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THE THERMODYNAMICS OF PURELY ELASTIC SCATTERING THEORIES AND CONFORMAL PERTURBATION THEORY

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We discuss the thermodynamic Bethe ansatz, and explain how it allows one to reduce the infinite-volume thermodynamics of a (1 + 1)-dimensional purely elastic scattering theory to the solution of a set of integral equations for the one-particle excitation energies. The free energy at zero chemical potential(s) and temperature T is related to the ground state energy $E_0(R)$ of the theory on a cylinder of circumference $R = 1/T$. $E_0(R)$ determines properties of the CFT describing the UV limit of the given massive theory. These include the central charge (which we investigated in earlier work), the scaling dimension d of the conformal field whose perturbation leads to the massive theory, the coefficients in the conformal perturbation theory (CPT) expansion of $E_0(R)$ in powers of R^{2-d}, and the bulk term in the CPT calculation of the ground-state energy. We determine the bulk term analytically, and obtain numerically the first six coefficients in the expansion of $E_0(R)$ for many purely elastic scattering theories, including the scaling limit of the $T = T_c$ Ising model in a magnetic field. The perfect agreement with (more limited) direct CPT results provides further strong support for the identification of these theories as specific perturbed CFTs. We suggest that the singularities of $E_0(R)$, the first of which is responsible for the finite radius of convergence of CPT, are square-root branch points and related to the zeros of the partition function of the corresponding lattice model.

1. Introduction and summary

Recent progress in (1 + 1)-dimensional quantum field theory (QFT) includes the discovery of many new integrable massive QFTs [1–14]. This was possible due to an interplay and convergence of several ideas. One of these, initiated by A.B. Zamolodchikov [1, 2], is to consider a massive QFT as a certain relevant perturbation of the conformal field theory (CFT) describing its UV limit. Since such a perturbation corresponds to a super-renormalizable interaction in standard QFT

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language, it is assumed that there is a one-to-one correspondence between the fields in the CFT and those in the perturbed massive theory. Recall that there are infinitely many chiral fields in a CFT, i.e. (anti)holomorphic currents, that give rise to infinitely many integrals of motion. Zamolodchikov gave a sufficient condition, now know as the "counting argument", to determine if some combination(s) of integrals of motion of a given Lorentz spin survive the perturbation of the CFT. If some do survive, and if the perturbed theory is purely massive, as one can argue in many cases, then it must be describable by a factorizable S-matrix. The values of the Lorentz spins of the integrals of motion restrict the possible bound-state structure and mass ratios in the theory. The bootstrap principle [2, 15, 16] then allows one to actually construct a conjecture for the S-matrix of the theory, in the process discovering its particle content (see ref. [3] and sect. 2 for more details). Especially the last step involves several assumptions that are difficult to justify from the pure S-matrix or perturbed CFT poit of view, beyond the fact that they lead to self-consistent results. In particular, there are usually ambiguous factors in the S-matrix elements – two-dimensional CDD factors [17] with unphysical poles.

To check these conjectures for the S-matrices another idea proves to be very useful. It has been known for a long time [18] that the infinite-volume thermodynamics of a massive QFT can be expressed solely in terms of its S-matrix. In addition, in a euclidean formulation it is obvious (see sect. 4) that the free energy of a theory on an infinite line at temperature T and zero chemical potential(s) is related in a simple way to the ground-state energy $E_0(R)$ of the same QFT on a periodic space of length $R = 1/T$*, i.e. on an infinitely long cylinder. Therefore $E_0(R)$ can also be calculated in terms of S-matrix data. Now the point is that $E_0(R)$ contains information about the CFT describing the UV limit of the given massive theory. Explicitly, normalizing the ground-state energy to vanish as $R \to \infty$, it must be of the form

$$E_0(R) = -\frac{\pi \tilde{c}(r)}{6R}, \tag{1}$$

where $\tilde{c}(r)$ is a function of $r \equiv Rm$ (m being, say, the smallest mass in the theory) which vanishes at infinity. (This simple scaling behaviour holds for all the theories considered in this paper, as they are each characterized by a single dimensionful coupling.) $\tilde{c}(0)$ is known [19, 20] to be equal to $\tilde{c} \equiv c - 12d_0$, where c is the central charge and d_0 the lowest scaling dimension of the UV CFT. The small-r expansion of $\tilde{c}(r)$ also allows one to extract the scaling dimension d_Φ of the conformal field Φ by which one has to perturb the UV CFT to obtain the massive theory in question. Furthermore, the coefficients in the expansion can be calculated in conformal perturbation theory (CPT) – until one or one's computer is exhausted.

* We set $\hbar$, c, and Boltzmann's constant equal to 1 in this paper.

which is usually the case after the first or second term – and compared with the corresponding results obtained by the above method (where several more coefficients can be calculated numerically before exhaustion occurs).

This method, when applied to a factorizable S-matrix theory, has recently become known as the *thermodynamic Bethe ansatz* [21] (TBA). So far, the TBA has achieved extensive use [3, 21, 22] only for theories with a diagonal S-matrix, also known as *purely elastic scattering theories* (we will say more about these theories shortly). For such theories the TBA can be applied in a straightforward and explicit way, as we will see.

If the application of the TBA to a conjectured S-matrix leads to values of $\tilde{c}$ and d_Φ which are those of the CFT whose perturbation is supposed to give rise to the scattering theory in question, this provides very strong evidence that the conjectured S-matrix is correct. The previously mentioned ambiguous factors in the S-matrices can be fixed in this way [3]. Note that the consistency of the TBA with CFT requirements might also be considered as a posteriori evidence for the assumption underlying the whole perturbed-CFT approach, namely that the somewhat formal procedure of perturbing a CFT really leads to consistent QFTs. Conversely, if a given S-matrix does *not* lead to "reasonable" fractions for $\tilde{c}$ and d_Φ, the S-matrix is presumably not that of any consistent QFT. (This seems to be the case for some of the scattering theories discussed in ref. [8], which were already problematic on the pure S-matrix level.)

Al.B. Zamolodchikov [21] first calculated $\tilde{c}(r)$ for the perturbed Yang–Lee CFT and the scaling 3-state Potts model (whose $\tilde{c}(r)$ functions just differ by a factor of 2, cf. below). We then [3] calculated $\tilde{c}(0)$ for many classes of purely elastic scattering theories, clarifying some issues in their identification as perturbed CFTs. The purpose of this paper is to extend these works in two directions. On the one hand, we want to clarify the physical basis of the TBA and show how it allows one to calculate the general thermodynamics (i.e. at arbitrary chemical potentials) of a purely elastic scattering theory. This does not require a large extension of earlier work; nevertheless, because of the conceptual importance of being able to reduce the complete thermodynamics of a class of nontrivial interacting QFTs to simple integral equations, we felt it is worthwhile to present these considerations. Secondly, we perform extensive analytical and numerical studies of $\tilde{c}(r)$ for the (minimal, see below) purely elastic scattering theories considered in ref. [3], further supporting the identification of these theories as perturbations of specific CFTs. These studies also allow us to gain some insight into the singularity structure of $\tilde{c}(r)$.

Before giving an outline of the paper, let us say a few words about purely elastic scattering theories. In table 1 we have summarized important data of the purely elastic scattering theories we will consider. They are all related to some affine Lie algebra $\hat{\mathscr{G}}$ (listed in the first column), in that the Lorentz spins of the integrals of motion in a given S-matrix theory are the exponents of the corresponding affine

TABLE 1
Data of the perturbed CFTs and S-matrices considered

$\hat{\mathscr{G}}$	UV CFT	$\bar{c}$	y	A_{11}	Refs.
$A_n^{(1)}$	Z_{n+1} parafermions	$\frac{2n}{n+3}$	$\frac{2(n+1)}{n+3}$	$\left\{\frac{2}{n+1}\right\}$	[1, 27]
$A_{2n}^{(2)}$	$M_{2,2n+3}$	$\frac{2n}{2n+3}$	$\frac{4(2n+1)}{2n+3}$	$\left\{\frac{2}{2n+1}, \frac{2n-1}{2n+1}, 1\right\}$	[4–6]
$D_n^{(1)}$	$r_{\text{orb}} = \sqrt{n/2}$ orbifold	1	$\frac{2(n-1)}{n}$	$\left\{\frac{1}{n-1}, \frac{n-2}{n-1}, 1\right\}$	[3, 10]
$E_6^{(1)}$	Tricritical 3-st. Potts	$\frac{6}{7}$	$\frac{12}{7}$	$\left\{\frac{1}{6}, \frac{1}{2}, \frac{2}{3}\right\}$	[7, 11]
$E_7^{(1)}$	Tricritical Ising	$\frac{7}{10}$	$\frac{9}{5}$	$\left\{\frac{1}{9}, \frac{4}{9}, \frac{5}{9}, \frac{8}{9}, 1\right\}$	[5, 7, 8]
$E_8^{(1)}$	Critical Ising	$\frac{1}{2}$	$\frac{15}{8}$	$\left\{\frac{1}{15}, \frac{1}{3}, \frac{2}{5}, \frac{3}{5}, \frac{2}{3}, \frac{14}{15}, 1\right\}$	[2]

Lie algebra. In addition, the number of particles in the $\hat{\mathscr{G}}$-related theory is equal to the rank of $\hat{\mathscr{G}}$ (except for the somewhat special $A_{2n}^{(2)}$-related theories, which have n particles). Further relations of the masses and integrals of motion to the affine Lie algebra will be mentioned in sect. 2.

Actually there are two purely elastic scattering theories related to each Lie algebra, differing by CDD factors with unphysical poles. We will only consider the so-called *minimal* S-matrix theories where the additional CDD factors are absent (more in sect. 2). These theories are perturbations of nontrivial CFTs, which are indicated in column 2 of table 1. Besides the well-known CFTs indicated explicitly by name, note that some other familiar (perturbed) CFTs are hiding in this table: The thermal perturbation of the critical Ising model leads to the $A_1^{(1)}$-related model (the "Ising field theory", see sect. 6), the perturbation of the critical 3-state Potts model by the energy operator is described by the $A_2^{(1)}$-related theory [1], and the unique perturbation of the Yang–Lee CFT $M_{2,5}$* (which describes [23] the universality class of the Yang–Lee edge singularity [24, 25] in two dimensions) leads to the $A_2^{(2)}$-related theory.

We should also mention that the S-matrix of the $D_n^{(1)}$-related model differs from that of the sine-Gordon model, at the special value of the coupling where the $(n-1)$th breather is at threshold, only by the sign of some scattering matrix elements (see ref. [3] for a detailed discussion). This implies (cf. sect. 3) that these theories have the same infinite volume thermodynamics. The S-matrices of the models labelled by $A_{2n}^{(1)}$ and $A_{2n}^{(2)}$ are also closely related [3]. To each of the n particles in the $A_{2n}^{(2)}$-related theory there corresponds a particle and an anti-particle in the $A_{2n}^{(1)}$-related model. From the explicit S-matrices and the discussion in

* $M_{p,q}$ denotes the Virasoro minimal model with central charge $c = 1 - 6(p-q)^2/pq$ and diagonal modular invariant partition function.

sect. 3 below, one sees that the free energies of the two theories just differ by a factor of 2, if each member of a triplet of related particles in the two theories has the same chemical potential (note that a particle and its anti-particle can have identical chemical potentials in a purely elastic scattering theory since *all* particle numbers are strictly conserved; there is no pair creation or annihilation). In particular, setting all chemical potentials to 0, the $\tilde{c}(r)$ functions of these two theories are equal up to a factor of 2.

Recent work [14] suggests that the relation of the S-matrix theories of table 1 to affine Lie algebras can be understood as part of a larger picture in which integrable massive QFTs (generically with non-diagonal S-matrix) are associated to certain cosets of affine Lie algebras. Note that the S-matrix theories related to $A^{(2)}_{2n}$ are somewhat special. They are the only ones related to *twisted* affine algebras, and they are also the only ones which are perturbations of *non-unitary* [26] CFTs, namely the Virasoro minimal models $M_{2,2n+3}$. These scattering theories have been argued [6] to correspond to "restrictions" of the sine-Gordon model at special values of the coupling, where the solitons can be consistently eliminated from the spectrum of the theory. In terms of the "larger picture" alluded to above one might therefore consider these theories to be related to $A^{(1)}_1$, rather than $A^{(2)}_{2n}$, since the sine-Gordon model is the $A^{(1)}_1$ affine Toda theory with purely imaginary coupling.

$\tilde{c} \equiv c - 12d_0$ is presented in the third column of the table. For the non-unitary CFTs the scaling dimension d_0 of the field creating the ground state is negative, and so their $\tilde{c}$ is larger than their central charge; in particular, these $\tilde{c}$ are just one half those of the $A^{(1)}_{2n}$-related theories, in agreement with our earlier remarks about the $\tilde{c}(r)$ functions in these theories. The fourth column contains the renormalization group eigenvalue y of the perturbing field Φ, i.e. $y = 2 - d_\Phi$. Note that the perturbations we are considering are strongly relevant: $0 < d_\Phi \leq 1$ for all perturbations of unitary theories, and $-2 < d_\Phi < 0$ for the perturbations of the non-unitary models $M_{2,2n+3}$.

In the fifth column we give the set A_{11} of rational numbers which characterizes the S-matrix element describing the scattering of the lightest particles in the theory (if there are several species of lightest particles one can pick any one of them as "the lightest particle"). A_{11} will be defined in sect. 2. Finally, the last column contains the references in which the S-matrix of a theory was first presented and/or identified as a perturbed CFT. The reader should consult these references for the explicit form of the S-matrix elements; we of course use them in our numerical calculations of $\tilde{c}(r)$. (The $A^{(1)}_n$-, $A^{(2)}_{2n}$-, and $D^{(1)}_n$-related S-matrices are given in ref. [3] in the same notation as used here.)

The paper is organized as follows. In sect. 2 we present some details of the general structure of the scattering matrix elements of purely elastic scattering theories; in particular, we derive some properties of the phase shifts in these theories, eqs. (13), (14) and (17), which will be needed later. In sect. 3 we explain

how the TBA allows one to reduce the calculation of the complete infinite-volume thermodynamics of a purely elastic scattering theory (in its low-density phase) to the solution of a set of coupled nonlinear integral equations for the one-particle excitation energies. We will see that, roughly speaking, the thermodynamics of a purely elastic scattering theory is identical to that of a free theory, except that one has to use a nontrivial dispersion relation determined by the above integral equations. In sect. 4 we turn to the study of $\tilde{c}(r)$, by relating it to the free energy of the previous section, at zero chemical potential. We show that the leading correction to $\tilde{c}(0)$ is an r^2-term (corresponding to a bulk term in $E_0(R)$) whose coefficient can be expressed very simply in terms of S-matrix data, cf. eq. (65). Higher-order corrections are discussed in sect. 5, where we use CPT to show that these corrections take the form of a power series in $r^{\tilde{y}}$. Here

$$\tilde{y} = \begin{cases} 2y \\ y \end{cases}, \quad \text{if the UV CFT is} \quad \begin{cases} \text{unitary} \\ \text{non-unitary} \end{cases}. \tag{2}$$

We also calculate the first nontrivial coefficient of the CPT expansion analytically, and the second coefficient numerically in several cases. Sect. 6 is devoted to scattering theories with constant phase shifts, e.g. free theories or the Ising field theory. In these cases we have integral representations for $\tilde{c}(r)$ and can rewrite them to explicitly exhibit the singularity structure of the $\tilde{c}(r)$ and analytically obtain all the coefficients in their small-r expansions. This will be instructive and useful on several occasions. For instance, we use these results to supplement those of refs. [28,29] to give compact and illuminating expressions for the partition functions of free fermions, free bosons, and the Ising field theory in *finite* volume.

Our numerical work is presented in sect. 7. We numerically solve the TBA integral equations for the one-particle excitation energies to high precision, and calculate $\tilde{c}(r)$ for many different scattering theories. (For the important case of the magnetic perturbation of the Ising model at its critical temperature, the $E_8^{(1)}$-related theory, we present some of the calculated $\tilde{c}(r)$ values in table 2.) From the $\tilde{c}(r)$ data we extract $\tilde{y}$ (table 3) and six of the coefficients in the expansion of $\tilde{c}(r)$ in powers of $r^{\tilde{y}}$ (table 4). These results are in perfect agreement with predictions of CPT (whenever available), as can be seen in table 5 where we compare the TBA prediction for the second coefficient with the CPT result. This comparison is possible after obtaining the coefficient κ relating the perturbing parameter λ of CPT to the power $m_1^{\tilde{y}}$ of the lightest mass in the theory. κ is also given in table 5. Finally, we estimate the form and position of the first singularity of $\tilde{c}(r)$, which determines the finite, nonzero radius of convergence of (IR cutoff) CPT. The numerical results indicate (table 6) that these singularities are square-root branch points. This will be explained in sect. 8, where we show that the singularities of the eigenvalues of the perturbed CFT hamiltonian are a consequence of level-crossing at complex values of λ. We also outline a perhaps somewhat more physical way to

understand the singularities of $\tilde{c}(r)$ by providing evidence that they are related to the zeros of the partition function of the corresponding lattice model close to the critical point. The last section contains brief concluding remarks.

2. Purely elastic scattering theories

We briefly summarize the basic aspects of purely elastic scattering theories which will be used in later sections. For more details, including some slightly subtle issues that will not be mentioned here, we refer the reader to ref. [3].

We define *a purely elastic scattering theory* to be a (1 + 1)-dimensional QFT whose S-matrix is factorizable and diagonal. Factorizability means that the scattering amplitudes of any number of particles can be written as products of the two-particle amplitudes. Even though a diagonal factorizable S-matrix automatically satisfies the Yang–Baxter equation, this does not mean that the S-matrix is trivial, because it can have a highly complicated bound-state structure.

The scattering of particles a and b is described by the two-particle scattering amplitude S_{ab}, which is a function of the relative rapidity $\theta_{ab} = |\theta_a - \theta_b|$. Recall that the rapidity θ provides a convenient way of parametrizing the momentum of a particle in 1 + 1 dimensions. It is defined by

$$(p^0, p^1) = (m\cosh\theta, m\sinh\theta)\,. \tag{3}$$

In an obvious notation for states, the definition of $S_{ab}(\theta)$ reads

$$|a(\theta_a)b(\theta_b)\rangle_{\text{in}} = S_{ab}(\theta_{ab})|a(\theta_a)b(\theta_b)\rangle_{\text{out}}\,. \tag{4}$$

Note that $S_{ab}(\theta)$ is (for real, i.e. physical, rapidities) just the exponential of the phase shift of the in- with respect to the out-state, $S_{ab}(\theta) = \mathrm{e}^{i\delta_{ab}(\theta)}$.

When S_{ab} is expressed as a function of θ, the requirements of real analyticity, unitarity, and crossing read

$$\begin{aligned} &\text{Real analyticity:} && S^*_{ab}(\theta) = S_{ab}(-\theta^*)\,,\\ &\text{Unitarity:} && S_{ab}(\theta)S_{ab}(-\theta) = 1\,,\\ &\text{Crossing:} && S_{a\bar{b}}(\theta) = S_{ab}(i\pi - \theta)\,, \end{aligned} \tag{5}$$

where $\bar{b}$ denotes the antiparticle of b. Assuming, in addition, that scattering amplitudes are meromorphic in θ and polynomially bounded in the momenta then implies [3] that they are products of basic building blocks:

$$S_{ab}(\theta) = \prod_{\alpha\in\mathbf{A}_{ab}} f_\alpha(\theta)\,, \tag{6a}$$

where

$$f_\alpha(\theta) = \sinh \tfrac{1}{2}(\theta + i\alpha\pi)/\sinh \tfrac{1}{2}(\theta - i\alpha\pi)\,. \tag{6b}$$

Note that these building blocks are just two-dimensional CDD factors [17]. If all particles are stable, as we will assume, the numbers α constituting the sets A_{ab} are real, and we can choose $-1 < \alpha \leqslant 1$.

For $\alpha \neq 0, 1$ $f_\alpha(\theta)$ has a simple pole at $\theta = i\alpha\pi$, and a simple zero at $\theta = -i\alpha\pi$. We see that purely elastic scattering theories are nontrivial only because of these poles (paired with zeros via unitarity, eq. (5)), and are uniquely determined by the positions and orders of the poles, as encoded in the sets A_{ab}.

In this paper we will concentrate on purely elastic scattering theories which are perturbations of nontrivial CFTs (i.e. not a collection of free bosons). In these S-matrix theories the poles of all scattering amplitudes occur exclusively in the physical strip $0 < \operatorname{Im} \theta_{ab} < \pi$. The corresponding S-matrices are known as *minimal* S-matrices, as there exists a unique [3], one-parameter deformation of each of these theories whose scattering matrix elements have additional factors of $f_\alpha(\theta)$ with negative α. These latter *nonminimal* S-matrices are very likely [3, 8, 9, 30] those of (real-coupling) affine Toda field theories [31], with the one parameter of the deformation corresponding to the coupling constant of the Toda theories. The UV limits of (real-coupling) affine Toda field theories are free bosonic CFTs [3].

