_i = \sum_{j=2}^{\ell-1}x_{2j}. \tag{5.2}$$

Hence, the hyperbolic cosine factors in the denominators, involving all x_i's as well as the last two sums above, do not depend on $\theta_{2\ell-1}$, so that it is the large $|\theta_{2\ell-1}|$ behaviour of the integrand that determines the singularity at small rm. In the exponential, we have at large $|\theta_{2\ell-1}|$ and fix x_i's,

$$\sum_{i=1}^{2\ell-1} \cosh\theta_i + \cosh\left(\sum_{i=1}^{2\ell-1}\theta_i\right) \propto e^{|\theta_{2\ell-1}|}. \tag{5.3}$$

Hence, the exponential factor will display a jump of finite width from 1 to 0 around $|\theta_{2\ell-1}| \sim -\log(rm) + const.$ when rm is small, so that the leading small-rm behaviour can be obtained by omitting the exponential factor and replacing $\int d\theta_{2\ell-1}$ by $-2\log(rm)$. As a result, we find

$$e_\ell(rm) \sim g_\ell \log(rm) \tag{5.4}$$

where

$$g_\ell = \frac{(-1)^{\ell+1}}{8\ell}\left[\binom{2\ell-2}{\ell-1} J_\ell(0)^2 - \sum_{j=1}^{\ell}\sum_{k=1}^{j-1}\sum_{q=\pm}\binom{2\ell-1}{\ell-j}(-1)^j J_\ell\left(q(j-k)\right)^2\right] \tag{5.5}$$

with

$$J_\ell(a) = \left[\prod_{k=1}^{\ell-1}\int_{-\infty}^{\infty}\frac{dx_k}{4\pi\cosh\left(\frac{x_k}{2}+\frac{a\pi i}{2\ell}\right)}\right]\frac{1}{\cosh\left(\frac{1}{2}\sum_{j=1}^{\ell-1}x_j - \frac{a\pi i}{2\ell}\right)} \tag{5.6}$$

where we used the fact that the integrals factorise into even and odd-indexed x variables. The function $J_\ell(a)$ can be evaluated exactly:

$$J_\ell(a) = \frac{2^{-\ell+1}}{(\ell-1)!}\begin{cases} \csc(a\pi/2)(-1)^{\frac{\ell}{2}-1} a \displaystyle\prod_{j=1}^{\frac{\ell}{2}-1}(a^2-(2j)^2) & (\ell \text{ even}) \\ \sec(a\pi/2)(-1)^{\frac{\ell-1}{2}} \displaystyle\prod_{j=1}^{\frac{\ell-1}{2}}(a^2-(2j-1)^2) & (\ell \text{ odd}) \end{cases} \tag{5.7}$$

The expression for the number g_ℓ can be simplified to

$$\frac{1}{8\ell}\left(2^{3-2\ell}\binom{2\ell-3}{\ell-2} - \frac{h_\ell}{\pi^2(\ell-1)^2}\right) \tag{5.8}$$

where

$$h_\ell = \begin{cases} \displaystyle\binom{2\ell-2}{\ell-1}\binom{\ell-2}{\ell/2-1}^{-2} + 2\sum_{p=0}^{\ell/2-1}\binom{2\ell-2}{\ell-1+2p}\binom{\ell-2}{\ell/2-1+p}^{-2} & (\ell \text{ even}) \\ \displaystyle 2\sum_{p=0}^{\ell/2-3/2}\binom{2\ell-2}{\ell+2p}\binom{\ell-2}{\ell/2-3/2-p}^{-2} & (\ell \text{ odd}) \end{cases} \tag{5.9}$$

The sum over ℓ of the first term in (5.8) is readily seen to be 1/4, whereas the rest was verified to be consistent with $-1/12$ by summing 500 terms. Hence, we find

$$\sum_{\ell=1}^{\infty} g_\ell = \frac{1}{6} \tag{5.10}$$

in agreement with the known logarithmic behaviour from CFT. In appendix C, we provide a numerical analysis of the scaling dimension Δ_n characterising the short-distance behaviour of the full two-point function of twist fields from our form factor expansion. Agreement with the known CFT dimension provides an extremely non-trivial check of the validity of this form factor expansion.

5.2 Exact expression for $V(\kappa)$

From the results in the previous two sections, it is possible to derive an exact expression for $V(\kappa)$ appearing in (1.6).

First, comparing (4.6) to (3.54), we see that if we set the reflection matrices to 1, we have $2s_{2\ell}(2rm,\kappa) = e_\ell(2rm)$. The meaning of this is that the replacement $R \to 1$ in $\sum_{\ell=1}^{\infty} s_{2\ell}(2rm,\kappa)$ precisely provides the leading small-distance behaviour of the entanglement entropy in the boundary case, which is related to the bulk case by $S_A^{\text{boundary}}(rm) \sim \frac{1}{2} S_A^{\text{bulk}}(2rm)$ $(rm \to 0)$ (up to a finite term). The term $s_1(2rm,\kappa)$ in the boundary case only contributes a finite term as $rm \to 0$, and this holds as well as for all other terms $s_{2\ell+1}(2rm,\kappa)$ for $\ell = 1,2,3,\ldots$.

In order to understand this, consider first the expression for $s_{2\ell}$ in (3.54). The leading small-t behaviour of the integrals in the square brackets comes from the region of large rapidities which is not damped by the hyperbolic cosine factors in the denominator. Integrating $\theta_{2\ell}$ using the delta-function, we can change variables to the set $x_i = \hat{\theta}_{i,i+1}$ for $i = 1,\ldots,2\ell-2$, and $\theta_{2\ell-1}$. Then, we have

$$\theta_i = \sum_{j=i}^{2\ell-2} (-1)^{j-i} x_j + (-1)^{1+i} \theta_{2\ell-1} \tag{5.11}$$

and in particular,

$$\sum_{i=1}^{2\ell-1} \theta_i = \sum_{j=1}^{\ell-1} x_{2j-1} + \theta_{2\ell-1}, \quad \sum_{i=1}^{2\ell-2} \theta_i = \sum_{j=1}^{\ell-1} x_{2j-1}, \quad \sum_{i=2}^{2\ell-1} \theta_i = \sum_{j=2}^{\ell-1} x_{2j}. \tag{5.12}$$

Hence, the hyperbolic cosine factors in the denominators, involving x_i's and the last two sums above, do not depend on $\theta_{2\ell-1}$, so that it is the large $|\theta_{2\ell-1}|$ behaviour of the integrand that determines the singularity at small t. On the other hand, $\theta_{2\ell-1}$ is involved in the argument of every R-matrix. Since $R(i\pi/2 - \theta) \sim \pm i$ as $\text{Re}(\theta) \to \mp\infty$ for κ finite, and the opposite for $\kappa = -\infty$, one can see that the product of R matrices goes to 1 as $\theta_{2\ell-1} \to \pm\infty$ for any κ. This shows that the replacement $R \to 1$ gives the leading behaviour as $rm \to 0$.

