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Operator dimensions and surface exponents for the non-linear Schrödinger model at $T=0$

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Abstract. Using the Euler-Maclaurin formula, we compute finite-size corrections to the ground- and excited-state energies and momenta. This enables us to obtain all possible operator scaling dimensions at the critical point ($T=0$) and surface exponents for a variety of boundary conditions. We extend the predictions of conformal invariance to include Green functions with oscillating terms.

1. Introduction

Recently there has been a resurgence of interest in exactly integrable models. This interest is justified by two reasons. Firstly, some exactly intergrable models, like the Potts model, are of intrinsic interest in statistical mechanics. Secondly, they present us with patterns for the behaviour of other quantum field theories which can only be approached through approximations.

In exactly integrable models, it is generally true that the spectrum is far easier to obtain than the correlation functions. The Bose gas with pairwise repulsive delta function interaction (also called the non-linear Schrödinger, or NLS, model) is no exception. It is defined by the second quantised Hamiltonian:

$$\hat{H}=\int_0^L \mathrm{d}x(\phi^{+\prime}(x)\phi'(x)+g\phi^+(x)\phi^+(x)\phi(x)\phi(x)-\mu_0\phi^+(x)\phi(x)) \tag{1.1}$$

where μ_0 is the chemical potential and $g>0$ is the strength of the repulsive interaction. Using the Bethe ansatz [1], Lieb and Liniger [2] obtained the spectrum in the thermodynamic limit. They also obtained the many-body wavefunction exactly. In principle, all the information about particle correlations is contained in the wavefunction. The difficulty arises because the wavefunction is a sum of $N!$ terms (for N particles) and correlation functions typically involve $(N!)^2(N-1)$ integrals, of which many are destined to cancel. Substantial progress in calculating correlation functions was not made until the 1980s [3, 4].

The structure of the general correlation functions in this model is still an open problem (see, however, [5]). At $T=0$, however, there is a major simplification. The correlation functions computed above show that the correlation length goes to infinity as $T\to 0$, signalling a second-order phase transition. Since this is a theory with short-ranged interactions and a linear dispersion law we expect it to show conformal invariance at this point.

Conformal invariance in two spacetime dimensions has proven to be a very powerful constraint on the structure of quantum field theories. This was an idea first proposed by Polyakov [6]. In their seminal work [7], Belavin *et al* (hereafter referred to as BPZ) investigated the consequences of conformal invariance. A key object in the theory is the stress tensor which can be decomposed into analytic and antianalytic pieces at the scale-invariant point:

$$T(z) = T_{11} - T_{22} + 2\mathrm{i}T_{12} \qquad \bar{T}(\bar{z}) = T_{11} - T_{22} - 2\mathrm{i}T_{12}. \tag{1.2}$$

These can now be expanded in Laurent series and the coefficients, which generate infinitesimal conformal transformations, obey the Virasoro algebra with central extension:

$$\begin{aligned} T(z) &= \sum_{-\infty}^{\infty} \frac{L_n}{z^{n+2}} \\ \bar{T}(\bar{z}) &= \sum_{-\infty}^{\infty} \frac{\bar{L}_n}{\bar{z}^{n+2}} \\ [L_m, L_n] &= (m-n)L_{m+n} + \tfrac{1}{12}c(m^3 - m)\delta_{m+n,0} \\ [\bar{L}_m, \bar{L}_n] &= (m-n)\bar{L}_{m+n} + \tfrac{1}{12}c(m^3 - m)\delta_{m+n,0} \\ [L_m, \bar{L}_n] &= 0. \end{aligned} \tag{1.3}$$

The fields in the theory which transform in the simplest possible manner under conformal transformations (i.e. homogeneously) are called primary fields. All other fields can be constructed from them. The primary fields obey the following commuation relations with the Virasoro generators:

$$\begin{aligned} [L_n, \phi(z, \bar{z})] &= z^{n+1}\partial\phi/\partial z + (n+1)\Delta z^n \phi \\ [\bar{L}_n, \phi(z, \bar{z})] &= \bar{z}^{n+1}\partial\phi/\partial \bar{z} + (n+1)\bar{\Delta} \bar{z}^n \phi. \end{aligned} \tag{1.4}$$

Under finite conformal transformations

$$\begin{aligned} &z \to w(z) \qquad \bar{z} \to \bar{w}(\bar{z}) \\ &\phi(z, \bar{z}) \to \left(\frac{\partial z}{\partial w}\right)^{\Delta} \left(\frac{\partial \bar{z}}{\partial \bar{w}}\right)^{\bar{\Delta}} \phi(z(w), \bar{z}(\bar{w})). \end{aligned} \tag{1.5}$$

BPZ found that if the number of primary fields was to be finite then the central extension (also called the conformal anomaly) must be quantised:

$$c = 1 - \frac{6}{m(m+1)} \tag{1.6}$$

where m is rational. In this case the possible scaling dimensions are also restricted, given by the Kac formula [8]

$$\Delta_{p,q} = \frac{[(m+1)p - mq]^2 - 1}{4m(m+1)}. \tag{1.7}$$

Following this up, Friedan *et al* [9] found that unitarity restricts the value of m to be an integer greater than 2 if $c < 1$. For $c \geqslant 1$ there is no restriction.

It is possible to extend the definition of a primary conformal field to include oscillations in the Green functions. This new primary field obeys the commutation relations with the following generators:

$$\begin{aligned}[L_n, \phi_q(z, \bar{z})] &= z^{n+1}(\partial\phi/\partial z + \mathrm{i}q\phi) + (n+1)\Delta z^n\phi \\ [\bar{L}_n, \phi_q(z, \bar{z})] &= \bar{z}^{n+1}(\partial\phi/\partial \bar{z} + \mathrm{i}q\phi) + (n+1)\bar{\Delta}\bar{z}^n\phi.\end{aligned} \tag{1.8}$$

The two-point correlator of a 'scalar' field defined as

$$\Phi_q(z, \bar{z}) = \frac{\phi_q(z, \bar{z}) + \phi_{-q}(z, \bar{z})}{2} \tag{1.9}$$

is

$$\langle \Phi_q(z_1, \bar{z}_1)\Phi_q(z_2, \bar{z}_2)\rangle = \frac{\cos[2q \operatorname{Re}(z_1 - z_2)]}{(z_1 - z_2)^{\Delta}(\bar{z}_1 - \bar{z}_2)^{\bar{\Delta}}}. \tag{1.10}$$

It is interesting to note that this is the most general definition of a primary field consistent with translation invariance of the Green functions. It should also be noted that $\exp(\mathrm{i}q \operatorname{Re}(z))\phi_q(z)$ behaves like a conventional primary field.