Unless otherwise stated, we will from now on restrict ourselves to minimal S-matrix theories. In such theories a simple pole of $S_{ab}(\theta)$ at $\theta_{ab} = iu^c_{ab}$ in the direct channel indicates that there exists a bound state c of a and b whose mass is

$$m_c^2 = m_a^2 + m_b^2 + 2m_a m_b \cos u^c_{ab}\,. \tag{7}$$

More generally, it seems [3, 8] that in the minimal S-matrix theories a particle appearing as *any* odd-order pole in the direct channel of a scattering amplitude should be considered to be a bound state. (In the nonminimal S-matrix theories on the other hand, one can argue [3] that *none* of the poles should be considered to be bound-state poles in any literal sense.)

The factorization of scattering amplitudes on simple poles implies that if c appears as a simple pole of $S_{ab}(\theta)$ (in the direct channel), its scattering amplitude with any other particle d must satisfy the *bootstrap equation* [2]

$$S_{cd}(\theta) = S_{ad}(\theta + i\bar{u}^{\bar{b}}_{a\bar{c}})S_{bd}(\theta - i\bar{u}^{\bar{a}}_{b\bar{c}})\,, \tag{8}$$

where $\bar{u}^c_{ab} \equiv \pi - u^c_{ab}$. This fundamental equation allows one to actually construct a purely elastic scattering theory once one knows – or has a conjecture for – the scattering amplitudes of the one or two fundamental particles (see ref. [3] for details). It is possible [2] to make a plausible conjecture for the amplitudes of the

fundamental particles, based on the knowledge of some of the (Lorentz) spins of the integrals of motion of the scattering theory.

If we assume that the conserved charges of a purely elastic scattering theory are local and diagonal on asymptotic one-particle states, then Lorentz covariance dictates that a conserved charge Q_s of spin s acts on an N-particle (asymptotic) state as follows:

$$Q_s|a_1(\theta_1)\dots a_N(\theta_N)\rangle = \sum_{i=1}^{N} \gamma_{a_i}^{(s)} e^{s\theta_i}|a_1(\theta_1)\dots a_N(\theta_N)\rangle, \tag{9}$$

where the $\gamma_{a_i}^{(s)}$ are some (real) coefficients. Note that for $s = 1$, corresponding to energy–momentum conservation, the $\gamma_a^{(s)}$ are just the masses m_a in the theory, up to an arbitrary overall factor.

If we require eq. (9) also to hold for imaginary values of the rapidities, corresponding to bound-state poles in certain channels, the statement "c is a bound state of a and b" leads to the following consistency condition [2] on the coefficients $\gamma_a^{(s)}$:

$$\gamma_c^{(s)} = \gamma_a^{(s)} e^{-is\bar{\theta}_{ac}^{b}} + \gamma_b^{(s)} e^{is\bar{\theta}_{bc}^{a}}. \tag{10}$$

This equation determines each of the vectors $\gamma^{(s)} \equiv (\gamma_a^{(s)})$ up to an overall factor. (The subscript a here runs over the different particles in the model, which are uniquely associated [3, 5, 9, 10] to the nodes of the Dynkin diagram of the corresponding (ordinary) Lie algebra. We will always choose $a = 1$ to correspond to the lightest particle in the model.) In previous work [3] we found that it is possible to state the values of the $\gamma_a^{(s)}$ in all the Lie-algebra related S-matrix theories in a rather elegant and concise way*. Let $h_{\mathscr{G}}$ denote the Coxeter number of the ordinary Lie algebra $\mathscr{G}$. Then, if s (mod $h_{\mathscr{G}}$) is not an exponent of $\mathscr{G}$, $\gamma^{(s)}$ of the $\hat{\mathscr{G}}$-related minimal or nonminimal S-matrix theory vanishes. On the other hand, if s is an exponent of $\mathscr{G}$, the vector $\gamma^{(s)}$ is an eigenvector of the incidence matrix $I_{\mathscr{G}}$ of $\mathscr{G}$ corresponding to the eigenvalue $2\cos(\pi s/h_{\mathscr{G}})$. Furthermore, $\gamma^{(s)} = \gamma^{(2h_{\mathscr{G}}-s)} = \gamma^{(s+2h_{\mathscr{G}})}$. The case of $\hat{\mathscr{G}} = A_{2n}^{(2)}$ has to be treated slightly differently; the above is still true if we set $h_{\mathscr{G}} = \frac{1}{2}h_{\mathscr{G}} = 2n + 1$, let the exponents run over the first n exponents of $A_{2n}^{(2)}$, and use for $I_{\mathscr{G}}$ the "generalized incidence matrix" [3] obtained by replacing the last 0 on the diagonal of the incidence matrix of A_n by 1.

As pointed out in ref. [10], it is not an accident that eq. (10) has a structure similar to the bootstrap equation (8). The relation between these equations can be seen as follows. Let us introduce

$$\varphi_{ab}(\theta) = -i\frac{d}{d\theta}\ln S_{ab}(\theta) = \sum_{\alpha \in A_{ab}} \varphi_\alpha(\theta). \tag{11}$$

* H. Braden and E. Corrigan have informed us that this was also noticed by P. Dorey.

where we defined

$$\varphi_a(\theta) = -i\frac{\mathrm{d}}{\mathrm{d}\theta}\ln f_a(\theta) = -\frac{\sin\alpha\pi}{\cosh\theta - \cos\alpha\pi}\,. \tag{12}$$

For $\theta \neq 0$ we can expand

$$\varphi_{ab}(\theta) = -\sum_{k=1}^{\infty}\varphi_{ab}^{(k)}\mathrm{e}^{-k|\theta|}, \tag{13}$$

with (see ref. [32], formula 1.461(1))

$$\varphi_{ab}^{(k)} = 2\sum_{\alpha\in\mathrm{A}_{ab}}\sin(k\alpha\pi)\,. \tag{14}$$

Inserting this expansion into the (logarithmic derivative of the) bootstrap equation we obtain

$$\varphi_{cd}^{(k)} = \varphi_{ad}^{(k)}\mathrm{e}^{-ik\bar{u}_{ac}^{b}} + \varphi_{bd}^{(k)}\mathrm{e}^{ik\bar{u}_{bc}^{a}}\,. \tag{15}$$

Comparing with eq. (10) we see that the linearly independent columns and rows of the matrix $\varphi^{(k)} = (\varphi_{ab}^{(k)})$ provide solutions (although not always nontrivial ones, see below) for the vectors $\gamma^{(s)}$ defining the action of local conserved charges on asymptotic states.

From our foregoing description of the conserved charges we know that there are no nontrivial charges if their spin is not one of the exponents of the Lie algebra in question; so we conclude that $\varphi^{(k)} = 0$ if k is not among the exponents. We have also verified this directly using the scattering amplitudes of the minimal and nonminimal S-matrix theories. If k is among the exponents it may still happen that there exists a nontrivial conserved charge of spin $s = k$ and yet the matrix $\varphi^{(k)}$ is identically 0. This happens in the cases (i) $\hat{\mathscr{G}} = \mathrm{A}_n^{(1)}$, n odd, $s = \frac{1}{2}(n+1)$; (ii) $\hat{\mathscr{G}} = \mathrm{D}_n^{(1)}$, $s = n-1$; and (iii) $\hat{\mathscr{G}} = \mathrm{E}_7^{(1)}$, $s = 9$.

Except in these special cases the matrix $\varphi^{(s)}$ has rank one if s is an exponent, and each of its rows and columns is proportional to the unique vector $\gamma^{(s)}$. (The only cases where two conserved charges of the same spin exist are for $\hat{\mathscr{G}} = \mathrm{D}_n^{(1)}$, $s = n-1$ when n is even; and in these cases the matrix $\varphi^{(s)}$ is identically 0.) We therefore conclude that

$$\varphi_{ab}^{(s)} = \varphi_{11}^{(s)}\gamma_a^{(s)}\gamma_b^{(s)}\,. \tag{16}$$

Here "1" refers to the lightest particle in the theory, and we have normalized the $\gamma^{(s)}$ so that $\gamma_1^{(s)} = 1$ (one can check that $\gamma_1^{(s)} \neq 0$ in the cases where the matrix $\varphi^{(s)}$ is nontrivial.)

In particular – and this will be important in sect. 4 – for $s = 1$ this reduces to

$$\varphi_{ab}^{(1)} = \varphi_{11}^{(1)} \hat{m}_a \hat{m}_b \,, \tag{17}$$

where $\hat{m}_a = m_a/m_1$. $\varphi_{11}^{(1)}$ can be calculated from eq. (14) and the set A_{11} given in table 1.

3. The thermodynamic Bethe ansatz

In this section we explain how the thermodynamic Bethe ansatz (TBA) allows one to reduce the calculation of the complete infinite-"volume" thermodynamics of a purely elastic scattering theory (in its low density phase, in case it also has a high-density phase) to the solution of a set of coupled nonlinear integral equations for the one-particle excitation energies and the rapidity distributions of the particles in the theory.

The thermodynamic Bethe ansatz technique has two parts. The first is based on the observation that for a system of particles with purely elastic scattering the asymptotic wave function, i.e. the wave function when all particles are far apart, has a very simple form. Putting the system in a box and requiring (anti)periodic boundary conditions for the asymptotic wave function then leads to quantization conditions on the momenta of the particles of the interacting system, known as the Bethe ansatz equations. The second part of the TBA is just statistical mechanics: Going to the thermodynamic limit one determines the dominant microscopic configurations of the system consistent with a given set of macroscopic variables. The Bethe ansatz equations then lead to the previously mentioned nonlinear integral equations.

The method just outlined seems to have been rediscovered several times [21, 33, 34]. Note that the word "ansatz" in most of the various names that have been used for this method is somewhat misleading: As we have outlined above and will see in detail below, the TBA just follows from the fact that the scattering is purely elastic; no additional assumption or input are involved. In particular, it is not necessary to know the lagrangian or hamiltonian of the theory considered. It is therefore conceptually quite different from the usual Bethe ansatz [35], where one starts with some hamiltonian and in principle has to *prove* that the Bethe ansatz provides a complete set of eigenstates.

3.1. THE ASYMPTOTIC WAVE FUNCTION

Consider a purely elastic scattering theory on a circle of circumference L (as we will see, the TBA becomes exact only in the limit $L \to \infty$; so one should always think of L as being very large). Let there be n different species of particles in the theory, and consider N particles N_a of which are of species a, at positions

$x_1, \ldots, x_N$. We will first consider a microscopic description of the system, so we can talk about its wave function; in subsect. 3.2 we will pass to a macroscopic thermodynamic description.

Because the scattering is purely elastic, all particle momenta are asymptotically conserved, and when all particles are far apart (i.e. much farther than the correlation length $R_c = 1/m_1$) the wave function of the system must be of the form

$$\psi(x_1, \ldots, x_N) = \exp\left(i \sum_j p_j x_j\right) \sum_{Q \in S_N} A(Q)\Theta(x_Q), \tag{18}$$

to which we will refer as the *asymptotic wave function*. Here the second sum runs over the $N!$ permutations $Q \in S_N$ of the N particle positions on the line segment $[-L/2, L/2]$, and the $A(Q)$ are coefficients depending on the momenta of the particles, whose ordering on the line is specified by

$$\Theta(x_Q) = \begin{cases} 1 & \text{if } x_{Q_1} < \ldots < x_{Q_N}, \\ 0 & \text{otherwise} \end{cases} \tag{19}$$

Up to an irrelevant overall factor the coefficients $A(Q)$ are determined by the S-matrix of the theory. If the permutations $Q = (\ldots, i, j, \ldots)$ and Q' differ only by the exchange of i and j, then

$$A(Q') = S_{ij}(\theta_i - \theta_j) A(Q). \tag{20}$$

Since particle momenta are (asymptotically) conserved, we can consider the momentum of an (asymptotic) particle as part of the quantum numbers characterizing it. "Identical particles" are then also meant to have identical momenta. The requirement that the asymptotic wave function (18) be (anti)symmetric under the exchange of identical (fermions) bosons can then lead to restrictions on the allowed rapidities of the particles. (Had we required the appropriate symmetry properties under exchange of particles of the same species of *arbitrary* momenta, the form of the asymptotic wave function (18) would have been more complicated, without changing the physics.) To state these restrictions, let us define the *type* [21] of a particle of species a as $t_a = -(-1)^{F_a} S_{aa}(\theta = 0)$, where $(-1)^{F_a} = \pm 1$ indicates if the particle is a boson or fermion, respectively. We will refer to particles of type $t_a = \pm 1$ as fermionic and bosonic type particles, respectively. It is then easy to see [21] that fermionic type particles of the same species are not allowed to have the same rapidity – i.e. obey an exclusion principle – whereas there is no restriction for bosonic type particles. Since it seems likely (cf. refs. [3] and references therein) that in a consistent, interacting QFT all particles are of fermionic type, we will concentrate on this case in the following. It is easy to make the appropriate changes for bosonic type particles (see refs. [3, 21]), if desired.

Let us return to the asymptotic wave function. Imposing periodic (anti-periodic) boundary conditions for bosons (fermions)*,

$$\psi(\ldots, x_i = -\tfrac{1}{2}L, \ldots) = (-1)^{F_i}\psi(\ldots, x_i = \tfrac{1}{2}L, \ldots) \qquad \text{for } i = 1, 2, \ldots, N, \quad (21)$$

leads to

$$A(i, Q_2, \ldots, Q_N) = (-1)^{F_i} e^{ip_iL} A(Q_2, \ldots, Q_N, i) \quad (22)$$

for any $Q \in S_N$ such that $Q_1 = i$. From eqs. (20) and (22) we now conclude that

$$\exp[iLm_i \sinh\theta_i] \prod_{j:\, j \neq i} S_{ij}(\theta_i - \theta_j) = (-1)^{F_i} \qquad \text{for } i = 1, 2, \ldots, N. \quad (23)$$

↳ contém interacções entre partículas de diferentes espécies

In terms of the phase shifts $\delta_{ij}(\theta_i - \theta_j) = -i \ln S_{ij}(\theta_i - \theta_j)$, the logarithm of this equation leads to a set of coupled transcendental equations for the rapidities, known as the *Bethe ansatz equations*:

$$Lm_i \sinh\theta_i + \sum_{j:\, j \neq i} \delta_{ij}(\theta_i - \theta_j) = 2\pi n_i \qquad \text{for } i = 1, 2, \ldots, N. \quad (24)$$

The $\{n_i\}$ can be considered to be the quantum numbers of the state of the multi-particle system; n_i is an integer (half-odd integer) if i is a boson (fermion).

For definiteness, one has to choose a branch of the logarithm in the definition of the phase shift $\delta_{ab}(\theta)$. Our convention will be to take $\delta_{ab}(\theta = 0)$ to be 0 or π if $S_{ab}(0)$ is equal to $+1$ or -1, respectively. In particular, since for all the Lie algebra related scattering theories considered in this paper $S_{ab}(0) = (-1)^{\delta_{ab}}$ (without the argument θ, δ_{ab} is Kronecker's delta!), we have $\delta_{ab}(\theta = 0) = \pi\delta_{ab}$ for these theories. Unitarity, eq. (5), then implies $\delta_{ab}(\theta) + \delta_{ab}(-\theta) = 2\pi\delta_{ab}$ in these cases.

The Bethe ansatz equations (24) allow one to calculate the individual momenta of a multi-particle state in a periodic box of size L, up to an error determined by how good the asymptotic wave function (18) describes the actual state of the system. A state with a given number of particles is very well described by eq. (18) if the average distance between the particles is much larger than the interaction range, which is roughly the Compton wavelength $1/m_1$ of the lightest particle. The differences between the true momenta and those determined by eq. (24) are expected to decrease exponentially with L for purely elastic scattering theories (this is certainly true for arbitrary multi-particle states in the Ising field theory whose energies can be calculated exactly, see sect. 6; in general this question

* In the infinite-volume limit, in particular for the infinite-volume thermodynamics (see subsect. 3.2), it does not matter which boundary conditions we impose. It is however important if we consider multi-particle states on a finite space, cf. the end of sect. 6 for an example.

deserves further investigation). For free theories the asymptotic wave function is exact, of course, and since $\delta_{ij}(\theta) \equiv 0$ we recover the usual quantization conditions for the momenta of free bosons and fermions from the Bethe ansatz equations. We stress that the TBA involves only the physical particles of the theory, not the *pseudo-particles* of the usual Bethe ansatz method [35], therefore all the rapidities θ_i are real.

3.2. THERMODYNAMICS

Before discussing the explicit details of the thermodynamics, let us answer an obvious question which comes to mind. Namely, how can the use of an *asymptotic* wave function lead to exact results if the system has a nonzero density, so that the average distance between particles is *finite*? The basic reason [18, 34] we expect exact results in the infinite-volume limit is the existence of a virial expansion for thermodynamic quantities. In this expansion the nth term is completely specified by the scattering matrix elements describing the scattering of n particles – i.e. a finite number – in an infinite volume, as shown by Dashen, Ma and Bernstein [18]. For finite-range interactions the virial expansion is expected to have a nonzero radius of convergence around zero density (this is rigorously known in many models), and if the singularity leading to the breakdown of convergence occurs at positive values of the density it indicates a phase transition from a low- to a high-density phase. What the TBA essentially does, is to give us an expression for a "summed up version" of the virial expansion, with the scattering of any (finite) number of particles taken into account exactly (in the infinite-volume limit). Therefore the thermodynamic Bethe ansatz should give exact results for any bulk quantity in the low-density phase (which for one-dimensional systems is usually the only phase).

In the thermodynamic limit both L and all N_a become infinite, with the densities N_a/L staying finite. We can then introduce the rapidity density $\rho_a^{(r)}(\theta)$ as the number of particles of species a with rapidities between θ and $\theta + \Delta\theta$ divided by $L\,\Delta\theta$. We are assuming that it is possible to choose the intervals $\Delta\theta$ ($\Delta\theta$ can depend on θ) large enough to have an appreciable number of rapidity levels in them, but small enough so that the $\rho_a^{(r)}(\theta)$ vary only on a scale larger than several $\Delta\theta$. Let us also introduce for each fixed $a = 1, \ldots, n$ the subsets $\{n_{a,i}\}$ of the set of all the n_i in eq. (24), where i is now running only over the particles of species a. Let $\theta_{a,i}$ be the rapidity values corresponding to these $n_{a,i}$. It will be convenient to assume from now on that the $\theta_{a,i}$ are ordered, $\theta_{a,i} < \theta_{a,i+1}$.

Consider the functions $J_a(\theta)$ defined by

$$J_a(\theta) = m_a \sinh\theta + 2\pi \sum_{b=1}^{n} (\delta_{ab} * \rho_b^{(r)})(\theta)\,. \tag{25}$$

where $*$ denotes the convolution

$$(f * g)(\theta) \equiv \int_{-\infty}^{\infty} \frac{d\theta'}{2\pi} f(\theta - \theta') g(\theta') . \tag{26}$$

It will become clear shortly that the functions $J_a(\theta)$ are monotonically increasing. The continuum version of eq. (24) then implies that for each a the sequence of $n_{a,i}$ is monotonically increasing with i. If $J_a(\theta) = 2\pi n_{a,i}/L$, then $\theta = \theta_{a,i}$. Such rapidities θ will be referred to as roots of species a. Note that their density is $\rho_a^{(r)}(\theta)$. If the increasing sequence of n_i skips some integers there will be values of θ not among the $\theta_{a,i}$ such that $(1/2\pi)LJ_a(\theta)$ equals these skipped integers. Such values of θ will be called holes of species a, and their density denoted by $\rho_a^{(h)}(\theta)$.

For particles of fermionic type the $n_{a,i}$ must form a *strictly* increasing sequence of integers because these particles are not allowed to have the same rapidity. We can therefore define a density of states (roots *and* holes) for the particles of species a, $\rho_a = \rho_a^{(r)} + \rho_a^{(h)}$, by

$$\rho_a(\theta) \equiv \frac{1}{2\pi} \frac{d}{d\theta} J_a(\theta) = \frac{m_a}{2\pi} \cosh\theta + \sum_{b=1}^{n} (\varphi_{ab} * \rho_b^{(r)})(\theta) , \tag{27}$$

where $\varphi_{ab}(\theta)$ was defined in eq. (11) as the derivative of the phase shift $\delta_{ab}(\theta)$. Since the density of states of any species has to be positive on physical grounds, eq. (27) implies that the $J_a(\theta)$ must be monotonically increasing functions. We believe that with some work it is possible to prove explicitly (using eqs. (32)–(34) below) that (27) is positive.