Second, let us consider a similar change of variable in the odd case (3.55), $x_i = \hat{\theta}_{i,i+1}$ for $i = 1,\ldots,2\ell-1$, and $\theta_{2\ell}$. Then,

$$\sum_{i=1}^{2\ell-1} \theta_i = \sum_{j=1}^{\ell} x_{2j-1} - \theta_{2\ell}, \quad \sum_{i=2}^{2\ell} \theta_i = \sum_{j=1}^{\ell-1} x_{2j} + \theta_{2\ell}, \tag{5.13}$$

so that all variables are involved in the hyperbolic cosine factors in the denominators. Hence, in this case the limit $t \to 0$ can be taken, and all integrals are still convergent.

Then, subtracting this leading behaviour, and using the known small-rm behaviour of the entanglement entropy in the bulk case, (1.7), we find that the small-rm behaviour in the boundary case is given by (1.6) with

$$V(\kappa) = \sum_{\ell=1}^{\infty} c_\ell(\kappa) \tag{5.14}$$

with $c_1(\kappa)$ given by (3.16) and where

$$c_{2\ell}(\kappa) = \frac{\pi^2(-1)^\ell}{2\ell}\left[\prod_{k=1}^{2\ell}\int_{-\infty}^{\infty}\frac{d\theta_k}{4\pi}\right]\delta(\theta)\left[\left(\begin{array}{c}2\ell-2\\ \ell-1\end{array}\right)\frac{\prod_{j=1}^{2\ell}R\left(\frac{i\pi}{2}-\theta_j\right)-1}{\prod_{j=1}^{2\ell}\cosh\frac{\hat\theta_{jj+1}}{2}}\right. \tag{5.15}$$

$$\left.-\sum_{j=1}^{\ell}\sum_{k=1}^{j-1}\sum_{q=\pm}\left(\begin{array}{c}2\ell-1\\ \ell-j\end{array}\right)(-1)^j\frac{\prod_{i=1}^{2\ell}R\left(\frac{i\pi}{2}-(\theta_i+q\frac{j-k}{2\ell}\pi i)\right)-1}{\prod_{i=1}^{2\ell}\cosh\left(\frac{\hat\theta_{i,i+1}}{2}+q\frac{j-k}{2\ell}\pi i\right)}\right]$$

and similarly

$$c_{2\ell+1}(\kappa) = \frac{\pi^2(-1)^\ell}{2\ell+1}\left[\prod_{k=1}^{2\ell+1}\int_{-\infty}^{\infty}\frac{d\theta_k}{4\pi}\right]\delta(\theta) \tag{5.16}$$

$$\times\sum_{j=1}^{\ell}\sum_{k=1}^{j}\sum_{q=\pm}\left(\begin{array}{c}2\ell\\ \ell-j\end{array}\right)(-1)^j q\prod_{i=1}^{2\ell+1}\frac{R\left(\frac{i\pi}{2}-(\theta_i+q\frac{j-k+1/2}{2\ell+1}\pi i)\right)}{\cosh\left(\frac{\hat\theta_{i,i+1}}{2}+q\frac{j-k+1/2}{2\ell+1}\pi i\right)},$$

both formulae for $\ell=1,2,3,\ldots$. These generalise $c_2(\kappa)$ given in (3.28) (recall that $\theta=\sum_j\theta_j$). The derivation of (5.14) is as follows:

$$\begin{aligned} S_A^{\rm boundary}(rm) &= \frac{1}{12}\log(m\epsilon)+\frac{U}{2}+\sum_{\ell=1}^{\infty}s_\ell(2rm,\kappa)\\ &\sim \frac{1}{12}\log(m\epsilon)+\frac{U}{2}+\sum_{\ell=1}^{\infty}c_\ell(\kappa)+\frac{1}{2}\sum_{\ell=1}^{\infty}e_\ell(2rm)\\ &= \frac{1}{12}\log(m\epsilon)+\frac{U}{2}+\sum_{\ell=1}^{\infty}c_\ell(\kappa)+\frac{1}{2}\left(S_A^{\rm bulk}(2rm)-U-\frac{1}{6}\log(m\epsilon)\right)\\ &\sim -\frac{1}{12}\log(2r/\epsilon)+\sum_{\ell=1}^{\infty}c_\ell(\kappa). \end{aligned} \tag{5.17}$$

Although we have provided arguments suggesting that the integrals defining $c_\ell(\kappa)$ are convergent, in order for (5.14) to be a correct representation of $V(\kappa)$, the infinite sum over ℓ should give a finite result. This is much more subtle, as form factor expansions are expected to provide convergent series expansion for finite distances, but not necessarily at zero distance. Exact evaluations of the first few coefficients $c_\ell(\kappa)$ for some κ below, and extrapolation to higher ℓ, give strong indications that the series is indeed convergent; hence (5.14) is a correct representation.

5.3 Exact and approximate re-summations

All integrals defining the coefficients $c_\ell(\kappa)$ can be evaluated exactly. For instance, a change of variable $x_j=e^{\theta_j}$ makes all integrands rational functions, and multiple integrals can bring logarithmic terms, which can all be integrated. We have been able to evaluate exactly all coefficients $c_\ell(0)$:

$$c_{2\ell}(0)=\frac{1}{8\ell(2\ell-1)},\qquad c_{2\ell+1}(0)=\frac{\pi}{2^{4\ell+1}}\left(\begin{array}{c}2\ell-1\\ \ell-1\end{array}\right)^2-\frac{1}{4(2\ell+1)}, \tag{5.18}$$

extrapolating from the exact values at $\ell = 1, 2, 3$ and 4 obtained with the help of Mathematica. Along with $c_1(0)$ from (3.16), these re-sum to:

$$V(0) = \frac{\pi - 2}{8} + \sum_{\ell=2}^{\infty} c_\ell(0) = \log\sqrt{2}. \tag{5.19}$$

¿From this, we directly obtain $V(-\infty)$, since $c_{2\ell}(-\infty) = c_{2\ell}(0)$ and $c_{2\ell+1}(-\infty) = -c_{2\ell+1}(0)$. This gives

$$V(-\infty) = \frac{2 - \pi}{8} + \sum_{\ell=1}^{\infty}(c_{2\ell}(0) - c_{2\ell+1}(0)) = 0. \tag{5.20}$$

We have also computed the values of $c_\ell(-1)$ for ℓ up to 8 and obtained the following exact expressions,

$$\begin{aligned}
c_2(-1) &= \frac{23}{120} = 0.191667...,\\
c_3(-1) &= \frac{247}{12} + \frac{65}{2\pi} - \frac{315\pi}{32} = 0.00335195...,\\
c_4(-1) &= \frac{7771}{5040} - \frac{134}{9\,\pi^2} = 0.0333052...,\\
c_5(-1) &= \frac{364737}{40} - \frac{11788}{\pi^3} + \frac{420483}{16\pi} - \frac{2787435\pi}{512} = 0.000454195...,\\
c_6(-1) &= \frac{133054637}{800800} + \frac{53609}{30\,\pi^4} - \frac{16387}{9\,\pi^2} = 0.0137526...,\\
c_7(-1) &= \frac{2756451471}{112} + \frac{10463106}{\pi^5} - \frac{413423405}{6\,\pi^3} + \frac{113700482239}{1152\,\pi} - \frac{35098069395\,\pi}{2048}\\
&= 0.0000023...,\\
c_8(-1) &= \frac{1205078334301}{17867850} - \frac{52153432}{105\,\pi^6} + \frac{222090851}{180\,\pi^4} - \frac{176750962}{225\,\pi^2} = 0.00753035...
\end{aligned} \tag{5.21}$$

These values already give a rather good approximation to $V(-1)$:

$$V(-1) \approx \frac{5}{4} - \frac{3\pi}{8} + \sum_{\ell=2}^{8} c_\ell(-1) = 0.321966... \tag{5.22}$$

which is compatible with the expected value of $\log\sqrt{2} = 0.346574...$. Therefore, as expected, in the UV limit the entropy only depends on whether the magnetic field h is finite (free boundary conditions) or infinite (fixed boundary conditions). An interpretation of these results for $V(\kappa)$ is provided in section 6.