Subsequently, it was discovered [10] that finite-size corrections are also restricted by conformal invariance. Specifically, it was shown that the finite-size corrections to the ground-state energy behave like

$$E_{\mathrm{g}}(L) = Le_{\infty} - \frac{\pi c v_{\mathrm{s}}}{6L} + \ldots \tag{1.11}$$

for periodic boundary conditions. Here v_{s} is the velocity of sound in the model. Also for each operator O_α with anomalous dimension x_α and spin s_α there exists a tower of excited states with energies and momenta

$$E^{\alpha}_{j,j'} = E_{\mathrm{g}}(L) + \frac{2\pi v_{\mathrm{s}}}{L}(x_\alpha + j + j') \qquad P^{\alpha}_{j,j'} = \frac{2\pi}{L}(s_\alpha + j - j') \tag{1.12}$$

where j and j' are integers.

This presents an alternate way of approaching the problem of correlation functions in exactly soluble models. Knowing the scaling dimension and spin of an operator corresponds to knowing the asymptotic behaviour of its two-point correlation. Thus, finite-size corrections offer a partial solution to the problem of correlation functions at the critical point.

Finite-size corrections to a number of problems have been obtained by different methods [11]. The one that we will be using makes crucial use of the Euler–Maclaurin formula:

$$\sum_{n_1}^{n_2} f(n) = \int_{n_1}^{n_2} f(x)\,\mathrm{d}x + \tfrac{1}{2}(f(n_1) + f(n_2)) + \sum_{1}^{\infty} \frac{B_{2p}}{2p!}(f^{(2p-1)}(n_2) - f^{(2p-1)}(n_1)) \tag{1.13}$$

where B_{2p} are the Bernoulli numbers and assuming, of course, that all the derivatives exist. This method was pioneered by Woynarovich and Eckle [12].

This paper is organised as follows. In § 2 we give a brief review of the thermodynamics of the non-linear Schrödinger model. Section 3 describes the actual computation of the finite-size corrections and main results for the case of periodic and twisted boundary conditions. In § 4 we demonstrate the integrability of a class of reflecting wall boundary conditions. Section 5 is devoted to obtaining the surface critical exponents for these boundary conditions. We end with a summary and conclusions.

2. The thermodynamics of the NLS

There are several ways of deriving the thermodynamic behaviour of the repulsive Bose gas. In this section we will follow the most obvious route, starting from the many-body Schrödinger equation in first-quantised notation

$$\left\{-\sum_{i=1}^{N}\frac{\partial^2}{\partial x_i^2}+2g\sum_{i<j}\delta(x_i-x_j)\right\}\psi(\{x_i\})=E\psi(\{x_i\}) \tag{2.1}$$

where N is the number of particles. We solve this equation using the Bethe ansatz:

$$\psi_{\{\lambda_j\}}(\{x_j\})=\sum_P a(P)\exp\left(\mathrm{i}\sum_{j=1}^{N}\lambda_{Pj}x_j\right) \tag{2.2}$$

in the fundamental domain $x_1<x_2<\ldots.<x_N$ where P denotes a permutation. The wavefunction in any other domain is related to this by Bose symmetry.

It turns out that one can satisfy the Schrödinger equation with

$$\psi_{\{\lambda_j\}}(\{x_j\})=\sum_P\left[\prod_{i<j}\left(1-\frac{\mathrm{i}g}{\lambda_{Pi}-\lambda_{Pj}}\right)\right]\exp\left(\mathrm{i}\sum_{j=1}^{N}\lambda_{Pj}x_j\right). \tag{2.3}$$

Assuming periodic boundary conditions for this section (boundary conditions do not alter the spectrum in the thermodynamic limit) we must impose

$$\psi(0,x_2,x_3,\ldots,x_N)=\psi(x_2,x_3,\ldots,L). \tag{2.4}$$

This immediately leads to a system of transcendental equations to be satisfied by $\{\lambda_j\}$:

$$\exp(\mathrm{i}\lambda_jL)=\prod_{k\neq j}\frac{\lambda_j-\lambda_k+\mathrm{i}g}{\lambda_j-\lambda_k-\mathrm{i}g}. \tag{2.5}$$

Taking the logarithm with an appropriate choice of branch we get

$$\lambda_jL+\sum_{k=1}^{N}\Theta(\lambda_j-\lambda_k)=2\pi n_j \tag{2.6}$$

where

$$\Theta(\lambda)=\begin{cases}\pi-2\tan^{-1}(g/\lambda) & \lambda>0\\ -\pi+2\tan^{-1}(-g/\lambda) & \lambda\leqslant 0\end{cases} \tag{2.7}$$

where the n_j are distinct integers (for N odd) or half-odd integers (for N even). The λ_j and hence the n_j must be distinct if the wavefunction is to be normalisable. For the ground state the n_j are consecutive integers or half-odd integers with $-(N-1)/2\leqslant n_j\leqslant(N-1)/2$.