We have now assembled all equations and definitions needed to derive the complete thermodynamics of purely elastic scattering theories. In fact, we can lift most of these results from the classic paper of Yang and Yang [36] on the thermodynamics of a nonrelativistic gas of bosons with a repulsive δ-function interaction. We just have to take into account that now we have relativistic kinematics and several species of particles, in general.

Because of the existence of holes (at nonzero temperature) and the assumed smoothness of the densities ρ_a and $\rho_a^{(r)}$, there are many microscopic sequences $n_{a,i}$ giving rise to the same macroscopic densities ρ_a and $\rho_a^{(r)}$. The associated entropy per unit length is given by the standard expression

$$\begin{aligned} s[\rho, \rho^{(r)}] &= \sum_{a=1}^{n} s_a[\rho_a, \rho_a^{(r)}] \\ &= \sum_{a=1}^{n} \int_{-\infty}^{\infty} d\theta \left[\rho_a \ln \rho_a - \rho_a^{(r)} \ln \rho_a^{(r)} - (\rho_a - \rho_a^{(r)}) \ln(\rho_a - \rho_a^{(r)}) \right] . \end{aligned} \tag{28}$$

known from quantum statistical mechanics. Eq. (27) allows one to express the $\rho_a^{(r)}$ in terms of the ρ_a. The equilibrium ρ_a are obtained by minimizing the free energy per unit length,

$$f[\rho] = h[\rho^{(r)}] - Ts[\rho, \rho^{(r)}] . \tag{29}$$

where

$$h[\rho^{(r)}] = \sum_{a=1}^{n} \int_{-\infty}^{\infty} \mathrm{d}\theta\, \rho_a^{(r)}(\theta) m_a \cosh\theta \tag{30}$$

is the energy per unit length of a given rapidity distribution, subject to the constraint of fixed particle densities

$$D_a \equiv \frac{N_a}{L} = \int_{-\infty}^{\infty} \mathrm{d}\theta\, \rho_a^{(r)}(\theta) . \tag{31}$$

The chemical potentials μ_a of the different species are introduced, as usual, as Lagrange multipliers for the densities D_a. Introducing $\epsilon_a(\theta)$ by

$$\frac{\rho_a^{(r)}(\theta)}{\rho_a(\theta)} = \frac{1}{\mathrm{e}^{\epsilon_a(\theta)} + 1} , \tag{32}$$

and defining

$$L_a(\theta) \equiv \ln(1 + \mathrm{e}^{-\epsilon_a(\theta)}) , \tag{33}$$

the extremum condition can be shown to lead to the following set of coupled nonlinear integral equations for the $\epsilon_a(\theta) \equiv \epsilon_a(\theta, r, \{\hat{\mu}_b\})$:

$$\epsilon_a(\theta) = -\hat{\mu}_a r + \hat{m}_a r \cosh\theta - \sum_{b=1}^{n} (\varphi_{ab} * L_b)(\theta) \qquad \text{for } a = 1, \ldots, n , \tag{34}$$

where $\hat{\mu}_a = \mu_a / m_1$ and $\hat{m}_a = m_a / m_1$. (Here, as in most formulas below, we use $r = Rm_1$ or $R = 1/T$ as the thermodynamic variable, instead of the temperature T. This will be convenient later.) Eq. (34) is the most important equation* of the

* Using the Leray–Schauder–Tychonoff fixed point theorem [37] and a few other facts of functional analysis we have proved that eq. (34) has a real solution $\epsilon_a \equiv \epsilon_a(\theta, r, \{\hat{\mu}_b\})$ for $r > 0$ and $\hat{\mu}_a \in \mathbb{R}$. Clearly any such solution is C^∞ in θ, and furthermore, using the fact that the φ_{ab} are analytic in θ in a neighborhood of the real axis, one can show that the same is true for the ϵ_a. It is then easy to see that the solution ϵ_a is unique. Analyticity properties of ϵ_a in r and the $\hat{\mu}_a$ are not quite as easily established rigorously. The standard way to prove such properties (cf. appendix D of ref. [36]) is to show that one can solve the integral equation for the ϵ_a iteratively and that the iteration converges uniformly in r and the $\hat{\mu}_a$ in sufficiently small complex neighborhoods of any fixed $r = r_0 > 0$ and $\hat{\mu}_a = \hat{\mu}_{a,0} \in \mathbb{R}$. The analyticity of any finite iterate $\epsilon_a^{(n)}$ in neighborhoods of the positive r- and the whole real $\hat{\mu}_a$-axes is then inherited by the solution $\epsilon_a = \lim_{n\to\infty} \epsilon_a^{(n)}$. We know from our numerical work in sect. 7 that one can modify the "naive" iteration of eq. (34) (which does *not* converge, see sect. 7), so that it converges to the unique solution for any $r > 0$ and $\hat{\mu}_a \in \mathbb{R}$. It is also clear that the convergence is locally uniform in r and $\hat{\mu}_a$ – at least for real r and $\hat{\mu}_a$. We are sure that with a little bit of effort one can prove analytically that a suitable form of the iteration converges locally uniformly in r, $\hat{\mu}_a$ (and θ for that matter). Note that the analyticity properties of ϵ_a imply, via eqs. (36) and (33), that the pressure $P(T, \mu)$ is analytic in neighborhoods of any $T > 0$ and $\hat{\mu}_a \in \mathbb{R}$, i.e. there are no phase transitions for physical temperatures and chemical potentials. We will see later, however, that the thermodynamics becomes nonanalytic for complex temperatures, and that at least in some cases these nonanalyticities are related to physically interesting phase transitions.

TBA, since all thermodynamic quantities can be expressed in terms of the $\epsilon_a(\theta)$, as we will see presently.

The extremal free energy per unit length $f(R,\mu)$ is determined by using eqs. (34) and (27) to rewrite (29) as follows:

$$f(R,\mu) = -\frac{1}{2\pi R}\sum_{a=1}^{n}\int_{-\infty}^{\infty} \mathrm{d}\theta\, L_a(\theta, r, \hat{\mu})\, m_a \cosh\theta + \sum_{a=1}^{n} \mu_a D_a(R,\hat{\mu}), \quad (35)$$

where μ denotes the set of all μ_a. Here the first term can be shown to be the negative of the pressure P,

$$P(T,\mu) = \frac{T}{2\pi}\sum_{a=1}^{n}\int_{-\infty}^{\infty} \mathrm{d}\theta\, L_a(\theta, m/T, \mu)\, m_a \cosh\theta, \quad (36)$$

as expected from the thermodynamical relation $f = -P + \sum_a \mu_a D_a$ (the fact that we freely trade variables like r for T or $\hat{\mu}$ for μ should not cause any confusion, we hope).

To summarize: In a given purely elastic scattering theory, a choice of temperature $T = 1/R$ and (dimensionless) chemical potentials $\hat{\mu}_a$ determines the $\epsilon_a(\theta)$ through eq. (34). Using (32) in eq. (27) then yields an integral equation determining the densities $\rho_a(\theta)$ (or $\rho_a^{(t)}(\theta)$). Any desired thermodynamic quantity can be calculated by using, for instance, eq. (36) and the thermodynamical relation $\mathrm{d}P = s\,\mathrm{d}T + \sum_a D_a\,\mathrm{d}\mu_a$.

We see that the basic objects determining the thermodynamics in the TBA are the $\epsilon_a(\theta)$. Their physical interpretation can be obtained as follows. Start with an equilibrium sequence for the n_i in the Bethe ansatz equations (24), and then raise one $n_{a,i}$, corresponding to the rapidity $\theta_a = \theta_h$ ("h" for hole), to a larger nonequilibrium value corresponding to $\theta_a = \theta_p$. This describes a one-particle excitation of species a. A simple calculation, exactly as in ref. [36], then shows that the energy of the state increases by $T\epsilon_a(\theta_p) - T\epsilon_a(\theta_h)$. Up to an additive constant we therefore identify $T\epsilon_a(\theta)$ as the "dressed" one-particle excitation energy $E_a(\theta)$. The "constant" could a priori be a (model dependent) function of r and the μ_a. We fix it by the requirement that the fraction of occupied states of species a can be written in the familiar form

$$\frac{\rho_a^{(t)}(\theta)}{\rho_a(\theta)} = \frac{1}{\mathrm{e}^{(E_a(\theta)-\mu_a)/T}+1}. \quad (37)$$

By eq. (32) this implies that $E_a(\theta) = T\epsilon_a(\theta) + \mu_a$.

Similarly, the "dressed" momenta of one-particle excitations of species a are given up to a "constant" by the function $J_a(\theta)$, defined in eq. (25). The constant can be fixed by the condition that the momentum vanish at $\theta = 0$. Our choice of

phase shift for the Lie-algebra related scattering theories (see the end of sect. 3.1) then implies that the one-particle momenta in these theories are given by $p_a(\theta) = J_a(\theta) - \pi D_a$. This expression for the dressed momenta has an obvious interpretation as the "naive" zero-temperature momentum $m_a \sinh\theta$ modified through the phase shift a particle of species a experiences in collisions with other particles.

Although eq. (34) for the $\epsilon_a(\theta, r, \hat{\mu})$ can in general only be solved numerically, in the low- or high-temperature limits many physical quantities can be obtained analytically. As an example of quantities which can be calculated exactly in the high-temperature limit, consider the densities D_a, eq. (31). As $r \to 0$, eqs. (27) and (34) imply that $2\pi R \rho_a^{(r)}(\theta)$ and $-\partial_\theta L_a(\theta)$ satisfy the same equation for positive θ (for any fixed values of the $\hat{\mu}_a$). By the uniqueness of the solution of this equation these quantities therefore become equal for positive θ as $r \to 0$. The fact that $\rho_a^{(r)}(\theta)$ is even in θ then implies

$$D_a = 2\int_0^\infty \mathrm{d}\theta\, \rho_a^{(r)}(\theta) = -\frac{1}{\pi R}\int_0^\infty \mathrm{d}\theta\, \partial_\theta L_a(\theta) = \frac{L_a}{\pi R} \qquad \text{as } R \to 0. \tag{38}$$

where $L_a = \lim_{r\to 0} L_a(\theta = 0, r, \hat{\mu})$, which is independent of $\hat{\mu}$. The L_a are determined by eq. (47) of sect. 4, and their values are known [3] for all the theories discussed in this paper. Note that eq. (38) is also true for a free fermionic type particle where $L_a = L_1 = \ln 2$.

We will not pursue the study of the general thermodynamics any further here: we leave this to future work.

4. The ground-state scaling function $\tilde{c}(r)$

As an important special case of the thermodynamic considerations of sect. 3 we can obtain the vacuum energy $E_0(R)$ of a purely elastic scattering theory restricted to a periodic space of length R. The vacuum energy $E_0(R)$ is related in a simple way to the free energy of the QFT on an infinite line at finite temperature $T = 1/R$ and zero chemical potentials, as we now explain.

Consider the QFT in its euclidean version on a torus of perpendicular cycles of lengths L and R. There are two natural ways to pass to a quantum mechanical formulation of the theory, namely to choose time in the L or in the R direction. If we choose time in the L direction and let $L \to \infty$ we have

$$E_0(R) = \lim_{L\to\infty} -\frac{1}{L}\ln\left(\mathrm{Tr}_{\mathscr{H}_R}\, \mathrm{e}^{-LH_R}\right), \tag{39}$$

where H_R is the hamiltonian of the theory on a (periodic) space of length R, and $\mathscr{H}_R$ the corresponding Hilbert space. Note that the trace in this equation is over the *full* Hilbert space of the theory, not just some N-particle sector; the trace is

therefore the partition function $Z(L, R)$ in the *grand canonical ensemble at zero chemical potential*(s).

On the other hand, if we choose time in the R direction, the same partition function now describes the theory with periodic time (period R), i.e. at finite temperature $T = 1/R$. The $L \to \infty$ limit is now the thermodynamic limit, and we obtain

$$Rf(R, \mu = 0) = \lim_{L \to \infty} -\frac{1}{L} \ln\left(\mathrm{Tr}_{\mathscr{H}_L} \mathrm{e}^{-RH_L}\right), \tag{40}$$

where $f(R, \mu)$ is the free energy per unit length of sect. 3. So we see that

$$E_0(R) = Rf(R, \mu = 0). \tag{41}$$

From the exact ground-state energy $E_0(R)$ of the massive QFT one can read off important properties of the theory. Let us first of all discuss the normalization of the ground-state energy. We would like to choose $E_0(R)$ to vanish for $R = \infty$. (In a path-integral representation of the partition function this is equivalent to normalizing the measure so that its integral is 1 at $R = \infty$.) For a generic definition of the partition function this will only be the case after subtracting a bulk term, BR, and a boundary term, which is just a constant, from $E_0(R)$. On the cylinder, the case we are interested in, the boundary term in $E_0(R)$ vanishes. In the TBA calculation of $E_0(R)$ as $Rf(R, \mu = 0)$ the bulk term is also zero, because the free energy per unit length, eq. (35), vanishes at zero temperature and chemical potential(s) (this can be traced to the absence of any additional term on the r.h.s. of eq. (30)). On the other hand, in sect. 5 we will calculate $E_0(R)$ using conformal perturbation theory (CPT). In this approach the bulk term does not vanish, and it seems almost impossible to calculate it using CPT alone. However, as we will see, the exact bulk term of CPT can be obtained relatively easily by comparison with the TBA results.

Next, consider the finite-size corrections to a possible bulk term. In all the massive theories discussed in this paper there is only one length scale in addition to the cylinder circumference R: In the language of the S-matrix theory we choose it to be the correlation length $R_c = 1/m_1$ corresponding to the lightest particle (other distinct masses, when present, do not introduce independent length scales since all the mass ratios are fixed). From the viewpoint of CPT R_c is related to the single coupling λ, as discussed in sect. 5.

We conclude, simply by dimensional considerations, that after subtracting a possible bulk term the vacuum energy $E_0(R)$ can be written in the exact form

$$E_0(R) = -\frac{\pi \tilde{c}(r)}{6R}, \tag{42}$$

where $\tilde{c}(r)$ is a function of the dimensionless scaling length $r \equiv R/R_c$. We will call

$\tilde{c}(r)$ the *ground-state scaling function*. Because of the exponential fall-off of massive propagators we expect $\tilde{c}(r)$ to vanish exponentially as $r \to \infty$. The TBA will allow us to easily demonstrate this asymptotic behaviour.

In the opposite limit of $r \to 0$ only high-momentum modes propagate around the cylinder, so that we effectively see the massless UV limit of the given scattering theory. It is known [19, 20] that

$$\tilde{c}(0) = \tilde{c} \equiv c - 12 d_0 , \tag{43}$$

where c is the central charge and d_0 the lowest scaling dimension of the CFT describing the UV limit of the given massive QFT (for a unitary CFT $\tilde{c} = c$).

In sect. 5 we will see that in addition to $\tilde{c}$, the small-r behaviour of $\tilde{c}(r)$ allows one to determine [21] the scaling dimension of the conformal field by which one has to perturb the UV CFT to obtain the massive QFT in question.

We now turn to the study of $\tilde{c}(r)$. From eqs. (35), (41), and (42) we see that $\tilde{c}(r)$ is given by

$$\tilde{c}(r) = \frac{3}{\pi^2} \sum_{a=1}^{n} \int_{-\infty}^{\infty} \mathrm{d}\theta \, L_a(\theta, r) \hat{m}_a r \cosh\theta . \tag{44}$$

The larger-r (low-temperature) behaviour of $\tilde{c}(r)$ can be readily determined because it is basically just that of a free theory with the same mass ratios as the interacting theory. Namely, in this limit we have

$$\epsilon_a(\theta) = r\hat{m}_a \cosh\theta + \mathrm{O}(\mathrm{e}^{-r}) , \tag{45}$$

where the $\mathrm{O}(\mathrm{e}^{-r})$ correction is understood to possibly include powers of r. This implies that as $r \to \infty$

$$\begin{aligned} \tilde{c}(r) &= \frac{6}{\pi^2} r \sum_{a=1}^{n} \hat{m}_a \int_0^{\infty} \mathrm{d}\theta \cosh\theta \, \mathrm{e}^{-r\hat{m}_a \cosh\theta} (1 + \mathrm{O}(\mathrm{e}^{-r})) \\ &= \frac{6}{\pi^2} r \sum_{a:\, \hat{m}_a < 2} \hat{m}_a K_1(\hat{m}_a r) + \mathrm{O}(\mathrm{e}^{-2r}) , \end{aligned} \tag{46}$$

where again, $\mathrm{O}(\mathrm{e}^{-2r})$ is meant to include powers of r, and $K_1(x)$ is the modified Bessel function of order one. It is possible [21] to work out the next correction to the behaviour (46) (at least for the perturbed Yang–Lee CFT), but further corrections are difficult to calculate explicitly.

Let us now discuss the small-r behaviour of $\tilde{c}(r)$. We explicitly evaluated $\tilde{c} = \tilde{c}(0)$ in ref. [3] for all purely elastic scattering theories considered in this paper (and, in addition, for the corresponding nonminimal S-matrix theories). As $r \to 0$

the $\epsilon_a(\theta)$ become essentially constant in the region $-\ln(2/r) \ll \theta \ll \ln(2/r)$, while growing exponentially for $|\theta| \gg \ln(2/r)$. Calling the $r \to 0$ limit of these constants ϵ_a, we see from eq. (34) that they are determined by

$$\epsilon_a = \sum_{b=1}^{n} N_{ab} \ln(1 + e^{-\epsilon_b}) = \sum_{b=1}^{n} N_{ab} L_b , \tag{47}$$

where we introduced the symmetric matrix N by

$$N_{ab} = -\int_{-\infty}^{\infty} \frac{d\theta}{2\pi} \varphi_{ab}(\theta) = -\frac{1}{2\pi}(\delta_{ab}(\infty) - \delta_{ab}(-\infty)) = \sum_{\alpha \in A_{ab}} (1 - |\alpha|) \operatorname{sgn} \alpha . \tag{48}$$

There is always a unique real solution to eq. (47) for the ϵ_a. [Consider the ath component of this equation. The l.h.s. is strictly increasing as ϵ_a increases and independent of the other ϵ_b, whereas the r.h.s. is a positive and strictly decreasing function of all the ϵ_b, since the entries of the matrix N are positive. So the two sides of this equation are equal for exactly one set of (positive) $\{\epsilon_a\}$.] We noticed [3] that the matrix N can be simply expressed in terms of the incidence matrix I of the (non-affine) Lie algebra to which the S-matrix theory is related, as $N = I(2 - I)^{-1}$. (For the $A_{2n}^{(2)}$-related S-matrix theory I is the "generalized incidence matrix" defined in sect. 2.) In particular, the N-matrices have rational entries and so the e^{ϵ_a} are algebraic numbers, which were given in ref. [3]. There we also found that $\bar{c}$ can be expressed in terms of the ϵ_a as follows:

$$\bar{c} = \sum_{a=1}^{n} \bar{c}_a = \sum_{a=1}^{n} \bar{c}_{t_a}(\epsilon_a) , \tag{49a}$$

where

$$\bar{c}_{\pm}(\epsilon) = \pm \frac{6}{\pi^2}\left[\int_{\epsilon}^{\infty} dx \ln(1 \pm e^{-x}) + \tfrac{1}{2}\epsilon \ln(1 \pm e^{-\epsilon})\right]$$

$$= \frac{6}{\pi^2} \times \begin{cases} L\left(\dfrac{1}{1 + e^{\epsilon}}\right) \\ L(e^{-\epsilon}) \end{cases} . \tag{49b}$$

Here t_a is the type of the particle a as defined in subsect. 3.1, and $L(x)$ is Rogers' dilogarithm function [38]

$$L(x) = -\frac{1}{2}\int_0^x dy \left[\frac{\ln y}{1 - y} + \frac{\ln(1 - y)}{y}\right] . \tag{50}$$

Using known sum rules [38] for the Rogers dilogarithm we evaluated the expression for $\tilde{c}$ for the known purely elastic scattering theories and obtained the values of $\tilde{c}$ of the CFTs, perturbations of which are conjectured to give rise to the corresponding S-matrix theories (for the E_n-related S-matrix theories we evaluated $\tilde{c}$ numerically, since the corresponding sum rules do not seem to be known in the literature).

Besides the value of $\tilde{c}(r)$ at $r = 0$ one can also evaluate the leading corrections [21]. We will now do so for the Lie-algebra related purely elastic scattering theories with a non-constant S-matrix. In our calculations it will be important that $2 < \tilde{y} < 4$ (cf. table 1 and eq. (2)) for these theories. In perturbations of free theories or the critical Ising model by a pure mass term, where $\tilde{y} = 2$, we can explicitly evaluate all terms in the expansion of $\tilde{c}(r)$ around $r = 0$. This will be done in sect. 6.