6 Discussion

We recall that our main results are 1) the full form factor expansion for the entanglement entropy in the boundary Ising model (3.56) for $\kappa \leq 0$, 2) the full form factor expansion in the bulk case (4.7), and 3) an expression for the short-distance constant $V(\kappa)$ (5.14) leading to its exact value (1.8). We now discuss our results for the boundary entanglement entropy in the large-distance and short-distance limits.

6.1 Infrared behaviour of the boundary entanglement entropy

The form factor expansion (3.56) converges rapidly for large distances. Hence we expect the 2- and 4-particle contributions evaluated in section (3.2) to provide a good approximation of the IR behaviour of the entanglement entropy for sufficiently large distances. Let us start by studying the behaviour of the correction (3.14) for $t = 2rm$ large. In this case it is possible to compute the leading contribution of the correction by expanding the integrand (except for the exponential term) in the variable $\cosh\theta - 1$ around the value zero. We find,

$$s_1(t, \kappa \neq -1, 1) = -\frac{1}{8}\sqrt{\frac{\pi}{2}}\frac{\kappa+1}{\kappa-1}\frac{e^{-t}}{t\sqrt{t}} + O(e^{-t}t^{-5/2}), \tag{6.1}$$

and

$$\begin{aligned} s_1(t, 1) &= \frac{1}{2}\sqrt{\frac{\pi}{2}}\frac{e^{-t}}{\sqrt{t}} + O(e^{-t}t^{-3/2}) \\ s_1(t, -1) &= \frac{3}{32}\sqrt{\frac{\pi}{2}}\frac{e^{-t}}{t^2\sqrt{t}} + O(e^{-t}t^{-7/2}). \end{aligned} \tag{6.2}$$

Recall that these hold for all $\kappa \leq 1$.

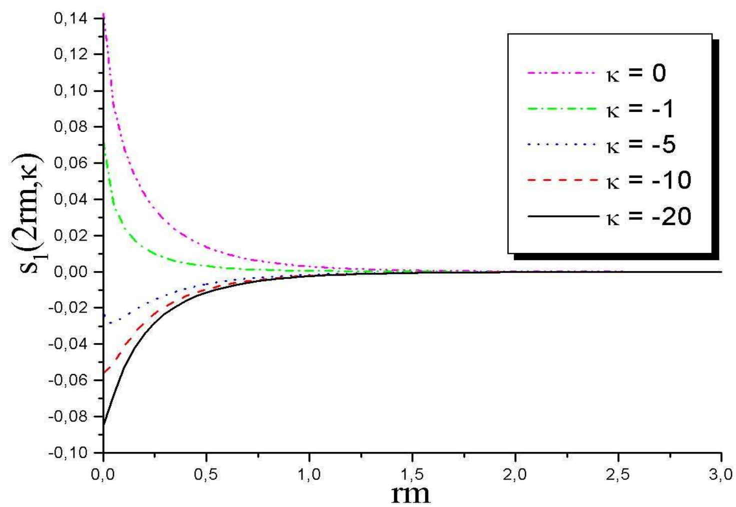

Figure 1: The function $s_1(2rm, \kappa)$ for several values of κ.

A similar computation for $s_2(t, \kappa)$ yields:

$$s_2(t, \kappa \neq -1) = -\frac{1}{64}\sqrt{\frac{\pi}{2}}\frac{(\kappa+1)^2}{(\kappa-1)^2}\frac{e^{-2t}}{2t\sqrt{2t}} + O(e^{-2t}(2t)^{-5/2}), \tag{6.3}$$

and

$$s_2(t, -1) = -\frac{15}{1024}\sqrt{\frac{\pi}{2}}\frac{e^{-2t}}{(2t)^3\sqrt{2t}} + O(e^{-2t}(2t)^{-9/2}), \tag{6.4}$$

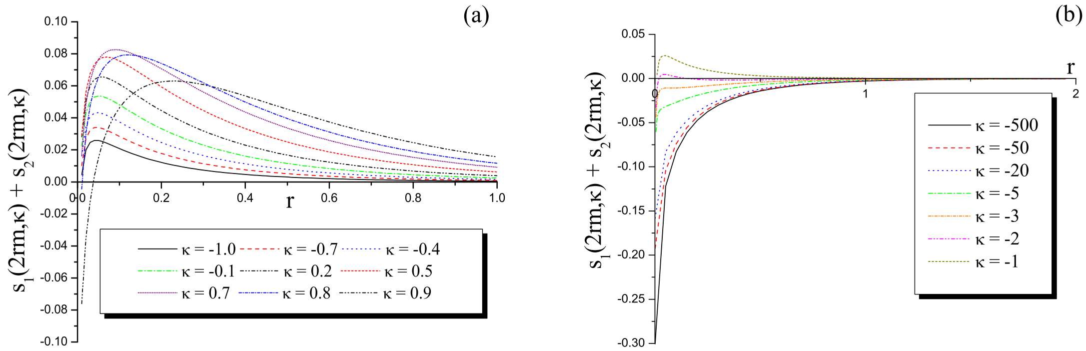

Figure 2: The function $s_1(2rm, \kappa) + s_2(2rm)$ for $0 < r \leq 2$. The value of rm for which the entropy is maximal for a given value of κ increases as κ gets closer to 1. As in figures 2 (a) and (b), the maximum of the entropy seems most pronounced for $\kappa = 0.7$ and rm around 0.1 and tends to shift and eventually disappear as $\kappa \to 1$. However, since the maximum occurs generally for rather small values of rm, its position may be affected significantly by higher order form factor corrections. Moreover, for $\kappa > 0$, additional contributions to s_2 may come from the boundary bound state. Yet, it is certain that there is a maximum for $\kappa \geq -1$ as in this case the function tends to zero from above as $rm \to \infty$.

which is clearly sub-leading comparing to the $s_1(t, \kappa)$ expansion. Note that there will be corrections to this sub-leading behaviour for $\kappa > 0$ due to the boundary bound state.