Continuing this equation to arbitrary values of λ and n we get

$$\frac{\lambda}{2\pi}+\frac{1}{2\pi L}\sum_{k=1}^{N}\Theta(\lambda-\lambda_k)=z(\lambda) \tag{2.8}$$

where

$$z(\lambda_j)=n_j/L \tag{2.9}$$

and the density of roots is

$$\rho(\lambda)=\mathrm{d}z/\mathrm{d}\lambda. \tag{2.10}$$

Taking the thermodynamic limit of this equation at constant density, i.e. $N \to \infty$, $L \to \infty$ but $N/L = D$ (density) fixed we get

$$\frac{\lambda}{2\pi}+\frac{1}{2\pi}\int_{-D/2}^{+D/2}\Theta(\lambda-\lambda(z'))\,\mathrm{d}z'=z. \tag{2.11}$$

Changing variables from z to λ inside the integral we get

$$\frac{\lambda}{2\pi}+\frac{1}{2\pi}\int_{-q}^{q}\Theta(\lambda-\mu)\,\mathrm{d}\mu\,\rho(\mu)=z. \tag{2.12}$$

q is akin to a Fermi momentum and is implicity defined by

$$\lambda(\pm D/2)=\pm q. \tag{2.13}$$

Differentiating equation (11) we have an integral equation for $\rho(\lambda)$:

$$\rho(\lambda)-\frac{1}{2\pi}\int_{-q}^{q}K(\lambda-\mu)\rho(\mu)\,\mathrm{d}\mu=\frac{1}{2\pi}\qquad K(\lambda)=\frac{2g}{\lambda^2+g^2}. \tag{2.14}$$

Unfortunately this equation cannot be solved in closed form. We can, however, introduce a formal inverse:

$$f(\lambda)-\frac{1}{2\pi}\int_{-q}^{q}K(\lambda-\mu)f(\mu)\,\mathrm{d}\mu=[(1-\hat{K}/2\pi)f](\lambda)=g(\lambda)$$

$$\Rightarrow f(\lambda)=[(1+\hat{M})g](\lambda)=g(\lambda)+\int_{-q}^{q}M(\lambda,\mu)g(\mu)\,\mathrm{d}\mu \tag{2.15}$$

where $M(\lambda,\mu)$ has the following property:

$$M(\lambda,\mu)-\frac{1}{2\pi}\int_{-q}^{q}M(\lambda,\nu)K(\nu-\mu)\,\mathrm{d}\nu=\frac{K(\lambda-\mu)}{2\pi}. \tag{2.16}$$

We can also expand M in a series in $1/g$:

$$M(\lambda,\mu)=\frac{1}{\pi g}+\frac{2q}{\pi^2g^2}+\frac{4q^2}{\pi^3g^3}-\frac{(\lambda-\mu)^2}{\pi g^3}+\dots. \tag{2.17}$$

Formal and series solutions for $\rho(\lambda)$ are

$$\rho(\lambda)=\frac{1}{2\pi}+\frac{1}{2\pi}\int_{-q}^{q}M(\lambda,\mu)\,\mathrm{d}\mu=\frac{1}{2\pi}\left(1+\frac{2q}{\pi g}+\frac{4q^2}{\pi^2g^2}+\frac{8q^3}{\pi^3g^3}-\frac{2q}{3\pi g^3}(q^2+3\lambda^2)+\dots\right). \tag{2.18}$$

The energy density of the ground state is

$$e_\infty=\int_{-q}^{q}(\lambda^2-\mu_0)\rho(\lambda)\,\mathrm{d}\lambda. \tag{2.19}$$

We can also consider particle and hole excitations at $|\lambda_{\mathrm{p}}|>q$ and $|\lambda_{\mathrm{h}}|<q$, respectively, with dressed energies

$$\varepsilon(\lambda)=[(1+\hat{M})(\lambda^2-\mu_0)] \tag{2.20}$$

and momenta

$$p(\lambda)=[(1+\hat{M})(\lambda)]. \tag{2.21}$$

From the above we can define the velocity of sound, which is the velocity of massless excitations following a linear dispersion law at the Fermi surface:

$$v_s \equiv \left.\frac{d\varepsilon(\lambda)}{dp(\lambda)}\right|_{\lambda=q} = \frac{2q+2\int_{-q}^{q} \lambda M(\lambda, q)\, d\lambda}{2\pi\rho(q)}. \tag{2.22}$$

This will be important to us in the following.

3. The finite-size corrections for periodic and twisted boundary conditions

Let us analyse in more detail the finite-size corrections in the case of periodic boundary conditions. The system of transcendental equations satisfied by the roots is

$$\exp(i\lambda_j L) = \prod_{k\neq j} \frac{\lambda_j - \lambda_k + ig}{\lambda_j - \lambda_k - ig}. \tag{3.1}$$

Taking the logarithm with a suitable choice of branch we obtain, as before,

$$\lambda_j L + \sum_k \Theta(\lambda_j - \lambda_k) = 2\pi n_j. \tag{3.2}$$

We will analyse excitations above the ground state which have zero energy in the thermodynamic limit. It is these states which are important for computing the asymptotic behaviour of correlation functions. The ground state for N particles is characterised by consecutive integers (or half-odd integers) n_j lying in the range $-(N-1)/2 \leq n_j \leq (N-1)/2$.

We create the most general excited state as follows.

(*a*) We add r extra particles to get the ground-state configuration for $N+r$ particles. This means that $-(N+r-1)/2 \leq n_j \leq (N+r-1)/2$.

(*b*) We shift all the integers (or half-odd integers) characterising the roots by an integer t. This means $-(N+r-1)/2+t \leq n_j \leq (N+r-1)/2+t$.

(*c*) Finally, we create particle–hole excitations near $\pm q$ by removing bare particles from $n_{h\pm}$ and putting it into $n_{p\pm}$. These pairs are labelled by two integers, $s_\pm$, the + and − indexing pairs at $\pm q$, respectively,

$$\begin{aligned} n_{h+} &= \frac{N+r-1}{2} + t - m_+(s_+) \\ n_{p+} &= \frac{N+r-1}{2} + t + n_+(s_+) \\ n_{h-} &= -\frac{N+r-1}{2} + t + m_-(s_-) \\ n_{p-} &= -\frac{N+r-1}{2} + t - n_-(s_-). \end{aligned} \tag{3.3}$$