Let us introduce the functions

$$\psi_a(\theta) \equiv \psi_a(\theta, r) = \left(\partial_r + \frac{1}{r}\partial_\theta\right)\epsilon_a(\theta, r), \tag{51}$$

which, by eq. (34) with $\hat{\mu}_a = 0$, satisfy the equations

$$\psi_a(\theta) = \hat{m}_a \mathrm{e}^{\theta} + \sum_{b=1}^{n}\left(\varphi_{ab} * \frac{\psi_b}{\mathrm{e}^{\epsilon_b} + 1}\right)(\theta). \tag{52}$$

Applying $r^{-1}(\mathrm{d}/\mathrm{d}r)$ to eq. (44) we get, after an integration by parts and using the fact that the $\epsilon_a(\theta, r)$ are even in θ,

$$\frac{1}{r}\tilde{c}'(r) = -\frac{3}{\pi^2}\sum_{a=1}^{n}\int_{-\infty}^{\infty}\mathrm{d}\theta\, \hat{m}_a \mathrm{e}^{-\theta}\frac{\psi_a(\theta, r)}{\mathrm{e}^{\epsilon_a(\theta, r)} + 1}. \tag{53}$$

The functions $\psi_a(\theta, r)$ are positive for all θ and $r > 0$ (their behaviour is described below), and hence the $\tilde{c}(r)$ are strictly monotonically decreasing functions of $r \geqslant 0$.

This expression can be calculated explicitly in the UV limit $r \to 0$. This is possible for the same reason that allowed the calculation of $\tilde{c}(0)$ in refs. [3, 21]. Namely, one can replace the functions $\epsilon_a(\theta, r)$ and $\psi_a(\theta, r)$ in eq. (53) by suitably chosen functions $\tilde{\epsilon}_a(\theta, r)$ and $\tilde{\psi}_a(\theta, r)$ without changing the $r \to 0$ limit of this expression, but now allowing one to evaluate it.

Let us define $\tilde{\epsilon}_a(\theta) \equiv \tilde{\epsilon}_a(\theta, r)$ as the solution of

$$\tilde{\epsilon}_a(\theta) = \tfrac{1}{2} r\hat{m}_a \mathrm{e}^{\theta} - \sum_{b=1}^{n}(\varphi_{ab} * \tilde{L}_b)(\theta), \tag{54}$$

where $\tilde{L}_a(\theta) = \ln(1 + \mathrm{e}^{-\tilde{\epsilon}_a(\theta)})$. Define $\tilde{\psi}_a(\theta) \equiv \tilde{\psi}_a(\theta, r)$ in terms of $\tilde{\epsilon}_a(\theta)$ in the same way that $\psi_a(\theta)$ is defined in terms of $\epsilon_a(\theta)$. $\tilde{\epsilon}_a(\theta)$ and $\tilde{\psi}_a(\theta)$ differ appreciably from

$\epsilon_a(\theta)$ and $\psi_a(\theta)$ only for θ smaller than $\theta \approx -\ln(2/r)$; $\tilde{\epsilon}_a(\theta)$ is now (approximately) constant for *all* $\theta \ll \ln(2/r)$.

The desired replacement is possible because the integrand in eq. (53) is concentrated around $\theta \approx \ln(2/r)$ as $r \to 0$. The integral $\int_{-\infty}^{0} d\theta\, e^{-\theta} \psi_a(\theta, r)/(e^{\epsilon_a(\theta)} + 1)$ in fact vanishes in this limit. This follows from the behaviour of the functions $\psi_a(\theta)$ in the $r \to 0$ limit. For $\theta \gg \ln(2/r)$ they are equal to $\hat{m}_a e^{\theta}$, up to double-exponentially small corrections, as is obvious from eq. (52). After a transition region around $\theta \approx \ln(2/r)$, $\psi_a(\theta) = O(e^{\eta\theta})$ for $|\theta| \ll \ln(2/r)$, where $\eta \equiv \tilde{y}/2$. There is another transition region around $\theta \approx -\ln(2/r)$; for smaller θ the $\psi_a(\theta)$ rapidly approach $K\hat{m}_a(\frac{1}{2}r)^{2(\eta-1)}e^{\theta}$, where K is a (model-dependent) constant of order 1. The details of the behaviour of the $\psi_a(\theta)$ are not trivial to prove; we have checked them numerically for many scattering theories. It implies that $\int_{-\infty}^{0} d\theta\, e^{-\theta} \psi_a(\theta, r)/(e^{\epsilon_a(\theta)} + 1)$ vanishes approximately like $r^{\eta-1}$ as $r \to 0$.

The point of introducing the "tilded" functions is that the r-dependence of $\tilde{\epsilon}_a(\theta, r)$ is trivial – it just amounts to a shift in θ. Defining the *r-independent* functions

$$\hat{\epsilon}_a(\theta) \equiv \tilde{\epsilon}_a(\theta, 2) = \tilde{\epsilon}_a\left(\theta + \ln\frac{2}{r}, r\right), \tag{55}$$

we see that

$$\tilde{\psi}_a(\theta, r) = \left(\partial_r + \frac{1}{r}\partial_\theta\right)\hat{\epsilon}_a\left(\theta - \ln\frac{2}{r}\right) = \frac{2}{r}\partial_\theta \hat{\epsilon}_a\left(\theta - \ln\frac{2}{r}\right). \tag{56}$$

Shifting the integration variable θ in eq. (53) (with the ψ_a replaced by $\tilde{\psi}_a$) by $\ln(2/r)$, we obtain

$$\frac{1}{r}\tilde{c}'(r)\Big|_{r=0} = \frac{3}{\pi^2}\sum_{a=1}^{n} \hat{m}_a \int_{-\infty}^{\infty} d\theta\, e^{-\theta}\partial_\theta \hat{L}_a(\theta) \equiv -\frac{3}{\pi^2}\sum_{a=1}^{n} \hat{m}_a T_a. \tag{57}$$

Note that $\tilde{\psi}_a(\theta, r)$ falls off like $e^{\eta\theta}$ for all $\theta \ll \ln(2/r)$. This implies that $\partial_\theta \hat{\epsilon}_a(\theta)$ and $\partial_\theta \hat{L}_a(\theta)$ are $O(e^{\eta\theta})$ for $\theta \ll 0$. The r.h.s. of eq. (57) therefore does not diverge, i.e. the leading term in the small r-expansion of $\tilde{c}(r)$ is $O(r^2)$. (The coefficient of the r^2-term is nonzero because the $\hat{L}_a(\theta)$ are strictly monotonically decreasing functions of $|\theta|$.) This r^2-term is in fact expected on physical grounds, cf. sect. 5, since it corresponds to a bulk term in $E_0(R)$.

We now evaluate the expression $\sum_a \hat{m}_a T_a$. To this end, consider [21] the convolution $\sum_b(\varphi_{ab} * \hat{L}_b)(\theta)$. Defining

$$\Delta_{ab}(\theta) \equiv \int_{-\infty}^{\theta} d\theta'\, \varphi_{ab}(\theta') = \delta_{ab}(\theta) - \delta_{ab}(-\infty), \tag{58}$$

we see after integrating by parts and using eq. (47) that

$$\sum_{b=1}^{n} (\varphi_{ab} * \hat{L}_b)(\theta) = -\epsilon_a + \frac{1}{2\pi} \sum_{b=1}^{n} \int_{-\infty}^{\infty} \mathrm{d}\theta' \Delta_{ab}(\theta - \theta') \partial_{\theta'} \hat{L}_b(\theta') . \tag{59}$$

Note that eqs. (13) and (48) imply that

$$\Delta_{ab}(\theta) = \begin{cases} -\Sigma_s \varphi_{ab}^{(s)} s^{-1} \mathrm{e}^{s\theta} & \theta < 0 \\ -2\pi N_{ab} + \Sigma_s \varphi_{ab}^{(s)} s^{-1} \mathrm{e}^{-s\theta} & \theta > 0 . \end{cases} \tag{60}$$

We conclude that

$$\sum_{b=1}^{n} (\varphi_{ab} * \hat{L}_b)(\theta) = -\epsilon_a + \frac{\mathrm{e}^{\theta}}{2\pi} \sum_{b=1}^{n} \varphi_{ab}^{(1)} T_b + \mathrm{O}(\mathrm{e}^{\eta\theta}) \qquad \text{as } \theta \to -\infty . \tag{61}$$

(Here we used the fact that $\eta < 2$ for all theories considered, otherwise $\mathrm{e}^{\eta\theta}$ might not be the leading correction.) Note that according to eq. (17) we have

$$\sum_{b=1}^{n} \varphi_{ab}^{(1)} T_b = \varphi_{11}^{(1)} \hat{m}_a \sum_{b=1}^{n} \hat{m}_b T_b , \tag{62}$$

so if we can evaluate the l.h.s. in another way, we know what the desired expression $\Sigma_b \hat{m}_b T_b$ is.

The convolution we have just been discussing can also be written as

$$\sum_{b=1}^{n} (\varphi_{ab} * \hat{L}_b)(\theta) = -\hat{\epsilon}_a(\theta) + \hat{m}_a \mathrm{e}^{\theta} , \tag{63}$$

simply by definition of $\hat{\epsilon}_a(\theta)$. Since $\hat{\epsilon}_a(\theta) - \epsilon_a$ vanishes like $\mathrm{e}^{\eta\theta}$ (i.e. faster than e^{θ}) as $\theta \to -\infty$, we see by matching the e^{θ} terms in eqs. (61) and (63) that $\hat{m}_a = (1/2\pi)\Sigma_b \varphi_{ab}^{(1)} T_b$, or, by eq. (62),

$$\sum_{a=1}^{n} \hat{m}_a T_a = \frac{2\pi}{\varphi_{11}^{(1)}} . = \frac{\pi}{2} \frac{1}{\tan \frac{\pi}{k}} \quad (k=h) \tag{64}$$

From eq. (57) we finally obtain

$$\tilde{c}(r) = \tilde{c} - \frac{3r^2}{\pi \varphi_{11}^{(1)}} + \Sigma(r) , \tag{65}$$

where $\Sigma(r)$ is a function of $\mathrm{o}(r^2)$, which will be studied in sect. 5. Recall that $\varphi_{11}^{(1)}$ is determined by eq. (14) and the set A_{11} given in table 1.

$\tilde{c}(r)' = -\frac{6r}{\pi \varphi_{11}^{(1)}}$; $\langle \Theta \rangle = -\frac{\pi^2}{3r} c'(r)$

$= \frac{4\pi}{}$

Before closing this section we should remark on some open problems of the TBA approach. We will see in sect. 5 by comparison with conformal perturbation theory on the cylinder that $\Sigma(r)$ has a power series expansion in $g = r^{\delta}$. If CPT has a nonzero radius of convergence (as widely believed and strongly suggested by our numerical results of sect. 7), $\Sigma(r)$ is analytic in g in some disk around $g = 0$. One would of course like to prove this directly within the TBA framework. Unfortunately, this seems to be a difficult – though intriguing – mathematical problem. There are indications that the first step in proving this is to show that the $\hat{\epsilon}_a(\theta)$ are analytic in $t \equiv e^{\eta\theta}$ in some disk around $t = 0$*. This is quite plausible, since we know from high-precision numerical results that $\hat{\epsilon}_a(\theta) = \epsilon_a + O(e^{\eta\theta})$ as $\theta \to -\infty$.

5. Conformal perturbation theory

Obtaining analytical information about the function $\Sigma(r)$ in eq. (65) directly from the nonlinear integral equations of the thermodynamic Bethe ansatz appears to be a very difficult mathematical problem, as just explained. At present, it seems that the best one can do in the framework of the TBA is to calculate it numerically. It is possible [21], however, to get some exact information about $\Sigma(r)$ by using a completely different approach, namely perturbation theory around the nontrivial CFT describing the UV limit of the massive QFT. This approach is called *conformal perturbation theory* (CPT).

In the cases we will consider, the CFT is perturbed by a single relevant spinless primary field Φ of scaling dimension $d_\Phi = 2 - y$ (we use the standard normalization [39] for Φ, namely $\langle \Phi(z,\bar{z})\Phi(0,0)\rangle = |z|^{-2d}$ at criticality on the plane). The (bare) euclidean action of the perturbed CFT is

$$\mathcal{S}_\lambda = \mathcal{S}_0 + \lambda \int d^2\xi\, \Phi(\xi)\,. \tag{66}$$

Note that λ has mass dimension y. We will choose positive λ (or positive imaginary λ in the case of the perturbed Yang–Lee CFT, see below) to correspond to the perturbation leading to the massive theory in question. This can always be achieved by a suitable choice of the overall sign of Φ. In some cases, e.g. the magnetic perturbation of the Ising model, both signs of λ lead to the same massive theory. This should be kept in mind, even though we will always take λ to be positive in the following.

The action of the unperturbed CFT, H_0, is in general not explicitly known. But the explicit form of H_0 is unnecessary anyhow; CPT is possible for the same

* The statement that the $\hat{\epsilon}(\theta)$ of the perturbed Yang–Lee CFT is analytic in $t = e^{\delta\theta/5}$ close to $t = 0$ first appeared in ref. [21].

reason that one can perturb around a free field theory – we know the *exact* correlation functions in the unperturbed theory. Correlation functions in the perturbed theory are then calculated in the standard way as if we actually had a functional integral representation for the theory: The expectation value of any operator A in the perturbed theory is

$$\langle A\rangle_\lambda = \frac{1}{Z_\lambda}\left\langle A\exp\left[-\lambda\int \mathrm{d}^2\xi\,\Phi(\xi)\right]\right\rangle_0$$

$$= \frac{1}{Z_\lambda}\sum_{n=0}^{\infty}\frac{(-\lambda)^n}{n!}\int \mathrm{d}^2\xi_1\ldots\mathrm{d}^2\xi_n\langle A\Phi(\xi_1)\ldots\Phi(\xi_n)\rangle_0, \tag{67}$$

with

$$Z_\lambda = \left\langle \exp\left[-\lambda\int \mathrm{d}^2\xi\,\Phi(\xi)\right]\right\rangle_0 . \tag{68}$$

Here the $\langle\ldots\rangle_0$ denote expectation values in the true ground state of the theory, created by the field Φ_0 of lowest scaling dimension; they can be expressed (see below) in terms of the usual CFT correlators, i.e. expectation values in the SL_2-invariant state created by the identity operator $\mathbb{1}$, which will not carry the subscript 0. In a unitary CFT $\Phi_0 = \mathbb{1}$, and this distinction is unnecessary.

The relevant perturbations considered in CPT correspond to super-renormalizable interactions. Therefore an arbitrary Green function can have *primitive* UV divergencies only in finitely many orders of CPT. By the same token, however, in the expansion around a massless theory IR problems will occur for all except a finite number of terms. As is well known, at least from examples (see e.g. ref. [40] and references therein), the perturbative IR problems are a sign that the Green functions of the "true" theory are not analytic in the coupling (the same reason suspected to be responsible for the UV problems of at least some perturbatively non-renormalizable theories). In our cases, where the perturbed theory is purely massive, the perturbative IR problems are "cured" in the true theory simply by virtue of the existence of a mass gap which acts as an IR cutoff.

Of course, the renormalization of IR divergencies [40] is not an easy task, so one would like to avoid it if possible. If one considers only slightly relevant perturbations the IR problems occur only in high orders and one can presumably trust RG-improved low order calculations (see e.g. refs. [41, 42]); this is the same idea as that underlying the ϵ-expansion. In our cases of strongly relevant perturbations, this approach of course cannot be taken.

Fortunately, for the quantity we are interested in here, the ground-state energy $E_0(R)$ on a cylinder, we do not use CPT on the plane but rather on the cylinder, whose radius acts as a natural IR cutoff; integrated *connected* correlators are IR finite on the cylinder.

We now show that in the cases we are considering there are also no UV problems in any order*. In the calculation of the vacuum energy on the cylinder we will encounter integrated correlators of the form

$$I_n = \int_\epsilon \mathrm{d}^2\xi_1 \ldots \mathrm{d}^2\xi_n \langle \Phi_0(i\infty)\Phi(\xi_n)\ldots\Phi(\xi_1)\Phi_0(-i\infty)\rangle\,, \tag{69}$$

where the ξ_i are integrated over the (IR regulated in the "time" direction) cylinder $\{\xi \mid \mathrm{Re}\,\xi \in [0, R),\ \mathrm{Im}\,\xi \in (-L/2, L/2)\}$, avoiding regions where the distances between them are smaller than the UV cutoff ϵ. In fact, we can easily generalize the discussion and consider integrals which show up in CFTs perturbed by more than one relevant field:

$$J_n = \int_\epsilon \mathrm{d}^2\xi_1 \ldots \mathrm{d}^2\xi_n \langle \phi_{n+1}(\xi_{n+1})\phi_n(\xi_n)\ldots\phi_1(\xi_1)\phi_0(\xi_0)\rangle\,. \tag{70}$$

where the ϕ_i are conformal fields of scaling dimension d_i. Now the unintegrated fields ϕ_0 and ϕ_{n+1} are located at $\xi_0 \neq \xi_{n+1}$ which are both either outside the integration region as in eq. (69), or inside it, a situation which is encountered in the CPT expansion of a two-point function in a perturbed unitary CFT. In the latter case the UV cutoff ϵ also prevents the integrated ξ_i from approaching ξ_0 and ξ_{n+1} too closely. Further generalization to include more unintegrated fields is straightforward.

In the space of integration variables $\xi_1, \ldots, \xi_n$ we have to consider the UV regions where any number $m = 2, \ldots, n$ of the ξ_i approach each other (the remaining ones kept fixed), or where $m-1$ approach one of the unintegrated points ξ_0 or ξ_{n+1}, if the latter are inside the full integration region. In both cases, the condition for UV finiteness is obtained by considering different fusion schemes (cf. ref. [43]) of m fields ϕ_{i_a}, $a = 1, \ldots, m$, leading to some "fused" field ϕ_i of dimension d_i: Let ξ_{i_1} be the point that the other ones, ξ_{i_b}, $b = 2, \ldots, m$, approach (the order of approach being specified by the fusion scheme; if ξ_0 or ξ_{n+1} is one of the $\xi_{i_1}, \ldots, \xi_{i_m}$ then ξ_{i_1} is ξ_0 or ξ_{n+1}). We change the integration variables ξ_{i_b}, $b = 2, \ldots, m$, by letting $\xi_{i_b} = \xi_{i_1} + \epsilon\zeta_{i_b}$, where the new variables are now restricted by the UV cutoff to obey $|\zeta_{i_b}| > 1$ and $|\zeta_{i_b} - \zeta_{i_c}| > 1$, for all $b \neq c$ (additional restrictions may arise from the fact that in a two-dimensional space there are not many directions along which points can approach each other!) Using the transformation properties of the CFT correlators under local scaling by $1/\epsilon$ (around ξ_{i_1}),

* In what follows we use the language of CPT on the cylinder, which will be needed for explicit calculations later on in this section. However, since the UV behaviour is independent of the global geometry, the condition for the absence of UV divergencies given below is just as true on the plane. One should however realize that IR divergencies on the cylinder as $\xi \to -i\infty$ naively appear as UV divergencies at $z = 0$ when transforming to the plane via $z = \exp(-2\pi i\xi/R)$.

we see that the contribution to J_n from the region considered behaves like ϵ to the power $2(m-1)-\sum_{a=1}^{m} d_{i_a}+d_f$, multiplied by the correlator of the field ϕ_f and the remaining $n+2-m$ fixed fields. We conclude that J_n is UV finite if the following condition is satisfied:

$$\sum_{a=1}^{m} y_{i_a} > y_f , \tag{71}$$

for all possible ϕ_f that can be obtained by fusing any m fields ϕ_{i_a} $(m=2,\ldots,n)$ and in addition are intermediate fields in the conformal blocks contributing to the full $(n+2)$-point function in the definition of J_n (namely, ϕ_f can be fused together with the $n+2-m$ remaining fields to give the identity).

Going back to the integrals I_n, eq. (69), we immediately see that in the perturbations of unitary CFTs (where $y_f \leqslant 2$ and $\Phi_0 = 1$) they are UV finite for all n provided that $y > 1$. This is the case for all the unitary theories we consider, except for the thermal perturbation of the Ising model where $y = 1$. But even in the latter case only the first nontrivial integrated correlator I_2 is UV divergent, all higher *connected* I_n are UV finite (cf. ref. [29] and sect. 6). For perturbations of the non-unitary models $M_{2,2n+3}$, where $y > 2$, $\Phi = \phi_{1,3}$ and $\Phi_0 = \phi_{1,n+1}$, we have to check that the condition (71) is satisfied when fusing m fields Φ. This is indeed the case, in fact, it is a consequence of the following more general result that is easy to verify: *Any* allowed fusion $\phi_a \times \phi_b \to \phi_c$ in the CFTs $M_{2,2n+3}$ satisfies $y_a + y_b - y_c > 2$. Summing up the relevant inequalities of this type along any "fusion path" of m fields Φ we get $my > y_f + 2(m-1)$, which of course implies (71). In these CFTs there are no UV divergencies in *any* integrated correlator.