Let us examine more carefully (6.1) and (6.2). The leading contribution to the entropy is negative, as long as $\kappa < -1$: the asymptotic value is approached from below. For $\kappa > -1$, however, a change of sign occurs: the asymptotic value is then approached from above, as can be seen in figure 1. This means that for values of $\kappa > -1$ the "saturation" value of the entropy in the infrared limit, $U/2$, is actually not the maximum value the entropy reaches. For $\kappa \geq -1$ there exists some finite value of rm for which the entropy has a maximum. From looking at the curves of $s_1(t, \kappa) + s_2(t, \kappa)$, this value seems to be moving towards higher rm as κ is decreased towards -1 – see figures 2 (a) and 2 (b). However, for $-1 < \kappa < 0$ the maximum is at very small values of rm, and for $\kappa > 0$, s_2 may receive extra boundary bound state contributions. Hence, this behaviour of the maximum cannot be conclusive.

The fact that the entanglement entropy is not monotonic for $\kappa > -1$ is not in contradiction with its fundamental properties. In particular, the fact that the entanglement entropy is an increasing function of rm in the bulk case follows from the "strong subadditivity theorem" and translation invariance, as proven in [32, 33]. Since translation invariance is broken in the boundary theory, the entanglement entropy in this case is not necessarily a monotonic function of rm.

As recalled in sub-section 2.4, for $\kappa > -1$, the R-matrix has a pole on the imaginary θ line, although it is only on the physical strip for $\kappa > 0$ (where a bound state is present). The value $\kappa = -1$ (corresponding to a magnetic field $h_c = 2\sqrt{m}$) is a "critical" value where the R-matrix has a third-order zero at $\theta = 0$. What we see here is that it is this critical value that plays an important role for seeing a maximum from the large-distance behaviour. Note that a similar sort of large-distance behaviour was observed for the one-point functions of the energy and spin operators in the boundary Ising model [29]. The explanation suggested was that while at short distances one sees the free boundary condition for any finite h, at large distances one observes the fixed boundary condition for $h > h_c$, and the free one for $h < h_c$. This gives rise to a cross-over behaviour in the h–mr plane for $h < h_c$, where we observe two separated regions, corresponding to increasing and decreasing entanglement entropy with distance.

6.2 Ultraviolet behaviour of the boundary entanglement entropy

6.2.1 Interpretation of $V(\kappa)$

It is natural to interpret $V(\kappa)$ as a "boundary entanglement": the contribution of the boundary to the entanglement between the region A and the rest. Naturally, for fixed boundary condition, there should be no contribution at all, since the boundary does not experience quantum fluctuations. Our result (1.8) shows that we have chosen the correct large-distance normalisation to have $V(-\infty) = 0$. On the other hand, for free boundary conditions, the boundary fluctuates and should participate to the entanglement. This is in agreement with $V(\kappa > -\infty) = \log\sqrt{2} > 0$.

In fact, we may connect $V(\kappa)$ to the *boundary entropy* s, a quantity that essentially counts the number of degrees of freedom pertaining to a boundary. This quantity is simply given by $s = \log g$ where g is the boundary degeneracy introduced by Affleck and Ludwig [25]. In particular for a bulk CFT, they showed that $g = \langle 0|\tilde{B}\rangle$ where $|0\rangle$ is the bulk CFT ground state, and $|\tilde{B}\rangle$ is a normalised boundary state in the bulk CFT Hilbert space (in particular, $s \leq 0$). It is considering the boundary entropy that Friedan and Konechny [34] were able to provide a proof of the "g-theorem": that the g-function decreases in the RG flow from UV to IR.

In order to derive the relation between $V(\kappa)$ and s, we first provide a direct connection between $V(\kappa)$ and entanglement entropies of the Ising model *at criticality*:

$$V(\kappa) = S_A^{\rm boundary}(r)_{\rm critical} - \frac{1}{2}S_A^{\rm bulk}(2r)_{\rm critical} + \log\sqrt{2}. \tag{6.5}$$

The result is independent of r, since both entanglement entropies have the same logarithmic r-dependence. Most importantly, both entanglement entropies must be evaluated in the same cut-off scheme; for instance, both should be evaluated on the same lattice, with the same lattice spacing. The entanglement entropies should be evaluated at the UV fixed point if κ is finite, and at the IR fixed point if $\kappa = -\infty$.

In quantum field theory, it is not easy to implement the same lattice spacing in the bulk and boundary situations, since the lattice spacing enters into non-universal constants. Using massive QFT, it is possible to solve this problem. Consider the entanglement entropy $S_A(r_1, r_2)$ of sub-section 2.1, but with a slightly different normalisation specified below; we will denote it $\tilde{S}_A(r_1, r_2)$. We may uniquely fix the cutoff, for instance by requiring the conformal normalisation as above, $\tilde{S}_A(r_1, r_2) \sim \frac{c}{3}\log((r_2 - r_1)/\varepsilon) + o(1)$ as $r_2 \to r_1$. This, then, is just the bulk critical entanglement entropy above: $S_A^{\rm bulk}(r)_{\rm critical} = \frac{c}{3}\log(r/\varepsilon)$. But using the same object, hence with the same lattice spacing, we can also define the critical entanglement entropy in the boundary case, $S_A^{\rm boundary}(r)_{\rm critical}$, following the arguments already outlined in sub-section 2.1. Note first that for $r_2 \gg r_1 \gg 0$, the entanglement entropy saturates to some constant $-\frac{c}{3}\log(m\varepsilon) + \tilde{U}$ thanks to the presence of the mass, and this saturation is a sum of the contributions of the two boundary points at r_1 and r_2. These contributions are equal, so that one boundary point contributes $-\frac{c}{6}\log(m\varepsilon) + \tilde{U}/2$. Now for $r_2 \gg r_1$ and $r_1 m$ finite, we get the entanglement entropy in the boundary case (i.e. with the region ending on the boundary being connected) and with a mass, but with an extra contribution of the boundary point r_2 (at infinity). Hence, we may define $\tilde{S}_A^{\rm boundary}(r) = \lim_{r_2\to\infty} S(r, r_2) + \frac{c}{6}\log(m\varepsilon) - \tilde{U}/2$. This quantity has large-rm asymptotic given by $-\frac{c}{6}\log(m\varepsilon) + \tilde{U}/2$. We then only need to take the critical bulk limit $rm \to 0$.

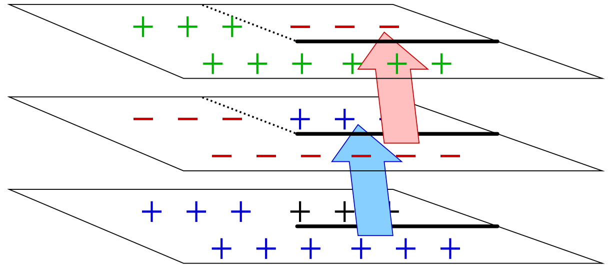

Figure 3: How a vacuum of the form $\cdots \otimes |0,+\rangle \otimes |0,-\rangle \otimes |0,+\rangle \otimes \cdots$ becomes a two-particle state after going through a branch-point twist field.