One can now write the system of the transcendental equations for the roots as

$$\begin{aligned} \frac{\lambda_j}{2\pi} + \frac{1}{2\pi L} \sum_{-(N+r-1)/2+t}^{(N+r-1)/2+t} \Theta(\lambda_j - \lambda_k) &= \frac{j}{L} - \frac{1}{2\pi L}\Bigg(\sum_{s+} [\Theta(\lambda_j - \lambda_{n_{p+}(s_+)}) - \Theta(\lambda_j - \lambda_{n_{h+}(s_+)})] \\ &\quad + \sum_{s-} [\Theta(\lambda_j - \lambda_{n_{p-}(s_-)}) - \Theta(\lambda_j - \lambda_{n_{h-}(s_-)})] \Bigg). \end{aligned} \tag{3.4}$$

We now use the Euler–Maclaurin formula to convert the sum into an integral and replace λ_j by $\lambda_L(z)$. We also make the ansatz

$$\lambda_L(z)=\lambda(z)+\frac{g_1(z)}{L}+\frac{g_2(z)}{L^2}+O\left(\frac{1}{L^3}\right) \tag{3.5}$$

where $\lambda(z)(=\lambda_\infty(z))$ is the function obtained in the limit $L\to\infty$. This ansatz is justified by self-consistency. It must also be noted at this point that the functions that appear naturally in this model are all analytic [2]. This means that we can take the Euler–Maclaurin series as far as we want. We now separate powers of $1/L$ to get integral equations for $\rho(\lambda)g_1(\lambda)$ and $\rho(\lambda)g_2(\lambda)$:

$$\begin{aligned}
\left(1-\frac{\hat{K}}{2\pi}\right)(\rho g_1)&=\frac{t}{2\pi}(\Theta(\lambda,q)-\Theta(\lambda,-q))+\frac{r}{4\pi}(\Theta(\lambda,q)+\Theta(\lambda,-q))\\
\left(1-\frac{\hat{K}}{2\pi}\right)(\rho g_2)&=\frac{1}{2}\left(1-\frac{\hat{K}}{2\pi}\right)'(\rho g_1^2)\\
&\quad+\frac{1}{4\pi}[(2t+r)g_1(q)K(\lambda,q)-(2t-r)g_1(-q)K(\lambda,-q)]\\
&\quad+\frac{1}{48\pi}\left([3(2t+r)^2-1]\frac{K(\lambda,q)}{\rho(q)}-[3(2t-r)^2-1]\frac{K(\lambda,-q)}{\rho(q)}\right)\\
&\quad+\frac{1}{2\pi}\left(\sum_{s_+}(m_+(s_+)+n_+(s_+))\frac{K(\lambda,q)}{\rho(q)}-\sum_{s_-}(m_-(s_-)+n_-(s_-))\frac{K(\lambda,-q)}{\rho(q)}\right)
\end{aligned} \tag{3.6}$$

where $\rho(\lambda)=\mathrm{d}z/\mathrm{d}\lambda$, $g_{1,2}(\lambda)=g_{1,2}(z(\lambda_\infty))$.

One can now use the formal inverse to 'solve' these integral equations and we get

$$\rho g_1(\lambda)=\tfrac{1}{2}r\mathscr{C}(\lambda)+t\mathscr{D}(\lambda)$$

where

$$\mathscr{C}(\lambda)=-\frac{(1+\hat{M})}{2\pi}(\Theta(\lambda,q)+\Theta(\lambda,-q))$$

$$\mathscr{D}(\lambda)=-\frac{(1+\hat{M})}{2\pi}(\Theta(\lambda,q)-\Theta(\lambda,-q))$$

$$\begin{aligned}
\rho g_2(\lambda)&=\tfrac{1}{2}(\rho g_1^2)'(\lambda)+\tfrac{1}{2}(\rho g_1^2(q)M(\lambda,q)-\rho g_1^2(-q)M(\lambda,-q))\\
&\quad+\tfrac{1}{2}[(2t+r)g_1(q)M(\lambda,q)-(2t-r)g_1(-q)M(\lambda,-q)]\\
&\quad+\frac{1}{24}\left([3(2t+r)^2-1]\frac{M(\lambda,q)}{\rho(q)}-[3(2t-r)^2-1]\frac{M(\lambda,-q)}{\rho(q)}\right)\\
&\quad+\sum_{s_+}(m_+(s_+)+n_+(s_+))\frac{M(\lambda,q)}{\rho(q)}-\sum_{s_-}(m_-(s_-)+n_-(s_-))\frac{M(\lambda,-q)}{\rho(q)}.
\end{aligned} \tag{3.7}$$

We now proceed to find the energy and momentum of the excited state. We start with

$$\begin{aligned}
E&=\sum_{-(N+r-1)/2+t}^{(N+r-1)/2+t}(\lambda_j^2-\mu_0)+\sum_{s_+}(\lambda_{\mathrm{p}_+}^2-\lambda_{\mathrm{h}_+}^2)+\sum_{s_-}(\lambda_{\mathrm{p}_-}^2-\lambda_{\mathrm{h}_-}^2)\\
P&=\sum_{-(N+r-1)/2+t}^{(N+r-1)/2+t}\lambda_j+\sum_{s_+}(\lambda_{\mathrm{p}_+}-\lambda_{\mathrm{h}_+})+\sum_{s_-}(\lambda_{\mathrm{p}_-}-\lambda_{\mathrm{h}_-}).
\end{aligned} \tag{3.8}$$