There is an important difference between CPT and perturbative expansions around free field theories: It is well known that, at least in bosonic theories, the perturbation expansion around free fields diverges even when IR and UV cutoffs are present, due to instantons. CPT on the other hand is expected [21, 44] to have a nonzero radius of convergence in such a situation (in the cases at hand even without the UV cutoff, of course).

The intuitive reason [44] for the benign behaviour of CPT is that a relevant perturbation of a CFT is not expected to worsen the asymptotic behaviour of the functional measure for large fields. This is clear, for instance, in the Landau–Ginzburg representation [45] of unitary minimal models. In the case of ordinary Rayleigh–Schrödinger perturbation theory in quantum mechanics the analogous results are of course rigorously known from the Kato–Rellich theory of regular perturbations (see e.g. ref. [46]). Consider, for instance, the perturbation of a hamiltonian $H_0 = p^2 + V_0(x)$ by a potential $\lambda V(x)$ which does not grow faster than $V_0(x)$ for large x. Then for sufficiently small λ a discrete nondegenerate eigenvalue E_0 of H_0 gets perturbed to a unique eigenvalue $E(\lambda)$ of $H_0 + \lambda V$, which is analytic in λ.

There is also a truly field theoretic example involving only bosons where a perturbation expansion around a free theory is known to have a nonzero radius of convergence, even without any cutoffs. The example is a massive free scalar field ϕ in $1+1$ dimensions perturbed by an interaction term of the form $\lambda\cos(\epsilon\phi+\theta)$ (the "massive sine-Gordon" model). It has been shown rigorously [47] that if the unperturbed boson has a sufficiently large mass, the perturbation series in λ is analytic in some disk around $\lambda = 0$. The intuitive reason for this is the same as mentioned above: The interaction is small compared to the mass term for large fields.

We will not attempt to prove here analytically that (IR cutoff) CPT has a nonzero radius of convergence. However, for the vacuum energy $E_0(R)$ of a purely elastic scattering theory on a cylinder of circumference R, our numerical results in sect. 7 indicate that this is indeed the case. Be that as it may, we know from our earlier remarks that

$\tilde{c} = -\frac{6}{\pi}R^2 B(\lambda) \rightarrow 1/R\,\frac{d\tilde{c}}{dR} \sim B(\lambda)$

$E_0(R) = -\frac{\pi\tilde{c}}{6R}$

$$E_0(R) = -\lim_{L\to\infty}\frac{1}{L}\ln\left\langle\exp\left[-\lambda\int_{\mathrm{cyl}}\mathrm{d}^2\xi\,\Phi(\xi)\right]\right\rangle_0 - B(\lambda)R - \frac{\pi\tilde{c}}{6R} \tag{72}$$

is well defined perturbatively. In the above expression we have subtracted a bulk term, whose coefficient $B(\lambda)$ should be chosen to cancel any bulk contribution arising from the first term. We have also included the "Casimir term" $-\pi\tilde{c}/6R$ in $E_0(R)$, so that at $\lambda = 0$ (where the first two terms on the r.h.s. vanish) we reproduce the value of the vacuum energy on the cylinder which corresponds to vanishing vacuum energy on the infinite plane. Expanding the expectation value in eq. (72) in powers of the dimensionless variable $R^y\lambda$ we obtain, using translational invariance on the cylinder,

$$E_0(R) = -\frac{\pi\tilde{c}}{6R} - B(\lambda)R - \frac{\pi}{6R}\sum_{n=1}^{\infty} C_n(R^y\lambda)^n, \tag{73}$$

where

$$C_n = 12\frac{(-1)^n}{n!}R^{2-ny}\int_{\mathrm{cyl}}\langle\Phi(0)\prod_{j=1}^{n-1}\Phi(\xi_j)\,\mathrm{d}^2\xi_j\rangle_{0,\mathrm{conn}} \tag{74}$$

and the subscript "conn" signifies that the correlators are connected.

Explicit calculations of the coefficients C_n will be deferred to the end of this section. Here we just note the consequences of nontrivial symmetries that are present in all the unitary CFTs whose perturbations we consider. In all these cases the perturbing field Φ belongs to a subalgebra of the operator algebra which has a $\mathbb{Z}_2$ symmetry, and Φ is odd with respect to this symmetry. (Except for the

$E_8^{(1)}$-related model, this fact is understood by observing that the above $\mathbb{Z}_2$ symmetry reflects the Kramers–Wannier duality of the corresponding lattice model; Φ is the energy density operator which is coupled to the temperature, and therefore is odd under this duality. In the $E_8^{(1)}$-related case, Φ is the spin operator of the Ising model and the $\mathbb{Z}_2$ symmetry is just the spin-flip symmetry.) It follows that correlators of an odd number of Φ's vanish identically, and hence $C_n = 0$ for odd n in all the models related to the untwisted affine algebras. This is not the case in the $A_{2n}^{(2)}$-related models, since the fusion rules of the unperturbed non-unitary CFTs $M_{2,2n+3}$ imply that the correlators in eq. (74) do not vanish for any n.

So we see that in the unitary as well as non-unitary cases the CPT prediction for the ground-state scaling function $\tilde{c}(r)$ is

$\tilde{y} = 2y$ (unitary UV CFT)
$\tilde{y} = y$ (non-unitary UV CFT)

$$\tilde{c}(r) = \tilde{c} + \frac{6}{\pi} B(\lambda) R^2 + \sum_{n=1}^{\infty} \tilde{C}_n (R^{\tilde{y}} \lambda^{\tilde{y}/y})^n , \tag{75}$$

$y = 2 - \Delta_\phi$

with $\tilde{y}$ defined in eq. (2), and

$$\tilde{C}_n = \begin{cases} C_{2n} & \text{(unitary cases)} \\ C_n & \text{(non-unitary cases)} . \end{cases} \tag{76}$$

Comparing with our final result for $\tilde{c}(r)$ from the TBA, eq. (65), we can conclude three things:

$$B(\lambda) = -\frac{m_1^2}{2\varphi_{11}^{(1)}} , \tag{77}$$

$$\Sigma(r) = \sum_{n=1}^{\infty} a_n (r^{\tilde{y}})^n , \qquad \text{for some } a_n \in \mathbb{R} , \tag{78}$$

and

$$a_n m_1^{n\tilde{y}} = \tilde{C}_n \lambda^{n\tilde{y}/y} \qquad \text{for all } n . \tag{79}$$

It is not surprising that we find a nonzero bulk term in the perturbative part of the ground-state energy as calculated by CPT, because, after all, we are expanding around a conformal theory in which fluctuations on all length scales contribute to the energy. In the corresponding statistical mechanics system this bulk term, proportional to $\lambda^{2/y}$, of course signals the phase transition: In the unitary cases it leads to the divergence of the "susceptibility" (second derivative of the free energy with respect to λ) at criticality; in the non-unitary cases already the "magnetiza-

tion" (first derivative of the free energy with respect to λ) diverges. Note that it would have been *extremely* difficult to obtain the bulk term coefficient $B(\lambda)$ within CPT alone: We would have had to analytically continue the power series in eq. (73), which (for fixed λ) converges only for small R, to large values of R and find the term proportional to R. But in most cases it is already quite difficult (see below) to calculate the second coefficient in this power series – even numerically.

In the TBA framework it is not yet possible to prove analytically that $\Sigma(r)$ has a power series expansion in r^{ν} (it can however be checked numerically at least for the first term, as we will see). But once we know this from the comparison with CPT, it is much easier to use the TBA to calculate the a_n than to obtain the C_n in CPT. So our approach will be to make several checks verifying the consistency of these two methods and then use the TBA to obtain further results. The first six coefficients a_n will be extracted from a numerical solution of the TBA eq. (34) (the details will be discussed in sect. 7). In particular, a_1 can be evaluated to very high accuracy. Eq. (79) for $n = 1$, with the exact value of $\tilde{C}_1$ (obtained analytically below), then allows us to accurately determine the coefficient κ,

$$\lambda = \kappa m_1^{\nu}, \tag{80}$$

relating the perturbing parameter to the lowest mass in a given theory. Consistency requires

$$\tilde{C}_n = a_n \kappa^{-n\nu/\nu}, \tag{81}$$

for $n > 1$, in particular. We will check this for $n = 2$ in the $A_2^{(2)}$-, $A_3^{(1)}$-, $D_{4-6}^{(1)}$-, and $E_8^{(1)}$-related cases (see below and sect. 7).

To conclude this section, we turn to the calculation of the coefficients C_n using the CPT approach. When calculating integrals of correlation functions in the CFT it is more convenient to work on the punctured plane, rather than the cylinder. This can be achieved by performing the conformal transformation $z = e^{-2\pi i \xi/R}$, for which we know how the critical correlators transform. Eq. (74) then yields

$$C_n = 12\frac{(-1)^n}{n!}(2\pi)^{1-\nu}\int_{\mathrm{pl}}\prod_{j=1}^{n-1}\frac{d^2z_j}{(2\pi|z_j|)^{\nu}} \sim e^{\frac{1}{(2\pi)^{\nu}}\ln n}$$

$$\times\left\langle \Phi_0(\infty,\infty)\Phi(1,1)\prod_{j=1}^{n-1}\Phi(z_j,\bar{z}_j)\Phi_0(0,0)\right\rangle_{\mathrm{conn}}. \tag{82}$$

Note the extra factors $|z_j|^{-\nu}$ in the integrand which are absent in CPT on the plane.

For the perturbed unitary CFTs we find [42, 48]

$$\bar{C}_1 = C_2 = 6(2\pi)^{1-2y}\int d^2z|z|^{-y}|1-z|^{-2(2-y)}$$

$$= 3(2\pi)^{2-2y}\gamma^2(1-\tfrac{1}{2}y)\gamma(y-1) \qquad \text{(unitary cases)}, \tag{83}$$

where $\gamma(s) = \Gamma(s)/\Gamma(1-s)$. (The integral converges for $1 < y < 2$, which is the case in all the models considered in this section.)

In the non-unitary CFTs $M_{2,2n+3}$ the first nonvanishing coefficient is

$$\bar{C}_1 = C_1 = -12(2\pi)^{1-y}C_{\Phi_0\Phi\Phi_0} \qquad \text{(non-unitary cases)}, \tag{84}$$

where the OPE coefficient is given by [48, 49]

$$(C_{\Phi_0\Phi\Phi_0})^2 = \frac{\gamma^2\left(\dfrac{1}{2n+3}\right)\gamma^3\left(\dfrac{2}{2n+3}\right)}{\gamma\left(\dfrac{4}{2n+3}\right)\gamma\left(-\dfrac{2n-1}{2n+3}\right)\gamma\left(-\dfrac{2n-3}{2n+3}\right)\gamma^2\left(\dfrac{2n}{2n+3}\right)}. \tag{85}$$

Note that $C_{\Phi_0\Phi\Phi_0}$ is real for $n > 1$, but purely imaginary for $n = 1$, indicating that the first model in the $A^{(2)}_{2n}$-related family, the perturbed Yang–Lee CFT, is somewhat special.

The sign of $C_{\Phi_0\Phi\Phi_0}$, as the sign of any other nontrivial OPE coefficient, is only determined after fixing the ambiguity in the overall signs of conformal fields. As indicated earlier, we have chosen the signs of the fields so that perturbations with positive λ (positive imaginary λ for the Yang–Lee CFT) lead to the massive theories considered.

As an example of the work involved in calculating the next coefficient $\bar{C}_2$ we consider the case of the $D^{(1)}_n$-related theories. (For $n = 3$ the following calculation gives us the coefficient $\bar{C}_2$ of the $A^{(1)}_3$-related theory, because the latter theory is identical to the $D^{(1)}_3$-related theory [3].) The $D^{(1)}_n$-related cases are relatively easy, as the critical correlators involved can be written in terms of those of a free boson $\varphi(z, \bar{z})$ (with no "screening"); namely, $\Phi(z, \bar{z}) = \sqrt{2}\ :\cos\varphi(z, \bar{z}/\sqrt{n}):$, so that

$$\left\langle \prod_{j=1}^{4}\Phi(z_j, \bar{z}_j)\right\rangle_{\text{conn}} = \tfrac{1}{4}\sum_s \prod_{1\le j<k\le 4}|z_j - z_k|^{2s_{jk}} - (|z_1 - z_2|\,|z_3 - z_4|)^{-4/n}$$

$$- (|z_1 - z_3|\,|z_2 - z_4|)^{-4/n} - (|z_1 - z_4|\,|z_2 - z_3|)^{-4/n}, \tag{86}$$

where $s_{jk} = 2s_js_k/n$ and the summation is over all $s = (s_1, s_2, s_3, s_4)$, $s_i = \pm 1$, such that $\sum_{i=1}^4 s_i = 0$. As in ref. [29], we expand factors of the form $|z_1 - z_2|^\alpha$ in a double

binomial series, and perform the integrations term by term using polar coordinates for the z_j. The integral for $\tilde{C}_2 = C_4$ is then replaced by the following sum, which is easier to control numerically:

$$\tilde{C}_2(D_n^{(1)}) = \tfrac{3}{8}(2\pi)^{-4+8/n} \sum_s \sum{}' (-1)^{m_1+n_1+m_3+n_5+m_6+n_6}$$

$$\times A_s(m_1, n_1, \ldots, m_6, n_6)\left(m_1 + m_2 + m_3 + \frac{1}{n}\right)^{-1}$$

$$\times\left(m_3 + m_5 + m_6 + \frac{1}{n}\right)^{-1}\left(m_2 + m_3 + m_4 + m_5 + \frac{2}{n} + s_{34}\right)^{-1}$$

$$-\tfrac{1}{4}(2\pi)^{-2+4/n}\tilde{C}_1(D_n^{(1)}) \sum_{k=0}^{\infty}\binom{-2/n}{k}^2\left(k + \frac{1}{n}\right)^{-2}. \tag{87}$$

Here $\sum'$ runs over $m_1, m_2, m_3, m_4, n_4, m_5, n_5, m_6, n_6$ from 0 to ∞, ignoring terms whose denominator vanishes (this reflects the cancellation between the IR non-integrable terms in the full and disconnected correlators), and

$$A_s(m_1, n_1, \ldots, m_6, n_6)$$

$$= \binom{s_{12}}{m_1}\binom{s_{12}}{n_1}\binom{s_{13}}{m_2}\binom{s_{13}}{n_2}\binom{s_{14}}{m_3}\binom{s_{14}}{n_3}\binom{s_{23}}{m_4}\binom{s_{23}}{n_4}\binom{s_{24}}{m_5}\binom{s_{24}}{n_5}\binom{s_{34}}{m_6}\binom{s_{34}}{n_6}, \tag{88}$$

with $n_1 = m_1 - m_4 + n_4 - m_5 + n_5$, $n_2 = m_2 + m_4 - n_4 - m_6 + n_6$, and $n_3 = m_3 + m_5 - n_5 + m_6 - n_6$. We evaluated $\tilde{C}_2(D_n^{(1)})$ numerically for $n = 3, 4, 5, 6$ by truncating the sum $\sum'$ above common values $N \leqslant 14$ for the 9 indices of summation, and then using rational extrapolation [50] with respect to $N^{-\omega}$ with ω chosen to give the best fit. The sum in the last line of eq. (87) was evaluated separately to a much higher accuracy. (The final results for $\tilde{C}_2$ are given in table 5 of sect. 7, where the error estimates reflect deviations between different extrapolations.)

6. Free bosons, free fermions and the Ising field theory

If the derivatives of the phase shifts of an S-matrix theory vanish, one can trivially solve the TBA equations and obtain explicit integral representations for all thermodynamic quantities. Not only free theories with trivial S-matrix $\mathcal{S} \equiv 1$, but also theories whose S-matrix differs from the trivial one by some scattering matrix elements that are equal to -1 have constant phase shifts (and this is the only other possibility allowed by unitarity, eq. (5)). From the TBA point of view, these latter theories are therefore equivalent to free theories, i.e. they have the same

infinite-volume thermodynamics. To avoid repeating the phrase "theories with constant phase shifts", we will refer to such S-matrix theories as *generalized* free theories, for short.

For free theories it is of course not necessary to use the TBA to calculate the thermodynamics. It is however quite instructive to do so for (generalized) free theories, in particular because one can rewrite the ground state scaling functions $\bar{c}(r)$ of these theories to explicitly exhibit their singularity structure. As a bonus, we will see that by combining these results with those of refs. [28, 29], we can obtain very compact expressions for the partition functions of free massive bosons and fermions, and of the Ising field theory, on the torus.

Recall that the *Ising field theory* [51] is obtained by a massive scaling limit (from above the critical temperature) of the Ising model at zero magnetic field. The theory contains a single (bosonic) particle in its spectrum, corresponding to the order variable σ of the Ising model, and its S-matrix is simply $S(\theta) \equiv -1$ (the $A_1^{(1)}$-related S-matrix theory). Its *infinite*-volume thermodynamics is therefore equal to that of a free fermion, since both theories describe a free fermionic type particle from the TBA point of view. We will explicitly see however, that its *finite*-volume thermodynamics differs from that of a free fermion – as it should.

Consider the purely elastic scattering theories of a single free fermionic and a single free bosonic type particle. With the derivative of the phase shift vanishing, the solution of eq. (34) (at zero chemical potential) is simply

$$\epsilon(\theta) = r \cosh \theta , \tag{89}$$

in both cases (we drop the subscript a, as there is only one particle species in each case). As expected, in generalized free theories the "dressed" one-particle energy $\epsilon(\theta)/R$ is equal to the "bare" one-particle energy $m \cosh \theta$. Denoting the ground-state scaling functions $\bar{c}(r)$ of free fermions and bosons by $c_{1/2}(r)$ and $c_0(r)$, respectively, eq. (44) then reads

$$c_{1/2,0}(r) = \pm \frac{6}{\pi^2} \int_0^\infty \mathrm{d}\theta \, r \cosh \theta \ln(1 \pm \mathrm{e}^{-r \cosh \theta}) . \tag{90}$$

In agreement with the general discussion in subsect. 3.2, these expressions are – up to a factor $-\pi/6R^2$ – just the free energies (or pressures) of ideal relativistic Fermi/Bose gases at $T = 1/R$ and $\mu = 0$.

We now rewrite these expressions to explicitly exhibit the singularities of the functions $c_{1/2,0}(r)$. First we expand the logarithm in eq. (90) in powers of $\mathrm{e}^{-r \cosh \theta}$ and integrate the resulting sum term by term. This gives

$$c_{1/2,0}(r) = \frac{6r}{\pi^2} \sum_{k=1}^{\infty} \frac{(\mp 1)^{k-1}}{k} K_1(kr) , \tag{91}$$

where $K_1(x)$ is a modified Bessel function. Taking first the $r \to 0$ limit, we obtain

$$c_{1/2,0}(0) = \frac{6}{\pi^2} \sum_{k=1}^{\infty} \frac{(\mp 1)^{k-1}}{k^2} = \begin{cases} \frac{1}{2} \\ 1 \end{cases} . \tag{92}$$

Next, using $[xK_1(x)]' = -xK_0(x)$, we find

$$\frac{1}{r}\frac{\mathrm{d}}{\mathrm{d}r} c_{1/2,0}(r) = -\frac{6}{\pi^2} \sum_{k=1}^{\infty} (\mp 1)^{k-1} K_0(kr) . \tag{93}$$

[This can also be obtained by first differentiating eq. (90) with respect to r,

$$\frac{\mathrm{d}}{\mathrm{d}r} c_{1/2,0}(r) = -\frac{6r}{\pi^2} \int_0^{\infty} \frac{\mathrm{d}\theta}{\mathrm{e}^{r\cosh\theta} \pm 1} , \tag{94}$$

from which the monotonic decrease of the $c_{1/2,0}(r)$ with r is manifest.] These sums of transcendental functions are of Schlömilch type and can be rewritten as sums of rational functions using formulas 8.526(1–2) of ref. [32]. A simple integration then gives

$$c_{1/2}(r) = \tfrac{1}{2} - \frac{3r^2}{2\pi^2}\left[\ln\frac{1}{r} + \tfrac{1}{2} + \ln\frac{4}{\pi} - \gamma_{\mathrm{E}}\right] + \frac{6}{\pi}\sum_{k=1}^{\infty}\left(\sqrt{(2k-1)^2\pi^2 + r^2} - (2k-1)\pi - \frac{r^2}{2(2k-1)\pi}\right) \tag{95}$$

and

$$c_0(r) = 1 - \frac{3r}{\pi} + \frac{3r^2}{2\pi^2}\left[\ln\frac{1}{r} + \tfrac{1}{2} + \ln 4\pi - \gamma_{\mathrm{E}}\right] - \frac{6}{\pi}\sum_{k=1}^{\infty}\left(\sqrt{(2k\pi)^2 + r^2} - 2k\pi - \frac{r^2}{4k\pi}\right), \tag{96}$$

where $\gamma_{\mathrm{E}} = 0.57721566\ldots$ is the Euler–Mascheroni constant. As expected, these functions do not have any singularities for physical, that is positive, values of r. There is however a branch cut starting at $r = 0$ coming from the $r^2 \ln(1/r)$ term. One can trace its origin to the logarithmic term in the free energy of the corresponding lattice models. Presumably more representative of generic perturbations of CFTs are the square-root singularities of the infinite sums at negative values of r^2 (we will return to this point in the sect. 8). The radius of convergence of these sums, r_0, is determined by the $k = 1$ term, namely $r_0 = \pi$ in the fermionic, and $r_0 = 2\pi$ in the bosonic case. Expanding the sums around $r = 0$ one obtains the

following expressions:

$$c_{1/2}(r) = \tfrac{1}{2} - \frac{3r^2}{2\pi^2}\left[\ln\frac{1}{r} + \tfrac{1}{2} + \ln\pi - \gamma_E \right.$$
$$\left. -4\sum_{n=1}^{\infty}\binom{\frac{1}{2}}{n+1}(1-2^{-2n-1})\zeta(2n+1)\left(\frac{r^2}{\pi^2}\right)^n\right], \quad (97)$$

$$c_0(r) = 1 - \frac{3r}{\pi} + \frac{3r^2}{2\pi^2}\left[\ln\frac{1}{r} + \tfrac{1}{2} + \ln 4\pi - \gamma_E \right.$$
$$\left. -2\sum_{n=1}^{\infty}\binom{\frac{1}{2}}{n+1}\zeta(2n+1)\left(\frac{r^2}{4\pi^2}\right)^n\right], \quad (98)$$

valid for $|r| < r_0$. Here $\zeta(s)$ is the Riemann zeta function.