At this point it would seem natural to identify $\tilde{U}$ with U, the bulk saturation constant, and then have $\tilde{S}_A^{\rm boundary}(r) = S_A^{\rm boundary}(r)$. However, this does not hold. The main idea comes from the fact that in the bulk, the ground state is degenerate, with spins being asymptotically up or down, $|0,+\rangle$ and $|0,-\rangle$. If we allow fluctuations amongst the two degenerate ground states, as would be obtained from a large-volume limit of a periodic space, the bulk constant U should be identified with the two contributions from the boundary points, and an additional pure entropy contribution coming from this fluctuation, which should be $\log 2$ (for instance, an extra contribution of $\log 2$ due to zero-modes was present in results of [35]). Hence we must write

$$U = \tilde{U} + \log 2. \tag{6.6}$$

In the boundary case with any non-zero magnetic field, however, there is a definite ground state that is chosen at infinity, and the derivation above indeed involves only the boundary point contribution $\tilde{U}/2$. Hence the large distance limit of $\tilde{S}_A^{\rm boundary}(r)$ is $-\frac{c}{6}\log(m\varepsilon) + U/2 - \log\sqrt{2}$ so that from (1.6), $\tilde{S}_A^{\rm boundary}(r) = S_A^{\rm boundary}(r) - \log\sqrt{2}$. Then we find $S_A^{\rm boundary}(r)_{\rm critical} = \frac{c}{3}\log(r/\varepsilon) + V(\kappa) - \log\sqrt{2}$, which shows (6.5).

Technically, allowing fluctuations amongst the two degenerate ground states corresponds to choosing $|0\rangle = ((|0,+\rangle + |0,-\rangle)/\sqrt{2})^{\otimes n}$ in the n-copy model. Our branch-point twist field form factors as constructed in [6], and more generally here, assume the use of this ground state, since they are non-zero even in cases where there are sheets with *odd numbers* of particles. Recall that in the ordered regime, particles correspond to domain walls, separating spin-up and spin-down regions. Then, the only way to have *out*-states with, for instance, two particles on different sheets after the twist field, is to have an *in*-state with sheets on different ground states, see figure 3. A completely up ground state $|0,+\rangle^{\otimes n}$, for instance, wouldn't admit such form factors. Since all configurations of an even number of particles distributed amongst the n sheets are allowed, we must use the completely symmetric ground state.

The constant $\tilde{U}$ is the large-distance limit of the bulk entanglement entropy evaluated from $\langle 0,+|^{\otimes n}\tilde{\mathcal{T}}(r_1)\mathcal{T}(r_2)|0,+\rangle^{\otimes n}$, whereas U is that obtained from $\langle 0|\tilde{\mathcal{T}}(r_1)\mathcal{T}(r_2)|0\rangle$ with the symmetric ground state. The difference can be computed explicitly. First note that matrix elements

$$\langle 0,\epsilon_1'| \otimes \cdots \otimes \langle 0,\epsilon_n'|\tilde{\mathcal{T}}(r_1)\mathcal{T}(r_2)|0,\epsilon_1\rangle \otimes \cdots \otimes |0,\epsilon_n\rangle$$

have zero large-distance limit unless $\epsilon_i = \epsilon_j = \epsilon_j'$ for all i,j (that is, all signs are the same), since otherwise domain walls will have to propagate between the twist fields. Hence we immediately find

$$\langle 0|\tilde{\mathcal{T}}(r_1)\mathcal{T}(r_2)|0\rangle \sim 2^{1-n}\langle 0,+|^{\otimes n}\tilde{\mathcal{T}}(r_1)\mathcal{T}(r_2)|0,+\rangle^{\otimes n} \tag{6.7}$$

at large distances, so that, taking derivatives with respect to n, we have

$$-\left(\frac{d}{dn}\langle 0|\tilde{\mathcal{T}}(r_1)\mathcal{T}(r_2)|0\rangle\right)_{n=1} \sim \log 2 - \left(\frac{d}{dn}\langle 0,+|^{\otimes n}\tilde{\mathcal{T}}(r_1)\mathcal{T}(r_2)|0,+\rangle^{\otimes n}\right)_{n=1} \tag{6.8}$$

which gives (6.6).

Note that although the arguments above hold for finite, and perhaps only large enough, magnetic field, the constant $V(\kappa)$ is the same for any κ finite (see sub-section 2.2), hence the result (6.5) is valid in general[‡].

Finally, Calabrese and Cardy [36] proposed a formula for the boundary entropy, which amounts, from (6.5), to the statement

$$V(\kappa) = s + \log\sqrt{2}, \tag{6.9}$$

and which has been tested numerically in [37, 38] This is in agreement with our results (1.8), since $s = 0$ in the free boundary case, and $s = -\log\sqrt{2}$ in the fixed boundary case [26].

From these arguments, in general the shift $\log\sqrt{2}$ should be replaced by $-\log\mathcal{C}$ where $\mathcal{C}^2$ is the fraction of the ground state degeneracy broken by the boundary condition for large enough h. This implies (1.9). Such an "extra" contribution to $s = \log g$ was also found in [39] in calculations using Thermodynamic Bethe Ansatz techniques and was accounted for by means of similar arguments (it is important to note that the Thermodynamic Bethe Ansatz used there is fundamentally different from our approach based on form factors).

In [39] the flow of g between critical points was studied for several families of minimal Toda field theories with ground state degeneracy k and with a boundary completely breaking it. The factor $\mathcal{C} = 1/\sqrt{k}$ was termed "symmetry factor". Interestingly, it was shown that at the infrared point of these models, one gets $g = \mathcal{C}$. Hence, for massive models with spontaneously broken order-parameter symmetry, and with an order-parameter boundary perturbation, one should find $V(\kappa) = s - s_{IR} \geq 0$, where $s_{IR} = \log\mathcal{C}$ is the infrared value of s. For the same order-parameter perturbation both on the bulk and boundary, one should simply find $V(\kappa) = s \leq 0$. All these considerations should not depend on integrability.

Note that a more detailed study of $V(\kappa)$ may be useful in understanding if the boundary entropy s is always bounded from below.

6.2.2 Conformal bulk with non-conformal boundary

Taking the short-distance limit $mr \to 0$ while increasing the magnetic field with a fixed product $2\kappa mr = a$, we obtain a conformal bulk theory with a non-conformal boundary, with $a = h^2 r$ the dimensionless parameter relating the distance r to the boundary and the boundary magnetic field h. The entanglement entropy then interpolates between the UV free-boundary point $r \to 0$, and the IR fixed-boundary point $r \to \infty$. We observed explicitly this interpolation in the four-particle result in section 3.2, through the monotonic function $c_2^\natural(a)$ (3.34). It is a complicated matter to generalise this to higher particle contributions, but it would be interesting to understand if the function stays monotonic, as this gives a natural g-function flow.

7 Conclusion

The main technical results of this paper are exact infinite-series formulae for the bi-partite entanglement entropy of the Ising model with and without boundaries. We have used for this

[‡]We would like to thank here P. Calabrese and P. E. Dorey, for suggesting to us the possibility of a relationship between the degeneracy of the ground state and the $\log\sqrt{2}$ term in (6.5).

a relationship between entanglement entropy and the derivative with respect to n at $n = 1$ of correlation functions of branch-point twist fields in the model composed out of n non-interacting copies of the Ising model. In order to obtain our formulae, it has been necessary to tackle several non-trivial intermediate problems:

- finding closed expressions for all non-vanishing form factors of branch point twist fields in the n-copy theory,
- identifying the correct analytic continuation in n of the contributions of these form factors to correlation functions and evaluate their derivatives with respect to n, and
- checking both the form factor formulae and their analytic continuation for consistency.