We apply the Euler-Maclaurin formula, keep terms up to $1/L$, substitute for $\rho g_1(\lambda)$ and $\rho g_2(\lambda)$ and use the expression for v_s, equation (2.22), to get

$$E = Le_\infty - \frac{\pi v_s}{6L} + \frac{2\pi v_s}{L}\left(r^2 x_p + \frac{t^2}{4x_p} + \sum_{s_+}(m_+ + n_+) + \sum_{s_-}(m_- + n_-)\right)$$
$$P = 2\pi t D + \frac{2\pi}{L}\left(2rt + \sum_{s_+}(m_+ + n_+) - \sum_{s_-}(m_- + n_-)\right) \tag{3.9}$$

where

$$x_p = \tfrac{1}{4}[1 + \mathscr{C}(q)]^2 = v_s/4\pi D. \tag{3.10}$$

Also, e_∞ is the energy density in the thermodynamic limit. This model has $c = 1$ and is clearly in the universality class of the Gaussian model [13]. The mapping between the coupling constant K of the Gaussian model and g is given by

$$x_p(g) = 1/4\pi K. \tag{3.11}$$

Let us consider an excitation which has particle-hole pairs near $+q$ only. Calling $\Sigma_{s_+}(m_+(s_+) + n_+(s_+)) = j$ we have

$$E - E_g = \frac{2\pi v_s}{L}\left(r^2 x_p + \frac{t^2}{4x_p} + j\right) \qquad P = 2\pi t D + \frac{2\pi}{L}(2rt + j) \tag{3.12}$$

where E_g is the ground-state energy. For large j the dispersion law for this excitation is

$$E_j - E_g = v_s(P_j - 2\pi t D). \tag{3.13}$$

This is indeed a linear dispersion law but it differs from the standard case in being displaced by $2\pi t D$ in the momentum. This shift is precisely what causes oscillating terms to appear in the correlation functions. To show this let us turn to the spectral representation of the current-current correlator at equal time. The current, expressed as $\phi^+(x)\phi(x) = j(x)$, has $r = 0$ but couples to all t and j, j':

$$\langle J(x)J(0)\rangle = \sum_m \langle 0|J(x)|m\rangle\langle m|J(0)|0\rangle = \sum_m |\langle 0|J(0)|m\rangle|^2 \exp[\mathrm{i}(p_m - p_g)x] \tag{3.14}$$

where the sum is over all states $|m\rangle$ and p_m and p_g are the momenta of states $|m\rangle$ and $|0\rangle$. We now break up this sum into disjoint sums characterised by different t and therefore different macroscopic momenta. Schematically, we have

$$\langle J(x)J(0)\rangle = \sum_{t=-\infty}^{\infty} \exp[\mathrm{i}2\pi D t x] \sum_{j,j'} |\langle 0|J(0)|t, j, j'\rangle|^2 \exp\left(\frac{\mathrm{i}2\pi x}{L}(j - j')\right) A(t, j, j') \tag{3.15}$$

where $A(t, j, j')$ gives the multiplicity of the 'state' t, j, j'. It is the second sum that gives the power law decays for $x \ll L$. The oscillating factors $\exp[\mathrm{i}(2\pi D)t]$ still remain and will give oscillating contributions to the correlation function.

It might be argued that the theory is not conformal even at long distances due to the presence of oscillating terms in the Green functions. The use of conformal theory results is justified by two reasons. Firstly, the predictions of conformal finite-size scaling are verified by the comparison with the exact known results at $T = 0$ [14] of the current-current correlator.

Secondly, it is possible to have field theoretic representations of the conformal algebra in which some fields have oscillating Green functions. In this case, the primary fields of dimension $(\Delta, \bar{\Delta})$ and momentum $2q$ transform according to equations (1.8)–(1.10).

Thus, there is no contradiction in using the results of conformal theory to obtain scaling dimensions in this model. We can now write down the general asymptotic (in distance) series for the field-field and current-current correlators:

$$\langle\phi^+(x)\phi(0)\rangle = \sum_{t=0}^{\infty}\sum_{j,j'=0}^{\infty} A_1(t,j,j')\frac{\cos[2\pi tDx+\phi_1(t,j,j')]}{|x|^{2x_p+t^2/2x_p+j+j'}} \tag{3.16}$$

$$\langle J(x)J(0)\rangle = \sum_{t=0}^{\infty}\sum_{j,j'=0}^{\infty} A_2(t,j,j')\frac{\cos[2\pi tDx+\phi_2(t,j,j')]}{|x|^{t^2/2x_p+j+j'}}. \tag{3.17}$$

We extend the conformal hypothesis to the case of twisted boundary conditions for which no exact results are known.

Before we move on to twisted boundary conditions it should be noted that it is straightforward, though tedious, to extend the above analysis to higher-order corrections. These corrections embody information about irrelevant operators in the critical Hamiltonian and about some coefficients in the operator product expansion [15]:

$$H_{\text{critical}} = H_{\text{conformal}} + \sum_{n=1}^{\infty} a_{i_n} O_{i_n}. \tag{3.18}$$

For example, there are three irrelevant operators O_i of dimension 3 in the Hamiltonian.

All these considerations are easy to generalise to the case of twisted boundary conditions. Here the system in transcendental equations is

$$\exp(\mathrm{i}\lambda_j L) = \exp(\mathrm{i}2\pi\beta)\prod_{k\neq j}\frac{\lambda_j-\lambda_k+\mathrm{i}g}{\lambda_j-\lambda_k-\mathrm{i}g}. \tag{3.19}$$

where β is a real number lying between $-\frac{1}{2}$ and $\frac{1}{2}$. The equations are formally identical to an excited state of the system with periodic boundary conditions with t replaced by $t+\beta$.

The results are as follows. The general excited-state energy and momentum are given by

$$E = Le_\infty - \frac{\pi v_s}{6L} + \frac{2\pi v_s}{L}\left(r^2 x_p + \frac{(t+\beta)^2}{4x_p} + \sum_{s_+}(m_+ + n_+) + \sum_{s_-}(m_- + n_-)\right) \tag{3.20}$$

$$P = 2\pi(t+\beta)D + \frac{2\pi}{L}\left(2r(t+\beta) + \sum_{s_+}(m_+ + n_+) - \sum_{s_-}(m_- + n_-)\right). \tag{3.21}$$

Several points are noteworthy here. The vacuum (the lowest energy state) has a macroscopic momentum $(2\pi\beta D)$. Operator dimensions and spin in the bulk depend upon β:

$$x_\alpha = r^2 x_p + \frac{t^2+2t\beta}{4x_p} + j + j' \qquad s_\alpha = 2r(t+\beta) + j - j'. \tag{3.22}$$

Finally, the value of the conformal anomaly changes to

$$c = 1 - 12\beta^2/4x_p. \tag{3.23}$$

We now go on to the analysis of reflecting wall boundary conditions.