We now discuss the partition functions of generalized free theories in a finite "volume". The above results, valid only in infinite volume, have one advantage over other methods of calculating partition functions, namely that we know the explicit small- *and* large-r behaviour of $c_{1/2,0}(r)$. One can therefore use the above results, trivial as they may seem, to supplement other approaches which provide most – but not all – information about the partition functions of generalized free theories on the torus (we have now switched to a euclidean description).

Ferdinand and Fisher [28] evaluated the partition function of the Ising model on an $N_L \times N_R$ lattice in the scaling limit where $N_R \to \infty$ with $\xi = N_L/N_R$ and $\tau \sim N_R(T - T_c)/T_c$ fixed (T_c is the critical temperature of the Ising model). Unfortunately, their calculation of the (logarithm of the) partition function was restricted to a power series expansion in τ with a finite radius of convergence (corresponding to our small-r expansions of $c_{1/2,0}(r)$; in fact, their τ equals our $r/2$). The large-τ behaviour of the partition function therefore remained unknown. In particular it was not possible to normalize the (scaled) partition function, see below.

Saleur and Itzykson [29] used ζ-function regularization of path integrals to calculate the partition functions of generalized free theories in finite volume. Their final results depend on the mass scale one has to introduce to perform ζ-function regularization (although this mass scale does not appear explicitly in ref. [29]). This mass scale has to be fixed by a normalization condition on the partition function. As discussed in sect. 3, it is natural to require that the ground-state energy $E_0(R)$ of the theory on a cylinder of circumference R vanish as $R \to \infty$. Such a requirement could not be implemented in ref. [29], because ζ-function regularization gave the partition functions in a form, which, although well defined for arbitrary tori, made it very difficult to extract the behaviour when the length of one of the cycles diverges. Since the ground state scaling functions $c_{1/2,0}(r)$ implement the above

normalization condition, one can fix the mass scale by comparing the small-r expansion of these functions with the results of Saleur and Itzykson. (It turns out that this amounts to replacing the area A of the torus in their expressions by the dimensionless quantity m^2A/e.) Their results can then be compactly written in terms of the $c_{1/2,0}(r)$, as follows.

We restrict their general results to tori of perpendicular cycles L and R; the expressions for arbitrary tori involve no qualitatively new element, they are just more lengthy. The building blocks of the partition functions can be written in terms of the path integral for a free Majorana fermion with various boundary conditions. They now read simply

$$D_{\alpha,\beta}(m|L,R) = \mathrm{e}^{-\delta_\beta \pi L c_\beta(r)/6R} \prod_{n\in\mathbb{Z}+\beta} \left(1 - \delta_\alpha \mathrm{e}^{-L\varepsilon_n(r)/R}\right). \tag{99}$$

where $\alpha, \beta \in \{0, \frac{1}{2}\}$ label the boundary conditions, periodic or antiperiodic, in the L ("time") and R ("space") directions, respectively, $\delta_\alpha = \mathrm{e}^{2\pi i\alpha}$, and

$$\frac{\varepsilon_n(r)}{R} = \sqrt{m^2 + \left(\frac{2\pi n}{R}\right)^2} \tag{100}$$

are just the energies allowed for a free particle in a box of length R. The partition function of a free massive boson (periodic real scalar field) is

$$Z_0(m|L,R) = D_{0,0}^{-1}(m|L,R) = \mathrm{e}^{\pi L c_0(r)/6R} \prod_{n\in\mathbb{Z}} \left(1 - \mathrm{e}^{-L\varepsilon_n(r)/R}\right)^{-1}, \tag{101}$$

that of a free fermion reads

$$Z_{\frac{1}{2}}(m|L,R) = D_{\frac{1}{2},\frac{1}{2}}(m|L,R) = \mathrm{e}^{\pi L c_{1/2}(r)/6R} \prod_{n\in\mathbb{Z}+\frac{1}{2}} \left(1 + \mathrm{e}^{-L\varepsilon_n(r)/R}\right), \tag{102}$$

and, finally, that of the Ising field theory is

$$\begin{aligned} Z_{\mathrm{IFT}}(m|L,R) &= \tfrac{1}{2}\left(D_{\frac{1}{2},\frac{1}{2}} + D_{0,\frac{1}{2}} + D_{\frac{1}{2},0} - D_{0,0}\right)(m|L,R) \\ &= \tfrac{1}{2}\exp\left[\frac{\pi L}{6R} c_{\frac{1}{2}}(r)\right] \\ &\quad \times \left\{ \prod_{n\in\mathbb{Z}+1/2} \left(1 + \mathrm{e}^{-(L/R)\varepsilon_n(r)}\right) + \prod_{n\in\mathbb{Z}+1/2} \left(1 - \mathrm{e}^{-(L/R)\varepsilon_n(r)}\right) \right. \\ &\qquad + \exp\left[-\frac{\pi L}{6R}\left(c_0(r) + c_{\frac{1}{2}}(r)\right)\right] \\ &\qquad \left. \times \left[\prod_{n\in\mathbb{Z}} \left(1 + \mathrm{e}^{-(L/R)\varepsilon_n(r)}\right) - \prod_{n\in\mathbb{Z}} \left(1 - \mathrm{e}^{-(L/R)\varepsilon_n(r)}\right)\right]\right\}. \end{aligned} \tag{103}$$

Note that these partition functions have exactly the same form as their well known massless limits, except for the "scale dependent central charges" $c_\beta(r)$ and the energies $\varepsilon_n(r)/R$ appropriate to massive free particles. Although it is not manifest, these partition functions are invariant under exchange of L and R, as their derivation shows [29].

We should comment on the fact that we have *subtracted* the last term $D_{0,0}$ in Z_{IFT}, not added it as in ref. [29]. This follows from the results for the partition function on the lattice [28,52] (it is not possible to deduce the correct sign by requiring modular invariance as $D_{0,0}$ is modular invariant by itself, nor by looking at the massless limit of the partition function, since $D_{0,0}$ vanishes then). Furthermore, only in this way can Z_{IFT} be interpreted as the partition function of a massive QFT. To see this latter point, expand the products in eq. (103) to write Z_{IFT} in the form

$$Z(L,R) = \mathrm{e}^{-LE_0(R)}\left[1 + \sum_{k=1}^{\infty} \mathrm{e}^{-L(E_k(R)-E_0(R))}\right], \tag{104}$$

where $E_k(R)$ is the energy of the kth excited state (in order of, say, increasing energy) when the theory is restricted to a periodic space of length R. If the theory has a mass gap m, the first contribution to the sum, $E_1(R)-E_0(R)$, is the finite-size corrected mass $m(R)$, which should approach m exponentially fast as $R\to\infty$. Indeed, from eq. (103) we read off

$$\begin{aligned} m(R) &= m + \frac{\pi}{6R}\left(c_0(r)+c_1(r)\right) = m\left(1+\frac{2}{\pi}\sum_{n=0}^{\infty}\frac{1}{2n+1}K_1((2n+1)r)\right) \\ &= \frac{2\pi}{R}\left[\frac{1}{8}+\frac{r}{4\pi}+\frac{1}{2\pi}\sum_{n=1}^{\infty}\left(\sqrt{(2n-1)^2\pi^2+r^2}+\pi-\sqrt{(2n\pi)^2+r^2}\right)\right] \\ &= \frac{2\pi}{R}\left[\frac{1}{8}+\frac{r}{4\pi}+\frac{r^2}{4\pi^2}\left(\ln 2+2\sum_{n=1}^{\infty}\binom{\frac{1}{2}}{n+1}(1-2^{-2n})\zeta(2n+1)\left(\frac{r}{\pi}\right)^{2n}\right)\right], \end{aligned} \tag{105}$$

the last expansion valid for $|r|<\pi$. We also see from eq. (103) that the last two terms in Z_{IFT} contain a whole "one-particle mass shell of states" appropriate to a boson, i.e. states with energies $\varepsilon_n(r)/R$, $n\in\mathbb{Z}$ (up to the same exponentially small corrections by which $m(R)$ differs from m for large r). Recall [53] that in the conformal limit $m\to 0$, $E_k-E_0=2\pi d_k/R$, where d_k is the scaling dimension of the field creating the state k. Here $d_1=\frac{1}{8}=d_\sigma$, so we obtain the expected result that the (bosonic) one-particle state in the Ising field theory is created by a massive analog of the spin field σ of the critical Ising model.

When Z_{IFT} is written in the form (104), the sum of the first two terms in eq. (103) contains only states with an even number of particles (the $\mathbb{Z}_2$-even vacuum sector), whereas the difference of the last two terms contains only states with an odd particle number (the $\mathbb{Z}_2$-odd σ-sector). The "construction" of Z_{IFT} from the fermionic building blocks $D_{\alpha,\beta}$ is therefore a massive analog of the GSO projection [54] in string theory.

For $r = Rm \gg 1$ the Bethe ansatz equations (24) (with L replaced by R and $S(\theta) \equiv -1$) imply that the energy of a multi-particle state in the odd (even) particle sector is given by a sum of terms of the form $\varepsilon_n(r)/R$ with $n \in \mathbb{Z}$ ($n \in \mathbb{Z} + \frac{1}{2}$). This is indeed what we see in eq. (103). Furthermore, in the even-particle sector there are no small r corrections to these "free energy levels", and in the odd-particle sector they are universal – i.e. independent of the number and momenta of the particles – and given by $m(R) - m$. The latter quantity should therefore be interpreted as the "ground-state energy" of the σ-sector measured with respect to the vacuum (although, to be sure, this "ground state" is of course not part of the spectrum of the massive theory). All other features of the spectrum are easily understood in terms of the massive free Majorana fermion underlying the Ising field theory, quite similar to the massless case.

7. Numerical work

Only in the case of the (generalized) free theories discussed in sect. 6 can the calculation of the complete thermodynamics be reduced to quadratures. For a generic purely elastic scattering theory one has to solve the nonlinear integral equation (34) for $\epsilon_a(\theta, r, \mu)$, which can only be done numerically (except for $r = 0, \infty$). In our numerical investigation of the thermodynamics of purely elastic scattering theories we concentrated on the ground-state scaling function $\tilde{c}(r)$ as this allows us to obtain several quantities characterizing the massive scattering theory, and, in particular, its UV limit.

From our discussion of conformal perturbation theory in sect. 5 we know that the function $\Sigma(r)$ in eq. (65) should be considered as the "perturbative part" of $\tilde{c}(r)$. The small-r behaviour of $\Sigma(r)$ determines $\tilde{y}$ and therefore the scaling dimension of the perturbing field. We can then fit $\Sigma(r)$ to a polynomial in $g \equiv r^{\tilde{y}}$ to obtain the first few coefficients a_n in eq. (78). From the a_n we are able to calculate the coefficient κ relating the perturbing parameter λ to the lowest mass in a given theory, eqs. (79) and (80), and estimate the position g_0 and form of the singularity of $\Sigma(r(g))$. The reader not interested in details of our numerical work can go directly to tables 2 to 6, where important final results are summarized.

To calculate $\tilde{c}(r)$ we have to numerically solve the nonlinear integral equation (34) for $\epsilon_a(\theta, r, \mu = 0)$ with fixed r, and then (numerically) perform the integral in eq. (44) determining $\tilde{c}(r)$. Suppressing the r-dependence, let us write eq. (34) as

$$\epsilon_a(\theta) = F_a\left[\{\epsilon_b(\theta)\}\right]. \tag{106}$$

In the case of the boson gas with a repulsive δ-function interaction treated by Yang and Yang [36], their (nonrelativistic) analog of this equation was proved to be solvable by simply iterating it, $\epsilon_a^{(n+1)}(\theta) = F_a[\{\epsilon_b^{(n)}(\theta)\}]$, $\epsilon_a(\theta) = \lim_{n\to\infty} \epsilon_a^{(n)}(\theta)$, using as initial $\epsilon_a^{(0)}(\theta)$ the nonrelativistic analog of our $r\hat{m}_a \cosh\theta$. The $\epsilon_a^{(n)}(\theta)$ then in fact monotonically decrease (pointwise) towards the unique solution. In our case with attractive interactions, the phase shifts in eq. (34) have a different sign compared to the repulsive case, and it is in general not possible to solve eq. (106) simply by iteration, no matter what initial $\epsilon_a^{(0)}(\theta)$ one uses. Except for the first few models in the $A_n^{(1)}$- and $A_{2n}^{(2)}$-related S-matrix theories the iteration does not converge for values of r smaller than about 1 (depending on the specific model), but rather leads to a "2-cycle" with different limits for even and odd n. The problem can be easily seen by looking at the special values $\epsilon_a(\theta = 0)$ as $r \to 0$. These values were called ϵ_a in sect. 4 and are determined by

$$\epsilon_a = f_a(\epsilon) \equiv \sum_{b=1}^{n} N_{ab} \ln(1 + e^{-\epsilon_b}) . \tag{107}$$

Although this equation has a unique real solution (cf. the remarks in sect. 4), one cannot solve it numerically by simple iteration, because the matrix of derivatives $\partial_{\epsilon_b} f_a = -N_{ab}/(e^{\epsilon_b} + 1)$ has, in general, some negative eigenvalues of magnitude larger than 1 at the unique fixed point $\{\epsilon_a\}$. This is the origin of the "2-cycle" property mentioned above.

This problem is of course easily circumvented. Consider the equation

$$\epsilon_a = f_a^{(M)}(\epsilon) \equiv \sum_{b=1}^{n} (M_{ab} f_b(\epsilon) + (1 - M)_{ab}\epsilon_b) , \tag{108}$$

where $M = (M_{ab})$ is an invertible $n \times n$ matrix which can depend on the ϵ_a, and $\mathbb{1}$ is the identity matrix. Clearly this equation has the same solution $\{\epsilon_a\}$ as eq. (107). However, for suitably chosen M the solution can be obtained by iteration, $\epsilon_a^{(n+1)} = f_a^{(M)}(\epsilon^{(n)})$. A simple choice of M leading to a convergent iteration is $M = \frac{1}{2}\mathbb{1}$. One can however make an *optimal* choice of M by requiring that the derivative matrix $\partial_{\epsilon_b} f_a^{(M)}$ vanish. Neglecting the derivatives of M with respect to the ϵ_a (which vanish at the fixed point), this leads to the optimal choice

$$M = (1 + \bar{N})^{-1} ,$$

where

$$\bar{N}_{ab} = \frac{N_{ab}}{1 + e^{\epsilon_b}} . \tag{109}$$

Compared to the simple choice $M = \frac{1}{2}\mathbb{1}$, this M cuts down dramatically the

number of iterations required to find the solution of eq. (107) to a given accuracy – by a factor of about 10–20.

Exactly the same method can be used to iteratively solve the integral equation (106) for the $\epsilon_a(\theta)$. We discretize the θ-axis (in steps of $\Delta\theta$) and replace the integral implicit on the r.h.s. of eq. (106) by a sum. Since the $\epsilon_a(\theta)$ are symmetric functions we only have to consider $\theta \geqslant 0$, and since $\tilde{c}(r)$ depends on $\epsilon_a(\theta)$ only through $L_a(\theta) = \ln(1 + e^{-\epsilon_a(\theta)})$ we can restrict ourselves to $\theta < \theta_{max}$, where $L_a(\theta)$ is not negligible (θ_{max} can fortunately be predicted beforehand, since $\epsilon_a(\theta) \simeq rm_a \cosh\theta$ for θ much larger than $\ln(2/r)$). We know that for small r the $\epsilon_a(\theta)$ are close to ϵ_a in most of the region $|\theta| < \theta_{max}$, so that the choice of M given by eq. (109) with $\epsilon_b = \epsilon_b(\theta)$ is a good one. As r increases the choice of M becomes less important, and from some r-value on (which depends quite strongly on the model) no advantage is gained by using eq. (109) for M instead of $M = \frac{1}{2}\mathbb{1}$.

Depending on the model and the value of r, we found it necessary to use $\Delta\theta = 0.016$–0.05 to achieve double precision accuracy. Solving eq. (106) successively for increasing (or decreasing) values of r it is convenient to use the solution $\epsilon_a^{(\infty)}(\theta, r)$ as the ansatz $\epsilon_a^{(0)}(\theta, r + \Delta r)$ for the next r-value. For the first r-value we used $\epsilon_a^{(0)}(\theta) = r\hat{m}_a \cosh\theta$, if $r > \epsilon_1$. For smaller initial values of r we used as an ansatz a function interpolating between $r\hat{m}_a \cosh\theta$ for $|\theta| \gg \ln(2/r)$ and the constant ϵ_a for small θ. With these ansätze a maximum of about 60 iterations was sufficient to obtain $\tilde{c}(r)$ to double precision accuracy in all models for any value of r. (For very small and in particular for large r, a much smaller number of iterations is required.)

We calculated $\tilde{c}(r)$ and its perturbative part $\Sigma(r)$ for $r = 0.0$–2.0 in steps of $\Delta r = 0.01$ for the smallest models, up to $\Delta r = 0.025$ for the largest models we investigated, and with somewhat larger r steps for $r = 2.0$–15.0. For the physically important case of the $E_8^{(1)}$-related S-matrix theory some of the calculated $\tilde{c}(r)$ values are shown in table 2.

We usually also calculated $\tilde{c}(r)$ for a few very small r-values. Using the ratio of $\Sigma(r)$ for two small r-values we estimated $\tilde{y}$. In all cases we obtained the value expected from CFT (table 1, and eq. (2)) to high accuracy, as comparison with table 3 shows. (We have checked that the tiny deviation from the exact value is entirely due to a combination of numerical error in $\tilde{c}(r)$ and the fact that $\tilde{y}$ is extracted from finite, not infinitesimal, values of r.)