The first of these problems was easy to solve, as we are dealing with a free theory for which Wick's theorem applies. Hence, we have been able to show that all form factors of the twist field admit expressions in terms of a Pfaffian. Obtaining the right analytic continuation of every contribution to the form factor expansion of the twist-field boundary one-point function (or bulk two-point function) is a highly non-trivial problem. The main complication arises from the fact that the pole- and zero-structure of the form factors (in particular, the way some poles and zeroes cancel each other) changes substantially as soon as n is allowed to take non-integer values. As a consequence, the phenomenon observed in [6] of non-uniform convergence of form factors as $n \to 1$ is generalised to a non-uniform convergence as $n \to \ell'$ for all positive integers $\ell' \leq \ell$ for the 2ℓ-particle form factor. The problem was solved following the principle that the analytic continuation is obtained from the analytic function that describes form factor contributions at values of n large enough. This amounts to evaluating first the contribution we would obtain analytically continuing in n around some integer and then adding the residues of all the extra poles that are crossed by the integration contours when bringing n from infinity. This is however not the only analytic continuation that is possible and therefore it becomes quite crucial to find ways of checking it for consistency. In this paper we have been able to do this in a very precise manner by finding an explicit formula for the leading logarithmic behaviour both of the two-point function of the twist field in the bulk and of its derivative at $n = 1$ (that is, the bulk entanglement entropy). By a combination of analytical and numerical computations we have been able to extract both UV behaviours with extreme accuracy and to show that they agree with what is expected from CFT arguments.

The results just described have put us in the position to analyse another quantity of interest in this context, that is the contribution to the free energy that can be attributed exclusively to the presence of the boundary. This is essentially the boundary entropy, the natural logarithm of the boundary degeneracy or g-factor originally introduced by Affleck and Ludwig in [25]. In our analysis we have computed the universal quantity $V(\kappa)$ which is closely related to g (where κ is related to the boundary magnetic field in the Ising model). We have defined $V(\kappa)$ as a certain rm independent contribution to the boundary entanglement entropy in the UV limit. We have found an exact formula for $V(\kappa)$ and evaluated it exactly at $\kappa = 0, -\infty$ to $V(0) = \log\sqrt{2}$ and $V(-\infty) = 0$. We have also gathered strong numerical evidence that $V(\kappa)$ is in fact constant and equal to $V(0)$ for any finite values of κ. These two values of $V(\kappa)$ would correspond to the two conformal invariant boundary conditions that are known for the Ising model: the free and fixed boundary conditions. The fact that $V(\kappa)$ is larger for free boundary conditions (finite magnetic field) and that $V(0) - V(-\infty) = \log\sqrt{2}$ are properties which also hold for $\log g$. However, it is known from Cardy and Lewellen's work [26] that $g_{\text{free}} = 1$ and $g_{\text{fixed}} = 1/\sqrt{2}$, hence

$$V(\kappa) - \log g = \log\sqrt{2}. \tag{7.1}$$

In this paper we have identified the difference between these two quantities as an IR contribution to the entanglement entropy coming from the ground state degeneracy in the periodic case that is broken in the boundary case. We have proposed a generalisation of this to more general models with relevant boundary perturbations.

We have also found interesting results for the IR behaviour of the entanglement entropy: it is known that the bulk entropy saturates for large distances (in the Ising model, the saturation value is given by the constant U given in (2.24)). In particular, the fact that the entropy is an increasing function of rm follows from the "strong subadditivity theorem" and translation invariance, as proven in [32, 33]. Since translation invariance is broken in the boundary theory, the entanglement entropy in this case is not necessarily a monotonic function of rm. Indeed, we find that, for a range of values of κ, it has a maximum for some value of rm before reaching its asymptotic value $U/2$. This range of values of κ starts precisely at $\kappa = -1$ which corresponds to a value of the magnetic field for which, in a sense, the boundary becomes "critical".

There are many open problems related to the present work and in general, to the computation of the entanglement entropy in integrable QFT. In the case of the bulk Ising model, it is known that the entanglement entropy can be described via Painlevé transcendents [30, 31]. It would be interesting to check the consistency of this representation with our full form factor expansion. In the boundary Ising case, it is known that the one-point function of the order parameter has a Fredholm determinant representation for any magnetic field, from which differential equations can be derived [29]. It would be interesting to see if similar formulae hold for the branch-point twist field. In the general QFT case, the most obvious problem is perhaps to extend the present analysis to theories other than the Ising model. We believe that this should be possible to some extent but it is very unlikely that re-summations can be done analytically for interacting models. Yet an independent check of (1.9) in the more general situation would be useful. It would also be interesting to apply the form factor approach employed here and in [6, 7, 8] to the computation of the entanglement entropy of multiply connected regions, both for bulk and boundary theories and also to extend the analysis of the present paper to the finite temperature situation.

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A Re-summation of fully connected terms

In this appendix we would like to provide a proof by induction of the equalities (3.41)-(3.42). Let us then assume that (3.41) is true for some value of ℓ and try to obtain (3.42) from it. If (3.41) holds, then it will also hold when the variable $x_{2\ell}$ is shifted as $x_{2\ell} \to x_{2\ell} - 2\pi i p$. We will do this and introduce at the same time one extra sum in the variable p and one factor $K(y^p)$,

$$\sum_{j_1,\ldots,j_{2\ell-1},p=0}^{n-1} K((-x_1)^{j_1})K(x_2^{j_1-j_2})\ldots K(x_{2\ell-1}^{j_{2\ell-2}-j_{2\ell-1}})K(x_{2\ell}^{j_{2\ell-1}-p})K(y^p) = \frac{(-1)^\ell 2i\sinh(\frac{x}{2})}{\prod_{i=1}^{2\ell} 2\cosh\frac{x_i}{2}}$$
$$\times \sum_{p=0}^{n-1}\sum_{j=1}^{\ell} \left(\begin{array}{c} 2\ell-1 \\ \ell-j \end{array}\right) \left[K(x^{j-p}-i\pi)+K(x^{-j-p}+i\pi)\right] K(y^p), \quad (A.1)$$

where, as before $x := \sum_{i=1}^{2\ell} x_i$. We can now employ (3.40) in order to carry out the sum in p in the second line,

$$\sum_{p=0}^{n-1} K(x^{\pm j-p} \mp i\pi)K(y^p) = \frac{i\cosh\left(\frac{x+y}{2}\right)}{2\sinh\frac{x}{2}\cosh\frac{y}{2}}\left(K(x+y\pm 2\pi i j)+K(x+y\pm 2\pi i(j-1))\right). \quad (A.2)$$