4. Algebraic Bethe ansatz for reflecting wall boundary conditions

In this section we will derive Bethe ansatz equations for the NLS model with non-periodic boundary conditions, which are compatible with exact integrability.

Consider the Hamiltonian

$$\hat{H}=\int_{x_-}^{x_+}\left(\frac{\partial\psi^+}{\partial x}\frac{\partial\psi}{\partial x}+g\psi^+\psi^+\psi\psi\right)\mathrm{d}x+\sum\alpha_\pm\psi^+(x_\pm)\psi(x_\pm) \tag{4.1}$$

where the boundary terms in (1) correspond to the following boundary problem for the wavefunction $\phi(x_1,\ldots,x_N)$ in the N-particle sector:

$$\left(\frac{\partial}{\partial x_j}+\alpha_\pm\right)\phi(x_1,\ldots,x_N)|_{x_j=x_\pm}=0 \qquad j=1,\ldots,N. \tag{4.2}$$

Although this problem can be solved by means of the explicit coordinate Bethe ansatz construction of the wavefunction (see, for example [16]), here instead we will use the modern technique, based on the quantum inverse scattering method (QISM) [17], which reduces the Bethe ansatz to elegant operator algebra. This technique, also known as the algebraic Bethe ansatz, was generalised recently by Sklyanin [18] to incorporate the non-periodic boundary conditions (4.2). Central to the QISM is the auxiliary linear equation

$$\frac{\partial T(\lambda,x)}{\partial x}=:L(\lambda,x)T(\lambda,x): \tag{4.3}$$

where λ is a complex spectral parameter and $T(\lambda,x)$ and $L(\lambda,x)$ are 2×2 matrices of operator fields. In particular, for the NLS model,

$$L(x,\lambda)=\begin{pmatrix}-\mathrm{i}\lambda/2 & \mathrm{i}\sqrt{g}\psi^+(x)\\ -\mathrm{i}\sqrt{g}\psi(x) & \mathrm{i}\lambda/2\end{pmatrix}. \tag{4.4}$$

It is often useful to consider a lattice approximation to the field and the auxiliary equation. With the replacements

$$L(x,\lambda)\to L_n(\lambda)=\begin{bmatrix}1-\mathrm{i}\lambda\Delta/2 & \mathrm{i}\sqrt{g}\psi_n^+\Delta\\ -\mathrm{i}\sqrt{g}\psi_n(x)\Delta & 1+\mathrm{i}\lambda\Delta/2\end{bmatrix} \tag{4.5}$$

$$x\to n\Delta \tag{4.6}$$

equation (4.3) assumes the form

$$T_{n+1}(\lambda)=:L_n(\lambda)T_n(\lambda):. \tag{4.7}$$

It is easy to construct the solution of (6) on the interval $(-N,+N)$

$$T_N(\lambda)=:L_N(\lambda)L_{N-1}(\lambda)\ldots L_{-N}(\lambda):=\begin{bmatrix}A_N(\lambda) & B_N(\lambda)\\ C_N(\lambda) & D_N(\lambda)\end{bmatrix}. \tag{4.8}$$

Complete integrability of this and related models is guaranteed by the so-called Yang–Baxter relations satisfied by the local matrices $L_n(\lambda)$ [17]. In the NLS model these identities take the form:

$$R(\lambda-\mu)L_n^1(\lambda)L_n^2(\mu)=L_n^2(\mu)L_n^1(\lambda)R(\lambda-\mu) \tag{4.9}$$

where $L_n^1=L_n\otimes I_{v_2}$; $L_n^2=I_{v_1}\otimes L_n$ and the 4×4 matrix $R(\lambda)$ is given by

$$R(\lambda)=\lambda-\mathrm{i}g\hat{P}=\begin{bmatrix}\lambda-\mathrm{i}g & 0 & 0 & 0\\ 0 & \lambda & -\mathrm{i}g & 0\\ 0 & -\mathrm{i}g & \lambda & 0\\ 0 & 0 & 0 & \lambda-\mathrm{i}g\end{bmatrix}. \tag{4.10}$$

Here, $\hat{P}$ is the permutation operator in $V_1 \otimes V_2$. It is trivial to verify that solution (4.8) satisfies its own Yang–Baxter relations, namely

$$R(\lambda-\mu)T_N^1(\lambda)T_N^2(\mu)=T_n^2(\mu)T_N^1(\lambda)R(\lambda-\mu). \tag{4.11}$$

In the case of periodic boundary conditions, one can make use of (4.11) to show that $\tau(\lambda)$, as defined as

$$\tau(\lambda)=\operatorname{tr} T_N(\lambda)=A_N(\lambda)+D_N(\lambda) \tag{4.12}$$

is the generator of mutually commuting conserved quantities, one of which is the Hamiltonian (1.1) and $B_N(\lambda)$ and $C_N(\lambda)$ operators are creation and destruction operators, correspondingly [17]. To generalise this construction in order to describe the Hamiltonian (4.1), which contains non-trival boundary terms, let us introduce two new matrices $K_+(\lambda)$ and $K_-(\lambda)$, defined by the given R matrix (4.10) and the Sklyanin relations [18]:

$$R(\lambda_{12})K_-^1(\lambda_1)R(\tilde{\lambda}_{12}+\mathrm{i}g)K_-^2(\lambda_2)=K_-^2(\lambda_2)R(\tilde{\lambda}_{12}+\mathrm{i}g)K_-^1(\lambda_1)R(\lambda_{12}) \tag{4.13}$$

$$\begin{aligned}R(-\lambda_{12})K_+^{1t_1}(\lambda_1)&R(-\tilde{\lambda}_{12}+\mathrm{i}g)K_+^{2t_2}(\lambda_2)\\ &=K_+^{2t_2}(\lambda_2)R(-\tilde{\lambda}_{12}+\mathrm{i}g)K_+^{1t_2}(\lambda_1)R(-\lambda_{12})\end{aligned} \tag{4.14}$$

where

$$\lambda_{12}=\lambda_1-\lambda_2 \qquad \tilde{\lambda}_{12}=\lambda_1+\lambda_2 \tag{4.15}$$