We then used standard fitting routines [50] to fit $\Sigma(r(g)) = \sum_{n=1}^{\infty} a_n g^n$ to a polynomial in $g \equiv r^{\tilde{y}}$, obtaining 6 of the coefficients a_n to at least 2 digits, with successively higher accuracy for smaller n. (In the fitting we do not let $\tilde{y}$ be a free parameter, but rather use the theoretical value, to obtain the a_n as accurate as possible.) It is difficult to obtain the higher a_n accurately because their magnitudes decrease rapidly with n (by roughly one order of magnitude from a_n to a_{n-1}), and for the fitting one can only use r-values quite a bit smaller than the radius of convergence of $\Sigma(r)$, which (see table 6 below) turns out to be smaller than 3.0 in

TABLE 2

Numerical results for the ground-state scaling function $\tilde{c}(r)$ of the $E_8^{(1)}$-related S-matrix theory, describing the scaling limit of the $T = T_c$ Ising model in a magnetic field.
The error in the last digit given for $\tilde{c}(r)$ is at most 2

r	$\tilde{c}(r)$	r	$\tilde{c}(r)$
0.025	$4.99926331494289 \times 10^{-1}$	3.4	$5.89376787062673 \times 10^{-2}$
0.050	$4.99705463734389 \times 10^{-1}$	3.5	$5.36363341869881 \times 10^{-2}$
0.075	$4.99337749094963 \times 10^{-1}$	3.6	$4.88053822691252 \times 10^{-2}$
0.100	$4.98823708366504 \times 10^{-1}$	3.7	$4.44052616117557 \times 10^{-2}$
0.125	$4.98164013110821 \times 10^{-1}$	3.8	$4.03991138110232 \times 10^{-2}$
0.150	$4.97359474791394 \times 10^{-1}$	3.9	$3.67527700509491 \times 10^{-2}$
0.175	$4.96411036991531 \times 10^{-1}$	4.0	$3.34346830588822 \times 10^{-2}$
0.200	$4.95319769399916 \times 10^{-1}$	4.1	$3.04158216805058 \times 10^{-2}$
0.225	$4.94086862928673 \times 10^{-1}$	4.2	$2.76695414108395 \times 10^{-2}$
0.250	$4.92713625608369 \times 10^{-1}$	4.3	$2.51714409580728 \times 10^{-2}$
0.275	$4.91201479039967 \times 10^{-1}$	4.4	$2.28992123033228 \times 10^{-2}$
0.300	$4.89551955257350 \times 10^{-1}$	4.5	$2.08324896610729 \times 10^{-2}$
0.325	$4.87766693897389 \times 10^{-1}$	4.6	$1.89527011496462 \times 10^{-2}$
0.350	$4.85847439601564 \times 10^{-1}$	4.7	$1.72429257623807 \times 10^{-2}$
0.375	$4.83796039590923 \times 10^{-1}$	4.8	$1.56877573125159 \times 10^{-2}$
0.400	$4.81614441368206 \times 10^{-1}$	4.9	$1.42731763438564 \times 10^{-2}$
0.425	$4.79304690509478 \times 10^{-1}$	5.0	$1.29864305021782 \times 10^{-2}$
0.450	$4.76868928513721 \times 10^{-1}$	5.2	$1.07511126086937 \times 10^{-2}$
0.475	$4.74309390683407 \times 10^{-1}$	5.4	$8.90111763998775 \times 10^{-3}$
0.50	$4.71628404012539 \times 10^{-1}$	5.6	$7.36978174473723 \times 10^{-3}$
0.55	$4.65911837798670 \times 10^{-1}$	5.8	$6.10203326568294 \times 10^{-3}$
0.60	$4.59739597956175 \times 10^{-1}$	6.0	$5.05237182434778 \times 10^{-3}$
0.65	$4.53133378846928 \times 10^{-1}$	6.2	$4.18319533612114 \times 10^{-3}$
0.70	$4.46116124267222 \times 10^{-1}$	6.4	$3.46341882149619 \times 10^{-3}$
0.75	$4.38711944036403 \times 10^{-1}$	6.6	$2.86733577979935 \times 10^{-3}$
0.80	$4.30946022694608 \times 10^{-1}$	6.8	$2.37368010496008 \times 10^{-3}$
0.85	$4.22844519254401 \times 10^{-1}$	7.0	$1.96485327374165 \times 10^{-3}$
0.90	$4.14434457231968 \times 10^{-1}$	7.2	$1.62628750899834 \times 10^{-3}$
0.95	$4.05743604488329 \times 10^{-1}$	7.4	$1.34592073600149 \times 10^{-3}$
1.0	$3.96800342745280 \times 10^{-1}$	7.6	$1.11376344671011 \times 10^{-3}$
1.1	$3.78272335483171 \times 10^{-1}$	7.8	$9.21541152655297 \times 10^{-4}$
1.2	$3.59084195897229 \times 10^{-1}$	8.0	$7.62399044331348 \times 10^{-4}$
1.3	$3.39469629401242 \times 10^{-1}$	8.2	$6.30657883863993 \times 10^{-4}$
1.4	$3.19656811102667 \times 10^{-1}$	8.4	$5.21612128671341 \times 10^{-4}$
1.5	$2.99862888891790 \times 10^{-1}$	8.6	$4.31362894900813 \times 10^{-4}$
1.6	$2.80288817111835 \times 10^{-1}$	8.8	$3.56679686270771 \times 10^{-4}$
1.7	$2.61114884078821 \times 10^{-1}$	9.0	$2.94885890913750 \times 10^{-4}$
1.8	$2.42497252776712 \times 10^{-1}$	9.2	$2.43763930448659 \times 10^{-4}$
1.9	$2.24565739146455 \times 10^{-1}$	9.4	$2.01476668087547 \times 10^{-4}$
2.0	$2.07422923049108 \times 10^{-1}$	9.6	$1.66502275571734 \times 10^{-4}$
2.1	$1.91144548068371 \times 10^{-1}$	9.8	$1.37580246020508 \times 10^{-4}$
2.2	$1.75781043829842 \times 10^{-1}$	10.0	$1.13666640726895 \times 10^{-4}$
2.3	$1.61359918347485 \times 10^{-1}$	10.5	$7.04809865230710 \times 10^{-5}$
2.4	$1.47888727315849 \times 10^{-1}$	11.0	$4.36676102507654 \times 10^{-5}$
2.5	$1.35358330353019 \times 10^{-1}$	11.5	$2.70340037942969 \times 10^{-5}$
2.6	$1.23746180823480 \times 10^{-1}$	12.0	$1.67240329807804 \times 10^{-5}$
2.7	$1.13019452151614 \times 10^{-1}$	12.5	$1.03387490242338 \times 10^{-5}$
2.8	$1.03137866044278 \times 10^{-1}$	13.0	$6.38716048950996 \times 10^{-6}$
2.9	$9.40561464929706 \times 10^{-2}$	13.5	$3.94345230989347 \times 10^{-6}$
3.0	$8.57260716570693 \times 10^{-2}$	14.0	$2.43326653171983 \times 10^{-6}$
3.1	$7.80981313371979 \times 10^{-2}$	14.5	$1.50058878860110 \times 10^{-6}$
3.2	$7.11228210605372 \times 10^{-2}$	15.0	$9.24924705350322 \times 10^{-7}$
3.3	$6.47516167162642 \times 10^{-2}$	15.5	$5.69818571906847 \times 10^{-7}$

TABLE 3

Numerical results for $\tilde{c}(r)$ and its perturbative part $\Sigma(r)$ for two small values of r, and the corresponding estimated $\hat{y} = (\ln(r_2/r_1))^{-1} \ln(\Sigma(r_2)/\Sigma(r_1))$. The error in the last digit given for $\tilde{c}(r)$ and $\Sigma(r)$ is at most 2

$\hat{\mathscr{G}}$	r	$\tilde{c}(r)$	$\Sigma(r)$	Estimated $\hat{y}$
$A_3^{(1)}$	0.01	0.999953262281947	$1.008764874 \times 10^{-6}$	
	0.02	0.999815419323971	$6.405255681 \times 10^{-6}$	2.66666621
$A_5^{(1)}$	0.025	1.24965844965296	$3.030212603 \times 10^{-6}$	
	0.05	1.24864591940887	$2.424164742 \times 10^{-5}$	2.99999682
$A_7^{(1)}$	0.025	1.39957967500417	$1.698277372 \times 10^{-6}$	
	0.05	1.39832751334396	$1.5606436754 \times 10^{-5}$	3.19999717
$A_2^{(2)}$	0.001	0.399999735051974	1.0716422×10^{-8}	
	0.002	0.399998953903823	5.6561614×10^{-8}	2.4000000
$A_4^{(2)}$	0.02	0.571329513317953	$1.349135659 \times 10^{-6}$	
	0.04	0.571036717982579	$9.775539116 \times 10^{-6}$	2.85714085
$A_6^{(2)}$	0.02	0.666545062218714	$5.35639773 \times 10^{-7}$	
	0.04	0.666182734494727	$4.628178962 \times 10^{-6}$	3.11110966
$A_8^{(2)}$	0.02	0.727124515842661	$3.49252212 \times 10^{-7}$	
	0.04	0.726681859963654	$3.375420041 \times 10^{-6}$	3.27272588
$D_4^{(1)}$	0.01	0.999972507850553	7.4295324×10^{-8}	
	0.02	0.999890328583463	$5.94362547 \times 10^{-7}$	2.9999999
$D_5^{(1)}$	0.025	0.999789631890275	$6.43526875 \times 10^{-7}$	
	0.05	0.999161867194632	$5.913741029 \times 10^{-6}$	3.19999876
$D_6^{(1)}$	0.025	0.999746644718168	$4.92120032 \times 10^{-7}$	
	0.05	0.998989570647096	$4.960254554 \times 10^{-6}$	3.33333201
$E_6^{(1)}$	0.025	0.857016839032789	$1.07128409 \times 10^{-7}$	
	0.05	0.856639509661813	$1.153472868 \times 10^{-6}$	3.42857104
$E_7^{(1)}$	0.02	0.699928050129612	2.1005502×10^{-8}	
	0.04	0.699712371203531	$2.54707093 \times 10^{-7}$	3.5999999
$E_8^{(1)}$	0.025	0.499926331494289	1.4570792×10^{-8}	
	0.05	0.499705463734389	$1.96040398 \times 10^{-7}$	3.7499998

all models. The values of the first six a_n are shown in table 4 for the models we investigated.

In tables 3 and 4 we have not given results for the $A_{2n}^{(1)}$-related theories. The reason is that the $\tilde{c}(r)$ and $\Sigma(r)$ functions in the $A_{2n}^{(1)}$-related theory are just twice those of the $A_{2n}^{(2)}$-related theory, as remarked in sect. 1. They therefore have the same $\tilde{y}$, and their a_n differ by a factor of 2.

From a_1 and the first nonvanishing coefficient $\tilde{C}_1$ of CPT (given analytically in eqs. (83) and (84) of sect. 5) we can obtain the coefficient κ relating the perturbation parameter λ to the lightest mass in the theory, cf. eqs. (79) and (80). $\tilde{C}_1$ and κ are shown in table 5. To compare the TBA with CPT we have calculated the TBA prediction for $\tilde{C}_2$ from eq. (81) (with a_2 from table 4), and included it in table 5 with the CPT result for $\tilde{C}_2$, whose calculation was outlined in sect. 5 for the $A_3^{(1)}$- and $D_{4-6}^{(1)}$-related models. For the Yang–Lee CFT (the $A_2^{(2)}$-related model) $\tilde{C}_2$

TABLE 4
The first coefficients a_n in the small g expansion of $\Sigma(r(g))$, $g = r^{\hat{\gamma}}$.
The error in the last digit is given in parentheses

$\hat{\mathcal{G}}$	a_1	a_2	a_3
$A_3^{(1)}$	$2.1733181681754(2) \times 10^{-1}$	$-2.7508491350(5) \times 10^{-3}$	$9.7354738(5) \times 10^{-5}$
$A_5^{(1)}$	$1.9393366771633(4) \times 10^{-1}$	$-3.906611329(1) \times 10^{-3}$	$1.9026114(1) \times 10^{-4}$
$A_7^{(1)}$	$2.2730066166665(3) \times 10^{-1}$	$-7.295920479(2) \times 10^{-3}$	$5.4223150(4) \times 10^{-4}$
$A_2^{(2)}$	$1.6984384285839(1) \times 10^{-1}$	$-1.6304729871(2) \times 10^{-3}$	$5.7099303(2) \times 10^{-5}$
$A_4^{(2)}$	$9.6439673313328(1) \times 10^{-2}$	$-1.5383117495(4) \times 10^{-3}$	$6.2220872(5) \times 10^{-5}$
$A_6^{(2)}$	$1.0340876048977(2) \times 10^{-1}$	$-2.6333052786(5) \times 10^{-3}$	$1.5783872(6) \times 10^{-4}$
$A_8^{(2)}$	$1.2688336314925(7) \times 10^{-1}$	$-5.105047678(4) \times 10^{-3}$	$4.7049522(5) \times 10^{-4}$
$D_4^{(1)}$	$7.429532361212 1(5) \times 10^{-2}$	$-6.3767173643(5) \times 10^{-4}$	$1.28642333(5) \times 10^{-5}$
$D_5^{(1)}$	$8.6130844616 73(2) \times 10^{-2}$	$-1.2063008718(3) \times 10^{-3}$	$3.7603081(2) \times 10^{-5}$
$D_6^{(1)}$	$1.0771372826766(3) \times 10^{-1}$	$-2.378406774(1) \times 10^{-3}$	$1.1417359(1) \times 10^{-4}$
$E_6^{(1)}$	$3.3318219272 18(1) \times 10^{-2}$	$-2.835975423(2) \times 10^{-4}$	$5.1154305(5) \times 10^{-6}$
$E_7^{(1)}$	$2.7455231631 14(1) \times 10^{-2}$	$-2.916675500(2) \times 10^{-4}$	$6.402701(2) \times 10^{-6}$
$E_8^{(1)}$	$1.4832286811 47(1) \times 10^{-2}$	$-1.417067561(2) \times 10^{-4}$	$2.750083(1) \times 10^{-6}$
	a_4	a_5	a_6
$A_3^{(1)}$	$-4.38087(2) \times 10^{-6}$	$2.2147(4) \times 10^{-7}$	$-1.20(1) \times 10^{-8}$
$A_5^{(1)}$	$-1.175218(5) \times 10^{-5}$	$8.157(1) \times 10^{-7}$	$-6.06(3) \times 10^{-8}$
$A_7^{(1)}$	$-5.10918(4) \times 10^{-5}$	$5.410(1) \times 10^{-6}$	$-6.12(2) \times 10^{-7}$
$A_2^{(2)}$	$-2.556045(7) \times 10^{-6}$	$1.2857(2) \times 10^{-7}$	$-6.93(2) \times 10^{-9}$
$A_4^{(2)}$	$-3.19411(3) \times 10^{-6}$	$1.843(1) \times 10^{-7}$	$-1.14(1) \times 10^{-8}$
$A_6^{(2)}$	$-1.199577(4) \times 10^{-5}$	$1.0245(2) \times 10^{-6}$	$-9.37(4) \times 10^{-8}$
$A_8^{(2)}$	$-5.49745(5) \times 10^{-5}$	$7.217(1) \times 10^{-6}$	$-1.01(1) \times 10^{-6}$
$D_4^{(1)}$	$-3.26975(2) \times 10^{-7}$	$9.322(3) \times 10^{-9}$	$-2.85(3) \times 10^{-10}$
$D_5^{(1)}$	$-1.47374(1) \times 10^{-6}$	$6.476(2) \times 10^{-8}$	$-3.05(2) \times 10^{-9}$
$D_6^{(1)}$	$-6.88670(6) \times 10^{-6}$	$4.660(4) \times 10^{-7}$	$-3.40(5) \times 10^{-8}$
$E_6^{(1)}$	$-1.15671(2) \times 10^{-7}$	$2.931(2) \times 10^{-9}$	$-7.98(7) \times 10^{-11}$
$E_7^{(1)}$	$-1.7595(1) \times 10^{-7}$	$5.41(1) \times 10^{-9}$	$-1.8(1) \times 10^{-10}$
$E_8^{(1)}$	$-6.6752(2) \times 10^{-8}$	$1.814(3) \times 10^{-9}$	$-5.3(2) \times 10^{-11}$

was first calculated in ref. [21]. Our somewhat more accurate evaluation of the corresponding integral, included in table 5, was obtained by a technique similar to that used in the $D_n^{(1)}$ cases; but here the integral gives rise to an only triple-infinite sum, which allows us to obtain $\tilde{C}_2$ more accurately than with the TBA. This provides a successful test of the accuracy of our TBA results for the a_n. The value of $\tilde{C}_2$ for the $E_8^{(1)}$-related theory is from ref. [29]. Note that except for this latter value the agreement between the TBA and CPT predictions is perfect. We believe that the slight discrepancy in the E_8 case is due to the fact that the CPT result for $\tilde{C}_2$ of ref. [29] is not quite accurate to the precision given. (The value of $\tilde{C}_1$ given in ref. [29], where it was calculated numerically, also does not quite agree with our analytical result, eq. (83), for this coefficient.)

TABLE 5

The analytically known first coefficient $\tilde{C}_1$ of CPT, eqs. (83) and (84), the value of κ obtained as $(a_1/\tilde{C}_1)^{\nu/\hat{\nu}}$ (with a_1 from table 4), the TBA prediction for $\tilde{C}_2$, eq. (81), and the CPT result for $\tilde{C}_2$. The exact values for the Ising field theory ($A_1^{(1)}$) are shown for comparison

$\hat{\mathscr{G}}$	$\tilde{C}_1$	$\kappa = \lambda m_1^{-\nu}$	$\tilde{C}_2$ (TBA)	$\tilde{C}_2$ (CPT)
$A_1^{(1)}$	∞	$(2\pi)^{-1}$	$-21\zeta(3)/2$	$-21\zeta(3)/2^a$
$A_2^{(1)}$	12.58308592696532	0.1643033129407 28(5)	−4.4746422804(6)	
$A_3^{(1)}$	6.822131955170958	0.178484948224174(8)	−2.71056684756(5)	−2.7107(5)
$A_4^{(1)}$	5.016102325614698	0.196091906729 57(1)	−2.08082556 49(5)	
$A_5^{(1)}$	4.179611789057032	0.215406414960 93(2)	−1.8145363559(5)	
$A_6^{(1)}$	3.722555422994466	0.235707324291 18(2)	−1.7062351868(3)	
$A_7^{(1)}$	3.451207388176337	0.256634371184 02(2)	−1.6819799204(5)	
$A_8^{(1)}$	3.283893388644309	0.277985929252 74(8)	−1.709773346(1)	
$A_2^{(2)}$	$-1.750093194020531i$	$0.097048456298606(6)i$	0.1731156555(2)	0.1731156555 5984(2)
$A_4^{(2)}$	2.378996974689406	0.040537955423786(4)	−0.9360966167(2)	
$A_6^{(2)}$	5.198797174960418	0.019890901108401(4)	−6.655677855(1)	
$A_8^{(2)}$	8.177679609711356	0.015515814901646(9)	−21.20560281(2)	
$D_4^{(1)}$	4.179611789057032	0.133325360490478(5)	−2.0181158889(2)	−2.01812(3)
$D_5^{(1)}$	3.451207388176337	0.157976986177 75(2)	−1.9367802357(5)	−1.93676(4)
$D_6^{(1)}$	3.180437510254713	0.184031470214 51(3)	−2.0735654615(9)	−2.073565(1)
$E_6^{(1)}$	3.086187627468699	0.103903392586 19(2)	−2.433232175(2)	
$E_7^{(1)}$	3.185717895036244	0.092834392226 73(2)	−3.9269242 12(3)	
$E_8^{(1)}$	3.854530510914108	0.062032361354 76(2)	−9.5701182 1(1)	−9.5704(2)[a]

[a] From ref. [29].

To further demonstrate the accuracy of the TBA results as compared to other methods, we mention a universal quantity which is of interest in magnetic systems [29, 55–57]:

$$\mathscr{R} = -\tfrac{1}{3} \lim_{N_R \to \infty} \frac{m_4(N_R)}{[N_R m_2(N_R)]^2}, \tag{110}$$

where

$$m_2(N_R) = \lim_{N_L \to \infty} (N_L N_R)^{-1} \langle M^2 \rangle,$$

$$m_4(N_R) = \lim_{N_L \to \infty} (N_L N_R)^{-1} [\langle M^4 \rangle - 3\langle M^2 \rangle^2] \tag{111}$$

are the first cumulants of the total magnetization M on an $N_L \times N_R$ lattice (with periodic boundary conditions) at criticality. For the Ising model $\mathscr{R}$ was evaluated numerically using transfer matrix methods [56] and a Monte Carlo calculation [57]. The quoted result of both methods is 2.46044(2). CPT predicts $\mathscr{R} = -12\tilde{C}_2/(\pi\tilde{C}_1^2)$,

estimated [29] as $\mathscr{R} = 2.46048(5)$ (cf. table 5). From our TBA results for the $E_8^{(1)}$-related model we estimate $\mathscr{R} = -12a_2/(\pi a_1^2)$ to be 2.460399897(4).

If we assume that $\Sigma(r(g))$ has a singularity of the form

$$\Sigma(r(g)) \propto (g - g_0)^{\alpha} \qquad \text{as } g \to g_0, \tag{112}$$

we can estimate the position g_0 and exponent α of the singularity from the ratios of successive a_n. If (112) were true for all g, we would have

$$r_n \equiv \frac{a_{n+1}}{a_n} = \frac{1}{g_0}\left(1 - \frac{\alpha + 1}{n + 1}\right). \tag{113}$$

If there are additional singularities in (112) of the same form with a g_0 of larger magnitude, a larger α, or, in general, any weaker singularity (including regular contributions), there will be $o(1/n)$ corrections to the ratios r_n. A simple and efficient way to take these corrections into account when extrapolating the r_n to $n = \infty$ to obtain $g_0 = 1/r_\infty$, is to perform rational extrapolation [50] on the r_n considered as a function of $1/n$ (this gives much better results than, for instance, polynomial extrapolation in $1/n$). From the slope of the function obtained by extrapolating the r_n at $1/n = 0$ we can also obtain an estimate for the exponent α. In the extrapolation it is important to know as many a_n as accurate as possible; that is why we made some effort to calculate the $\bar{c}(r)$ to high precision.