Substituting these sums into (A.1) we obtain

$$\sum_{j_1,\ldots,j_{2\ell-1},p=0}^{n-1} K(-x_1^{j_1})K(x_2^{j_1-j_2})\ldots K(x_{2\ell-1}^{j_{2\ell-2}-j_{2\ell-1}})K(x_{2\ell}^{j_{2\ell-1}-p})K(y^p) = \frac{(-1)^{\ell+1} 2\cosh(\frac{x+y}{2})}{2\cosh\frac{y}{2}\prod_{i=1}^{2\ell} 2\cosh\frac{x_i}{2}}$$
$$\times \sum_{j=1}^{\ell} \left(\begin{array}{c} 2\ell-1 \\ \ell-j \end{array}\right) \left[K(x^j+y)+K(x^{j-1}+y)+K(x^{-j}+y)+K(x^{-j+1}+y)\right]. \quad (A.3)$$

The sum in j can be split as,

$$\sum_{j=1}^{\ell} \left(\begin{array}{c} 2\ell-1 \\ \ell-j \end{array}\right) \left[K(x^j+y)+K(x^{-j}+y)\right] + \sum_{j=0}^{\ell-1} \left(\begin{array}{c} 2\ell-1 \\ \ell-j-1 \end{array}\right) \left[K(x^j+y)+K(x^{-j}+y)\right]$$
$$= \left(\begin{array}{c} 2\ell \\ \ell \end{array}\right) K(x+y) + \sum_{j=1}^{\ell} \left(\begin{array}{c} 2\ell \\ \ell-j \end{array}\right) \left[K(x^j+y)+K(x^{-j}+y)\right], \quad (A.4)$$

where we have used the identities

$$2\left(\begin{array}{c} 2\ell-1 \\ \ell-1 \end{array}\right) = \left(\begin{array}{c} 2\ell \\ \ell \end{array}\right) \quad \text{and} \quad \left(\begin{array}{c} 2\ell-1 \\ \ell-j \end{array}\right) + \left(\begin{array}{c} 2\ell-1 \\ \ell-j-1 \end{array}\right) = \left(\begin{array}{c} 2\ell \\ \ell-j \end{array}\right). \quad (A.5)$$

This completes our proof, since by calling $y = x_{2\ell+1}$ our expression (A.3) is nothing but (3.42). In an entirely analogous way it is possible to obtain (3.41) starting with (3.42).

B Alternative formulae

In this section, we re-write formulae (3.54), (3.55), (4.6), (5.15) and (5.16). These are obtained using $\delta(\theta) = \int \frac{d\mu}{2\pi} e^{i\mu\theta}$ and shifting all contours in θ back to the real line. The results involve less and more symmetric multiple integrals, which is useful for numerical computations or exact evaluation of the integrals with the help of a symbolic mathematics computer application (like Maple or Mathematica).

With

$$
\begin{aligned}
A^e_\ell(\mu) &= \left(\begin{array}{c} 2\ell-2 \\ \ell-1 \end{array}\right) - \sum_{j=1}^{\ell}\sum_{k=1}^{j-1}\sum_{q=\pm}\left(\begin{array}{c} 2\ell-1 \\ \ell-j \end{array}\right)(-1)^j e^{\pi\mu q(j-k)} \\
A^o_\ell(\mu) &= \sum_{j=1}^{\ell}\sum_{k=1}^{j}\sum_{q=\pm}\left(\begin{array}{c} 2\ell \\ \ell-j \end{array}\right)(-1)^j q e^{\pi\mu q(j-k+1/2)},
\end{aligned}
\tag{B.1}
$$

we have

$$
\begin{aligned}
s_{2\ell}(t,\kappa) &= \frac{\pi^2(-1)^\ell}{2\ell}\int_{-\infty}^{\infty}\frac{d\mu}{2\pi}\left[\prod_{k=1}^{2\ell}\int_{-\infty}^{\infty}\frac{d\theta_k e^{-t\cosh\theta_k}R\left(\frac{i\pi}{2}-\theta_k\right)}{4\pi\cosh\frac{\hat\theta_{k,k+1}}{2}}\right]A^e_\ell(\mu)e^{i\mu\theta} \\
s_{2\ell+1}(t,\kappa) &= \frac{\pi^2(-1)^\ell}{2\ell+1}\int_{-\infty}^{\infty}\frac{d\mu}{2\pi}\left[\prod_{k=1}^{2\ell+1}\int_{-\infty}^{\infty}\frac{d\theta_k e^{-t\cosh\theta_k}R\left(\frac{i\pi}{2}-\theta_k\right)}{4\pi\cosh\frac{\hat\theta_{k,k+1}}{2}}\right]A^o_\ell(\mu)e^{i\mu\theta} \\
e_\ell(rm) &= \frac{\pi^2(-1)^\ell}{\ell}\int_{-\infty}^{\infty}\frac{d\mu}{2\pi}\left[\prod_{k=1}^{2\ell}\int_{-\infty}^{\infty}\frac{d\theta_k e^{-rm\cosh\theta_k}}{4\pi\cosh\frac{\hat\theta_{k,k+1}}{2}}\right]A^e_\ell(\mu)e^{i\mu\theta} \\
c_{2\ell}(\kappa) &= \frac{\pi^2(-1)^\ell}{2\ell}\int_{-\infty}^{\infty}\frac{d\mu}{2\pi}\left[\prod_{k=1}^{2\ell}\int_{-\infty}^{\infty}\frac{d\theta_k}{4\pi\cosh\frac{\hat\theta_{k,k+1}}{2}}\right]\left(\prod_{k=1}^{2\ell}R\left(\frac{i\pi}{2}-\theta_k\right)-1\right)A^e_\ell(\mu)e^{i\mu\theta} \\
c_{2\ell+1}(\kappa) &= \frac{\pi^2(-1)^\ell}{2\ell+1}\int_{-\infty}^{\infty}\frac{d\mu}{2\pi}\left[\prod_{k=1}^{2\ell+1}\int_{-\infty}^{\infty}\frac{d\theta_k R\left(\frac{i\pi}{2}-\theta_k\right)}{4\pi\cosh\frac{\hat\theta_{k,k+1}}{2}}\right]A^o_\ell(\mu)e^{i\mu\theta}.
\end{aligned}
\tag{B.2}
$$

C Scaling dimension from the form factor expansion of the bulk two-point function

The scaling dimension of branch-point twist fields was evaluated from their two-particle form factors, along with the known form factors of the trace of the stress-energy tensor, for arbitrary $n > 1$ in [6] using the Δ-sum rule [40]. This gave an exact result (in agreement with the CFT result), because in free models, the stress-energy tensor does not have form factors with more than two particles. The scaling dimension can also be recovered from the two-point function of twist fields themselves, by analysing its short-distance behaviour. This is not as convenient, however, since it involves re-summing an infinite number of terms, which contain more and more integrals (all form-factor contributions), and usually it is superfluous, since the Δ-sum rule already gives the scaling dimension. But in our case, it is cornerstone check, because the correct analytic continuations in n of higher-particle contributions to the two-point function of twist fields necessitated a non-trivial choice of integration contours, a problem which did not occur for the two-particle contribution.