and the symbol t_i stands for the transposition in the space V_i. It can be easily shown by inspection that

$$K_\pm(\lambda)=\mathrm{i}\xi_\pm+\mathrm{i}\sigma_3(\lambda\mp\tfrac{1}{2}\mathrm{i}g) \tag{4.16}$$

are indeed the solutions to equations (4.13) and (4.14). Introducing $U(\lambda)$, defined as

$$U(\lambda)=T_N(\lambda)K_-(\lambda)\sigma_2T_N^t(-\lambda)\sigma_2=\begin{pmatrix}\tilde{A}(\lambda) & \tilde{B}(\lambda)\\ \tilde{C}(\lambda) & \tilde{D}(\lambda)\end{pmatrix} \tag{4.17}$$

and making use of equations (4.11) and (4.13) one can prove that $U(\lambda)$ also satisfies the Sklyanin relations:

$$R(\lambda_{12})U^1(\lambda_1)R(\tilde{\lambda}_{12}+\mathrm{i}g)U^2(\lambda_2)=U^2(\lambda_2)R(\tilde{\lambda}_{12}+\mathrm{i}g)U^1(\lambda_1)R(\lambda_{12}). \tag{4.18}$$

Consider now the new object $t(\lambda)$

$$t(\lambda)=\operatorname{Tr}\{K_+(\lambda)U(\lambda)\}. \tag{4.19}$$

With the help of easily verifiable identities for the R matrix

$$\begin{aligned}&R(\lambda)R(-\lambda)=-(\lambda^2+g^2) \qquad R^{t_1}(\lambda)=R^{t_2}(\lambda)\\ &R^{t_1}(\lambda)R^{t_1}(-\lambda+2\mathrm{i}g)=-\lambda(\lambda-2\mathrm{i}g)\end{aligned} \tag{4.20}$$

and relations (4.14) and (4.18), one can get

$$[t(\lambda_1),t(\lambda_2)]=0. \tag{4.21}$$

Thus, $t(\lambda)$ is the generating function of the infinite set of mutually commuting quantities. These quantities are also conserved, since the Hamiltonian (4.1) is one of them (with $\alpha_\pm = \xi_\pm + \frac{1}{2}g$).

To find eigenvectors of $t(\lambda)$

$$
\begin{aligned}
t(\lambda) &= (\mathrm{i}\xi_+ + \lambda - \tfrac{1}{2}\mathrm{i}g)\tilde{A}(\lambda) + (\mathrm{i}\xi_+ - \lambda + \tfrac{1}{2}\mathrm{i}g)\tilde{D}(\lambda) \\
&= \frac{2\lambda - \mathrm{i}g}{2\lambda}(\mathrm{i}\alpha_+ + \lambda)\tilde{A}(\lambda) + \frac{1}{2\lambda}(\mathrm{i}\alpha_+ - \lambda)\tilde{\mathscr{D}}(\lambda)
\end{aligned} \tag{4.22}
$$

where

$$
\tilde{\mathscr{D}}(\lambda) = 2\lambda\tilde{D}(\lambda) + \mathrm{i}g\tilde{A}(\lambda) \tag{4.23}
$$

and therefore eigenvectors of the Hamiltonian (4.1), we will need commutation relations between various operator-valued entries of the $U(\lambda)$ matrix. Making use of equation (4.18) and the definition (4.17), one obtains

$$
[\tilde{B}(\lambda_1), \tilde{B}(\lambda_2)] = [\tilde{C}(\lambda_1), \tilde{C}(\lambda_2)] = 0
$$

$$
\begin{aligned}
\tilde{A}(\lambda_1)\tilde{B}(\lambda_2) &= \frac{(\lambda_{12}+\mathrm{i}g)(\tilde{\lambda}_{12}+\mathrm{i}g)}{\lambda_{12}\tilde{\lambda}_{12}}\tilde{B}(\lambda_2)\tilde{A}(\lambda_1) \\
&\quad - \frac{\mathrm{i}g(2\lambda_2+\mathrm{i}g)}{2\lambda_2\lambda_{12}}\tilde{B}(\lambda_1)\tilde{A}(\lambda_2) + \frac{\mathrm{i}g}{2\lambda_2\tilde{\lambda}_{12}}\tilde{B}(\lambda_1)\tilde{\mathscr{D}}(\lambda_2)
\end{aligned} \tag{4.24}
$$

$$
\begin{aligned}
\tilde{\mathscr{D}}(\lambda_1)\tilde{B}(\lambda_2) &= \frac{(\lambda_{12}-\mathrm{i}g)(\tilde{\lambda}_{12}-\mathrm{i}g)}{\lambda_{12}\tilde{\lambda}_{12}}\tilde{B}(\lambda_2)\tilde{\mathscr{D}}(\lambda_1) - \frac{\mathrm{i}g(2\lambda_1-\mathrm{i}g)(2\lambda_2+\mathrm{i}g)}{2\lambda_2\tilde{\lambda}_{12}}\tilde{B}(\lambda_1)\tilde{A}(\lambda_2) \\
&\quad + \frac{\mathrm{i}g(2\lambda_1-\mathrm{i}g)}{2\lambda_2\lambda_{12}}\tilde{B}(\lambda_1)\tilde{\mathscr{D}}(\lambda_2).
\end{aligned} \tag{4.25}
$$

Formulae (4.24) and (4.25) suggest that $\tilde{B}(\lambda)$ is the creation operator. Let us introduce the reference state $|0\rangle$, defined as

$$
\psi(x)|0\rangle = \tilde{C}(\lambda)|0\rangle = 0. \tag{4.26}
$$

Then one can show that $|0\rangle$ is the eigenvector of the operators $\tilde{A}(\lambda)$ and $\tilde{\mathscr{D}}(\lambda)$:

$$
\begin{aligned}
\tilde{A}(\lambda)|0\rangle &= (\lambda + \mathrm{i}\alpha_-)\exp(-\mathrm{i}\lambda L)|0\rangle = a(\lambda)|0\rangle \\
\tilde{\mathscr{D}}(\lambda)|0\rangle &= (2\lambda + \mathrm{i}g)(\mathrm{i}\alpha_- - \lambda)\exp(\mathrm{i}\lambda L)|0\rangle = d(\lambda)|0\rangle.
\end{aligned} \tag{4.27}
$$