Our results are shown in table 6. The error estimates for g_0 and α presented in this table were obtained by observing how g_0 and α vary as we fit $\Sigma(r(g))$ to

TABLE 6
Numerically obtained parameters of the first singularity of the perturbative part of the ground-state scaling function, $\Sigma(r(g)) \propto (g - g_0)^{\alpha}$ as $g \to g_0$. For comparison note the exact values of the Ising field theory

$\hat{\mathfrak{g}}$	g_0	$r_0 = \lvert g_0 \rvert^{1/\delta}$	α
$A_1^{(1)}$	$-\pi^2$	π	$\frac{1}{2}$
$A_2^{(1,2)}$	−13.9(1)	2.99(1)	0.49(5)
$A_3^{(1)}$	−13.8(2)	2.68(2)	0.51(5)
$A_4^{(1,2)}$	−12.0(2)	2.39(2)	0.50(5)
$A_5^{(1)}$	−10.1(2)	2.16(1)	0.49(6)
$A_6^{(1,2)}$	−8.2(2)	1.97(2)	0.49(5)
$A_7^{(1)}$	−6.6(2)	1.80(2)	0.48(7)
$A_8^{(1,2)}$	−5.4(2)	1.67(2)	0.5(1)
$D_4^{(1)}$	−24.5(2)	2.904(8)	0.52(6)
$D_5^{(1)}$	−15.9(2)	2.374(8)	0.51(5)
$D_6^{(1)}$	−10.5(3)	2.02(2)	0.50(8)
$E_6^{(1)}$	−27.7(3)	2.635(8)	0.50(3)
$E_7^{(1)}$	−22.9(2)	2.386(6)	0.47(6)
$E_8^{(1)}$	−25.8(2)	2.379(7)	0.50(4)

polynomials of different orders and as we vary the number of "data points" $\tilde{c}(r)$ using in the fitting process. (This is a safer method than just taking the "fitting run" with the smallest (reduced) χ^2, and take as error the error of the extrapolation for this one run.) Usually the last coefficient a_n determined in a specific fitting run has a much larger error than the other ones, and correspondingly the last ratio should not be considered in the extrapolation to $n = \infty$.

The above procedure gives relatively small errors. To be sure that there are no sources of systematic errors we have tested the whole method on the case of massive free fermions (see sect. 6), where we know the exact values of g_0 and α. In this case the calculation of $\tilde{c}(r)$ reduces to the numerical integration of the r.h.s. of eq. (90) and we now also subtract the $r^2 \ln(1/r)$ term in eq. (97) from $\tilde{c}(r)$ when calculating $\Sigma(r)$. Comparison of the results with the exact coefficients a_n, which can be read off from eq. (97), and with the exact values $g_0 = -\pi^2$ and $\alpha = \frac{1}{2}$ shows that our error estimates are reliable in this case, and therefore presumably in general.

In sect. 4 we mentioned various properties of the functions $\hat{\epsilon}_a(\theta, r, \mu = 0)$, $\psi_a(\theta, r)$ and $\tilde{\psi}_a(\theta, r)$. These were confirmed numerically for several models by solving the integral equations determining these functions using the method discussed for $\epsilon_a(\theta)$.

8. The singularity structure of $\tilde{c}(r)$

The exponent α of the leading singularity of $\Sigma(r(g))$ in table 6 is always very close to 0.5. In fact, we claim that $\alpha = \frac{1}{2}$ *exactly*. As we now explain, this is related to the well-known fact that at crossing points of eigenvalues of perturbed operators generically only two eigenvalues "collide". Another, perhaps more physical way to understand the singularities of $\Sigma(r(g))$ will be presented later in this section.

Consider first perturbation theory in a *finite*-dimensional Hilbert space [46]. The eigenvalues $E_n(\lambda)$ of a perturbed operator $H_\lambda = H_0 + \lambda V$ are then just branches of algebraic functions of the perturbing parameter λ, since they are solutions of the characteristic equation. The singularities of the eigenvalues are therefore (non-logarithmic) branch points. It is clear that for a branch point of order m to occur at some λ, at least m eigenvalues must degenerate at this λ. It is also easy to see that the eigenvalues stay finite at the branch points. Now, generically, at most two eigenvalues coincide at any given λ, so that all singularities are expected to be square-root branch points. (One can of course find examples in which three or more eigenvalues become degenerate at some point, but in the space of, say, hermitian matrices representing the operators H_λ such a situation occurs "very rarely", in a sense which can be made precise [58]. We are not aware of any field-theory-related examples in which higher branch points occur, although this might just be a sign that more complicated theories, which exhibit such behaviour, have not been studied yet.)

How are the above considerations related to our case of perturbations of CFTs, whose Hilbert space is infinite dimensional? Imagine *truncating* the Hilbert space of the theory to a finite-dimensional space of, say, dimension N. In a CFT the truncation can be performed very naturally according to the (left and right) conformal dimensions of the states, for instance [59]. For any fixed N the above remarks then apply, showing that the perturbative part of the (rescaled) ground state energy, $\Sigma^{(N)}(r(g))$ (cf. eq. (65)), has only square-root singularities in the truncated Hilbert space (modulo the possibility of higher order branch points). Let us denote the positions of the singularities of $\Sigma^{(N)}(r(g))$ by $g_n^{(N)}$. Unless one has chosen a very perverse sequence of truncations of the Hilbert space of the theory one would expect that as $N \to \infty$ the positions of the singularities stabilize, i.e. that at least for $n \ll N$ we can uniquely identify $g_n^{(N)}$ as N varies, and that $g_n = \lim_{N\to\infty} g_n^{(N)}$ exists. If the singularities are (square-root) branch points for finite N, they must remain so as $N \to \infty$. The qualitative nature of the singularities can change at $N = \infty$ only at values of g where the set of g_n has an accumulation point. Barring this latter possibility, $\Sigma(r(g))$ is expected to be a branch of an analytic function with square-root singularities. (We are ignoring all subtleties related to the fact $\Sigma(r(g))$ actually lives on some Riemann surface of infinite genus. Analytic continuation around one branch point can then actually lead to an eigenvalue *different* from the lowest one we started with! This in fact happens for the anharmonic oscillator [60–62] where all eigenvalues of a given parity live on one and the same Riemann surface, each sheet of the Riemann surface corresponding to one energy level.)

For perturbations of CFTs with $\tilde{y} > 2$ our numerical results clearly indicate that at least the first singularity g_0 is an isolated square-root singularity. The work of Yurov and Zamolodchikov [59], who numerically studied the eigenvalues of the hamiltonian of the perturbed Yang–Lee CFT at various truncation levels, shows that up to the largest $|g|$ they investigated only two eigenvalues collide at a time, so that the corresponding singularities are also square-root branch points. Their results also support the general scenario sketched above, with the stabilization of the g_n already occurring for relatively small N.

Note that this picture of "colliding eigenvalues" also explains certain qualitative features of our numerical results for the positions of the first singularity g_0, e.g. that in the $A_n^{(1)}$-, $A_{2n}^{(2)}$-, and $D_n^{(1)}$-related theories g_0 moves closer to the origin as n increases (cf. table 6). This is presumably related to the fact that in the corresponding unperturbed CFTs the gap between the ground state and the next energy level decreases as n increases; i.e. the difference between the lowest and the next-to-lowest scaling dimensions becomes smaller. If energy levels collide at some negative g, they will typically collide earlier if they start out closer together at $g = 0$!

For the perturbations of free theories or the critical Ising model by a pure mass term we know the exact analytical structure of their ground-state scaling functions

$\tilde{c}(r)$ from sect. 6. These perturbations are somewhat singular, as seen from the $r^2 \ln r$ term ($g = r^2$ here) in the corresponding $\tilde{c}(r)$ functions; all other singularities of $\tilde{c}(r)$ are however well-separated square-root branch points, which is presumably the generic situation.

Note that the positions of the singularities for the free theories are the solutions of the equations $\varepsilon_n(r) = 0$, where the $\varepsilon_n(r)/R$ are the energies allowed for a free particle in a box of length R, with periodic or antiperiodic boundary conditions for bosonic or fermionic type particles, respectively (cf. sect. 6). For the scaled anharmonic oscillator Shanley [62] has given arguments that the position of the real part of the singularities of its eigenvalues should approximately be determined by $E_n(g) = 0$, where the E_n denote the different eigenvalues of the scaled anharmonic oscillator. It would be nice if similar statements hold more generally. For some suggestions in this direction, see below.

If such results hold in general, one might immediately conclude that the only accumulation points of singularities is at infinity (at least if $\bar{y} > 2$). Here we just give an argument which suggests that the singularities do in fact accumulate at infinity. The point is simply that this will typically be the only way that $\Sigma(r)$ can grow like r^2 at large r, as we know from eq. (65) and the fact that $\tilde{c}(r) \to 0$ as $r \to \infty$. In fact, this known asymptotic behaviour of $\Sigma(r)$ leads to *quantitative* restrictions on the rate at which the positions of the typical singularities approach infinity (we say "typical", because a set of singularities of sufficiently small measure can do "wild things" without affecting the asymptotics of $\Sigma(r)$). Consider, as an example motivated by the free theories of sect. 6, the following form for $\Sigma(r(g))$:

$$\Sigma(r(g)) = \sum_{n=0}^{\infty} b_n\left(\sqrt{g - g_n} - \sqrt{-g_n}\right). \tag{114}$$

Assume that the g_n are negative (so that the b_n must be real) and that $g_n \simeq -g_1 n^{\gamma}$, $b_n \simeq b_1 n^{-\beta}$ for some $\gamma > 0$ and $\beta \in \mathbb{R}$, for large n. A simple calculation then shows that for large g

$$\Sigma(r(g)) \simeq O\left(g^{\frac{1}{2} + (1-\beta)/\gamma}\right), \tag{115}$$

so that matching to the known $O(r^2) = O(g^{2/\bar{y}})$ behaviour requires

$$\tfrac{1}{2} + \frac{1-\beta}{\gamma} = \frac{2}{\bar{y}}. \tag{116}$$

Note that $\bar{y} > 2$ implies that $\beta < 1$. The case of free theories corresponds to $\beta = 0$ and $\gamma = \bar{y} = 2$, cf. sect. 6. (In this case one has to perform an additional "subtraction" in eq. (114) to make $\Sigma(r(g))$ well defined, i.e. replace $\sqrt{g - g_n} - \sqrt{-g_n}$ by $\sqrt{g - g_n} - \sqrt{-g_n} - g/(2\sqrt{-g_n})$, which then implies that the large-g behaviour of

$\Sigma(r(g))$ is dominated by a $g \ln g$ term, as we know from sect. 6.)

We have not yet commented on the assumption we implicitly made in our numerical analysis of the last section, namely that the first singularity g_0 is *real*. If real, it is of course negative, since, as mentioned in sect. 4, it is rather clear that one can rigorously establish analyticity of the thermodynamics for physical values of temperature and chemical potentials. However, a priori the singularities might just as well occur as complex conjugate pairs in the g-plane; $\Sigma(r(g))$ is then still real. For the anharmonic oscillator, for instance, none of the singularities is at real coupling. For the theories of sect. 6, on the other hand, all singularities occur at real $g = r^2$.

For the Ising field theory (and similarly for free bosons and fermions) we can understand the mechanism that leads to this phenomenon, by following the derivation [28] of the scaling-limit partition function from that of the Ising model (at zero magnetic field H) on an $N_L \times N_R$ lattice with periodic boundary conditions [52]. This will also reveal the physical origin of the singularities from the point of view of the underlying lattice system. Each of the four "partial partition functions" of the isotropic lattice model (analogs of the $D_{\alpha,\beta}$ in eq. (99)) has $N_L \cdot N_R$ zeros in the complex temperature plane. In the thermodynamic limit these sets of zeros all approach the same continuous distribution, which is also the asymptotic distribution of zeros of the full partition function, at least close to T_c. The asymptotic zeros lie on two circles [63] (in an appropriate variable), one of which "pinches" the real T-axis at T_c at a right angle, with a density of zeros proportional to $|T - T_c|$ for small (imaginary) $T - T_c$. This form of the density of zeros directly implies [63] the logarithmic divergence of the specific heat at criticality.

In the scaling limit $N_R \to \infty$ with $\xi = N_L/N_R = L/R$ and $r = Rm \sim N_R(T - T_c)$ fixed, the region around $T = T_c$ is "blown up", and the zeros of the four partial partition functions are determined by

$$\left(\frac{2\pi n_1}{R}\right)^2 + \left(\frac{2\pi n_2}{L}\right)^2 = -m^2, \tag{117}$$

where n_1, n_2 are integers or half-odd integers, depending on which of the partial partition functions is considered. In fact, *schematically*, the lattice partial partition functions become

$$\text{“}\exp\left\{\frac{L}{2R}\sum_{n_1 \in \mathbb{Z}+\beta} \varepsilon_{n_1}(r)\right\}\text{”} \prod_{n_1 \in \mathbb{Z}+\beta} (1 \mp e^{-L\varepsilon_{n_1}(r)/R}) \tag{118}$$

in the scaling limit, where $\varepsilon_n(r)$ was defined in eq. (100). The zeros of this expression are given by $L\varepsilon_{n_1}(r)/R = 2\pi i n_2$, with n_2 an integer or a half-odd

integer, respectively, for the two signs in the above expression; this is the same condition as (117). The analysis of ref. [28] together with our discussion in sect. 6 shows* that the first exponential on the r.h.s. becomes the exponential of the free-theory scaling function $c_\beta(r)$; when combined with the infinite product it gives the building block $D_{\alpha,\beta}$ of Z_{IFT}, cf. eqs. (103), (99), and (95) and (96). So we see that the zeros of the infinite products correspond directly to those of the partial partition functions on the lattice, where their "pinching" of the real axis at T_c is responsible for the phase transition. Now the crucial point is that although these infinite products disappear in the limit $L \to \infty$, the scaling functions $c_\beta(r)$ still "remember" the position of these zeros (determined simply by $\varepsilon_{n_i}(r) = 0$ in this limit), but now they manifest themselves as square-root singularities!

We would like to suggest that the situation in all the other models is similar, namely that the singularities of the functions $\Sigma(r(g))$ correspond to the zeros of the partition functions of the relevant lattice models (in the scaling limit appropriate to the cylindrical geometry); moreover, the singularities of $\Sigma(r(g))$ are real and negative (at least the first, see below) because the partition-function zeros of the lattice model correspond to purely imaginary λ for perturbations of unitary CFTs (where $g \sim \lambda^2$), or negative λ for the non-unitary CFTs (where $g \sim \lambda$). For the case of the Ising model in a magnetic field we know from the Yang–Lee theorem [24] that all zeros of the partition function lie on the imaginary H-axis (although the exact positions for a finite lattice are not known), and that in the thermodynamic limit they accumulate on this axis, reaching the origin $H = 0$ if $T \leqslant T_c$. In the scaling limit leading to the $E_8^{(1)}$-related theory on the cylinder (taken at $T = T_c$, with $H \to 0$, $N_R \to \infty$, keeping $N_L/N_R = \xi = \infty$ and $N_R H^{1/\delta} = N_R H^{8/15} \sim r \sim \lambda^{8/15}$ fixed), the Yang–Lee zeros should become discretely located on the imaginary λ-axis, the first singularity of $\Sigma(r(g))$ found in the previous section corresponding to the zeros (two!) closest to the H-axis. This singularity is therefore related to the Yang–Lee edge singularity, though in the special case of $T = T_c$ where it leads to the phase transition of the Ising model at zero "imaginary" magnetic field.

In all other cases we lack information on the partition-function zeros of the corresponding lattice models, but here we turn the logic around: The fact that the exponent α of the first singularity g_0 of $\Sigma(r(g))$ came out to be very close to the expected value $\frac{1}{2}$ (cf. table 6), under the *assumption* that the first singularity is real, presumably means that this assumption is correct. Suppose now that the asymptotic density of zeros of the corresponding lattice model crosses the critical point along a line (i.e. does not fill out an *area* there) in the complex plane of the variable that becomes λ in the scaling limit. The reality of the first singularity g_0

* We are skipping a few subtleties here, related to the fact that the lattice version of what we schematically call $\Sigma_n \varepsilon_n(r)$ does not have a well-defined scaling limit since it contains a term of the form $r^2 \ln N_R$, see eq. (3.30) of ref. [28]. The remedy is to subtract a term $-r^2 \ln(T - T_c)$, which is the lattice analog of the subtraction of a bulk term to implement the normalization condition $c_\beta(\infty) = 0$.

implies then that this line is tangent to the imaginary axis in the unitary cases and the Yang–Lee model, while tangent to the real axis in all other non-unitary models. Since the scaling limit "blows up" an infinitesimal region around the critical point, it follows that *all* singularities of $\Sigma(r(g))$ are real*. Therefore eq. (114) might not be a bad guess for the form of $\Sigma(r(g))$ for all the purely elastic scattering theories with $\tilde{y} > 2$ considered here (although there are infinitely many other possibilities, e.g. replacing the linear terms under the square roots in eq. (114) by more complicated polynomials).

9. Concluding remarks

We have seen that the thermodynamic Bethe ansatz is a powerful method to establish exact (or at least numerically precise) results about the thermodynamics of certain nontrivial interacting (1 + 1)-dimensional QFTs. In particular, it allows one to obtain numerically highly accurate results for the ground-state energy of a purely elastic scattering theory on a circle of arbitrary radius, going far beyond the small volume expansion provided by CPT on the cylinder. In fact, after the first or second term even the perturbation expansion coefficients are easier to obtain using the TBA than with CPT itself.

Recently, Yurov and Zamolodchikov [59] have proposed a "truncated conformal space approach" (mentioned in sect. 8) to analyze perturbations, not necessarily integrable, of CFTs on the cylinder. In this approach one can study not only the ground-state energy, but also (multi-)particle excitations in the massive theory, allowing one to see the interpolation between them and the conformal states of the unperturbed theory (cf. the discussion after eq. (105) in sect. 6, and ref. [64]). They applied this approach to the perturbed Yang–Lee CFT and used the highly accurate TBA results for the ground-state energy as a check for the less accurate results of the "truncated conformal space" method (conversely, the latter method allows one to obtain the position of the first singularity g_0 of $\Sigma(r(g))$ more accurately than with the former, serving as a test of the TBA – or rather of the extrapolation method used to obtain g_0 within the TBA framework). In the further study of the perturbed CFTs considered here using the "truncated conformal space approach" or other approximate methods, our TBA results can be used to check the accuracy of these methods.

* We should remark that this argument actually also assumes that *all* the zeros of the lattice model close to the critical point are "generic", in the sense that they asymptotically lie on the line on which we assumed the zeros to become dense. But in principle, e.g. if a theorem of the Yang–Lee type (assuring us that already for a finite lattice the zeros lie on the same line on which they accumulate asymptotically) does not apply, some zeros might conceivably be non-generic, the asymptotic density of zeros being unaffected. Note that this "nasty possibility" is not realized for the scaling limit of the $H = 0$ Ising model, despite the fact that there is no Yang–Lee theorem in this case.

We think that the TBA, the bootstrap and related ideas can still teach us a lot about (integrable) massive QFTs in 1 + 1 dimensions. Some calculations, e.g. that of form factors [6, 64, 65] (thereby obtaining representations for the Green functions) for some of the more complicated S-matrix theories, seem possible in principle, but difficult in practice. For other projects, e.g. deriving general expressions for the energy levels of a finite-volume purely elastic scattering theory in terms of its S-matrix (at least for large volume, in other words, calculating the corrections to the leading behaviour determined by eq. (24)), there is more hope.

Other questions deserving further investigation are the observations we made in sect. 8 concerning the relation between the singularities of the ground-state scaling function $\tilde{c}(r)$ and the zeros of the partition function of the corresponding lattice model in the scaling region. The QFT as well as the statistical mechanics side of this issue should be interesting.

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Note added in proof

After submitting this work we became aware of ref. [66], where infinite sums like those appearing in our eqs. (95, 96) ("remnant functions") are studied in great detail. In particular, the results obtained there complement those of refs. [28, 29] and can be used to deduce the large-r behaviour of the partition function of the Ising field theory on the torus. We did this independently in sect. 6, using the integral representations (90) for the ground-state scaling functions of free particles, which do not appear in ref. [66], and in our opinion are quite illuminating. We also thank M. Henkel for pointing out that the finite-volume mass gap in the Ising field theory, eq. (105), was written down previously in ref. [67] (although again not using eq. (90)). Finally, we should remark that our conjecture at the end of sect. 8 about the asymptotic density of zeros of the lattice partition functions crossing the real axis vertically (in the unitary theories), has recently been proposed independently [68] for the special case of the 3-state Potts model, based on a numerical study of the zeros of the partition function on finite lattices.

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