The most convenient way to evaluate the scaling dimension from the form factor expansion of the two-point function in free models is to take the logarithm, so that we are looking for the coefficient of the small distance logarithmic divergency. Using the fact that all form factors can be evaluated using Wick's theorem, the logarithm of the two-point function is just the sum of all connected contributions. The analytic continuation in n of connected form factor contributions was obtained in (3.44). Using the same symmetry arguments as in section 4 in order to count the number of connected contributions of a given particle number, we find

$$\log\left(\frac{\langle 0|\tilde{\mathcal{T}}(r)\mathcal{T}(0)|0\rangle}{\langle\mathcal{T}\rangle^2}\right) = \sum_{\ell=1}^{\infty}\frac{1}{2\ell}\left[\prod_{j=1}^{2\ell}\int\frac{d\theta_j}{2\pi}e^{-rm\cosh\theta_j}\right]u_\ell(\theta_1,\ldots,\theta_{2\ell}) \tag{C.1}$$

where $u_\ell(\theta_1,\ldots,\theta_{2\ell})$ is n times the right-hand side of (3.44).

As in sub-section 5.1, it is possible to obtain the small-rm logarithmic divergency by integrating out the $\theta_{2\ell}$ variable, after the change of variables to the set $x_j = \hat{\theta}_{j,j+1}$, $j = 1,\ldots,2\ell-1$ and $\theta_{2\ell}$. Separating into even and odd-indexed x variables and using Fourier transform, we can evaluate all remaining integrals in a similar fashion to what was done in section 5.1. In fact, it is convenient to shift back all contours in (3.44) to unshifted contours, picking up residues. The contribution to $u_\ell(\theta_1,\ldots,\theta_{2\ell})$ of the sum of all unshifted contours is simply

$$\frac{n(-1)^\ell 2i\sinh\theta}{\prod_{j=1}^{2\ell}2\cosh\frac{\hat{\theta}_{j,j+1}}{2}}\sum_{j=1}^{\ell}\left(\begin{array}{c}2\ell-1\\ \ell-j\end{array}\right)F_\ell(\theta) \tag{C.2}$$

where $\theta = \sum_{j=1}^{2\ell}\theta_j$ and

$$F_\ell(\theta) = K(2\theta+(2j-1)i\pi)+K(2\theta-(2j-1)i\pi). \tag{C.3}$$

For the coefficient of $-\log rm$ this gives a contribution

$$\sum_{\ell=1}^{\infty}\frac{2ni}{(2\pi)^4\ell}\int_{-\infty}^{\infty}dyF_\ell(y)G_\ell^2(y)\sinh y \tag{C.4}$$

where

$$G_\ell(y) = \int_{-\infty}^{\infty}\frac{da}{2\pi}\frac{\pi^\ell e^{iay}}{\cosh^\ell a\pi}. \tag{C.5}$$

The sum of the residues taken when unshifting the contours gives the following corrections to this contribution:

$$\sum_{\ell=1}^{\infty}\sum_{j=1}^{\ell}\sum_{k=1}^{[j/n]}\sum_{q=\pm}{}'\frac{in(-1)^{k+\ell+1}}{8\pi\ell}\left(\begin{array}{c}2\ell-1\\ \ell-j\end{array}\right)\sinh\left(\left(nk-j+\frac{q+1}{2}\right)i\pi\right)\times$$
$$\times\mathrm{Re}\left(J_\ell^2\left(nk-j+\frac{q+1}{2}\right)\right) \tag{C.6}$$

where $[\cdot]$ means the integer part, and the function $J_\ell(a)$ was evaluated in (5.7). Here, the sum over q is restricted as follows:

$\sum_{q=\pm}{}'$: for $k=[j/n]$, the term with $q=+1$ is present if and only if $n[j/n]<j-1$.

The sum of (C.4) and (C.6) should be compared with $4\Delta_n = (n-1/n)/12$.

Taking about 30 terms in the sums over ℓ in both (C.4) and (C.6) and adding up both contributions gives the following numerical values, for n between 1 and 3 (see fig. 4):

n	1	1.1	1.2	1.3	1.4	1.5	1.6
$4\Delta_n$ exact	0	0.01591	0.03056	0.04423	0.05714	0.06944	0.08125
$4\Delta_n$ approx.	0	0.01583	0.03047	0.04417	0.05710	0.06941	0.08123

n	1.7	1.8	1.9	2	2.1	2.2	2.3
$4\Delta_n$ exact	0.09265	0.10370	0.11447	0.125	0.13532	0.14545	0.15543
$4\Delta_n$ approx.	0.09264	0.10370	0.11447	0.12500	0.13532	0.14545	0.15543

n	2.4	2.5	2.6	2.7	2.8	2.9	3
$4\Delta_n$ exact	0.16528	0.175	0.18462	0.19414	0.20357	0.21293	0.22222
$4\Delta_n$ approx.	0.16530	0.17499	0.18464	0.19415	0.20358	0.21293	0.22192

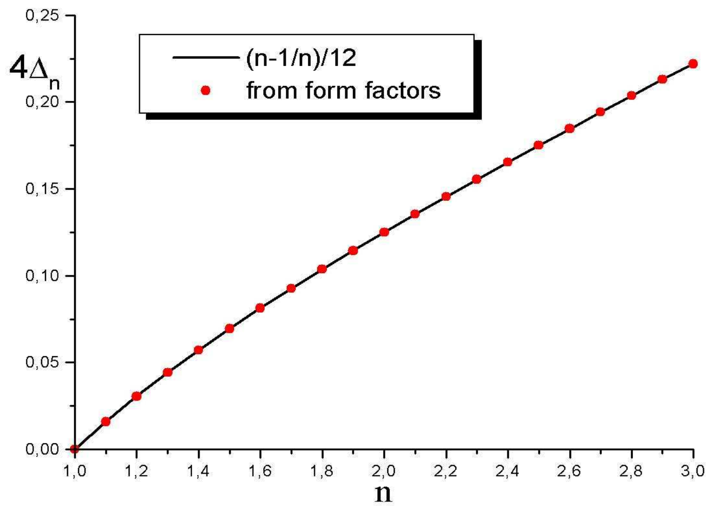

Figure 4: The exponent in the short-distance behaviour of the bulk two-point function, as function of the number of sheets n analytically continued to $n \geq 1$. This should be twice the scaling dimension, and the curve shows the expected value from CFT. The data points come from a re-summation of about 30 terms in the form factor expansion for the logarithm of the two-point function. For $n > 2$, an improvement using Euler's formula is needed in order to make the series convergent.

The corrections (C.6) are exactly zero when n is an integer: in these cases, no contour shift is necessary from the beginning. However, the numerical evaluation of (C.4) shows that this contribution is insufficient to reproduce the correct dimension formula for non-integer n, showing the necessity of the contour shifts. It is also interesting to note that the sum over ℓ in (C.4) is in fact a divergent alternating sum for $n > 2$. One can however make it convergent by using Euler's formula for improving convergence of alternating sums:

$$\sum_{\ell=1}^{\infty} a_\ell = \sum_{\ell=1}^{\infty} 2^{-\ell} b_\ell \ , \quad b_\ell = \sum_{k=1}^{\ell} \left(\begin{array}{c} \ell - 1 \\ k - 1 \end{array} \right) a_k. \tag{C.7}$$

The rationale behind this is that the sum is in fact convergent for any $rm > 0$, where Euler's formula can be used, which then gives a finite limit as $rm \to 0$.

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