The vector

$$
\phi(\{\lambda_j\}) = \prod_{i=1}^{N} \tilde{B}(\lambda_j)|0\rangle \tag{4.28}
$$

is the eigenvector of $t(\lambda_0)$:

$$
t(\lambda_0)\phi = \Lambda(\lambda_0)\phi \tag{4.29}
$$

where

$$\Lambda(\lambda_0) = a(\lambda_0)\frac{2\lambda_0 - ig}{2\lambda_0}(\lambda_0 + i\alpha_+)\prod_{i=1}^{N}\frac{(\lambda_{0i}+ig)(\tilde{\lambda}_{0i}+ig)}{\lambda_{0i}\tilde{\lambda}_{0i}}$$

$$+ d(\lambda_0)\frac{1}{2\lambda_0}(i\alpha_+ - \lambda_0)\prod_{i=1}^{N}\frac{(\lambda_{0i}-ig)(\tilde{\lambda}_{0i}-ig)}{\lambda_{0i}\tilde{\lambda}_{0i}} \tag{4.30}$$

if the pairwise distinct numbers $\{\lambda_j\}$ satisfy the following system of Bethe ansatz equations:

$$\exp(i2\lambda_i L) = \frac{(\lambda_i + i\alpha_+)}{(\lambda_i - i\alpha_+)}\frac{(\lambda_i + i\alpha_-)}{(\lambda_i - i\alpha_-)}\prod_{\substack{j=1\\ j\neq 1}}^{N}\frac{\lambda_{ij}+ig}{\lambda_{ij}-ig}\frac{\tilde{\lambda}_{ij}+ig}{\tilde{\lambda}_{ij}-ig}. \tag{4.31}$$

A proof can be constructed in a manner similar to that of the case of periodic boundary conditions [17] and makes use only of commutation relations (4.24) and (4.25) and formulae (4.27).

Since particle number ($\hat{N}$) and Hamiltonian ($\hat{H}$) operators belong to the infinite set of commuting conserved quantities, generated by $t(\lambda_0)$, we have

$$\hat{N}\phi(\{\lambda_i\}) = N\phi(\{\lambda_j\}) \qquad \hat{H}\phi(\{\lambda_i\}) = \sum_{j=1}^{N}\lambda_j^2 \cdot \phi(\{\lambda_j\}). \tag{4.32}$$

It should be noted that in the case of boundary conditions (4.2) the momentum operator $\hat{P}$ does not belong to the set of conserved quantities, in contrast to the case of periodic and twisted boundary conditions. This is quite natural, since in the presence of reflecting walls the transitional invariance is irretrievably lost.

Finally, returning to equation (4.31), we observe that this equation is symmetric under replacement $\lambda_j \to -\lambda_j$. To avoid the problem of double counting, we will assume below that all Bethe ansatz roots are positive.

5. The finite-size corrections for reflecting wall boundary conditions

In this section, we will consider the finite-size corrections to the spectrum of the system, given by the Hamiltonian (3.1) and will determine all surface critical exponents. Taking the logarithm of (4.31), we have

$$2\lambda_i L + \theta_+(\lambda_i) + \theta_-(\lambda_i) + \sum_{\substack{j=1\\ j\neq 1}}^{N}[\theta(\lambda_{ij}) + \theta(\tilde{\lambda}_{ij})] = 2\pi n_i \tag{5.1}$$

where $\theta_\pm(\lambda)$ is defined as $\theta(\lambda)$ with g replaced by $\alpha_\pm$, and integers $\{n_i\}$ belong to a set of unequal positive integers greater than zero.

One can rewrite (4.1) in a form similar to that of $2N+1$ particles in a box of length $2L$ with some extra terms:

$$\frac{\lambda_i}{\pi} + \frac{1}{2\pi L}[\theta_+(\lambda_i) + \theta_-(\lambda_i) - \theta(\lambda_i) - \theta(2\lambda_i)] + \frac{1}{2\pi L}\sum_{j=-N}^{N}\theta(\lambda_{ij}) = \frac{n_i}{L}. \tag{5.2}$$

In the last formula, we extended the limits of summation using the convention

$\lambda_{-i} = -\lambda_i$, $n_{-i} = -n_i$. The ground state is characterised by the set of consecutive integers j:

$$-N \leqslant j \leqslant N. \tag{5.3}$$

With the replacement

$$N \to N + r \tag{5.4}$$

one obtains Bethe ansatz equations for the ground state in the r-particle sector:

$$\begin{gathered}\frac{\lambda_i}{\pi} + \frac{1}{2\pi L}[\theta_+(\lambda_i) + \theta_-(\lambda_i) - \theta(\lambda_i) - \theta(2\lambda_i)] + \frac{1}{2\pi L}\sum_{j=-(N+r)}^{N+r}\theta(\lambda_{ij}) = \frac{i}{L}\\ -(N+r) \leqslant i \leqslant (N+r).\end{gathered} \tag{5.5}$$

Once again, let us define the new variable $z(\lambda_L)$ as

$$z(\lambda_L) = \frac{\lambda_L}{\pi} + \frac{1}{2\pi L}[\theta_+(\lambda_L) + \theta_-(\lambda_L) - \theta(\lambda_L) - \theta(2\lambda_L)] + \frac{1}{2\pi L}\sum_{j=-(N+r)}^{N+r}\theta(\lambda_L - \lambda_j). \tag{5.6}$$

Obviously, for $\lambda_L = \lambda_i$,

$$z(\lambda_L = \lambda_i) = i/L. \tag{5.7}$$

Applying the Euler–Maclaurin formula (1.13) to the sum on the RHS of the last equation and keeping terms up to order $1/L^2$, one obtains

$$\begin{aligned}&\frac{\lambda_L(z)}{\pi} + \frac{1}{2\pi L}[\theta_+(\lambda_L(z)) + \theta_-(\lambda_L(z)) - \theta(\lambda_L(z)) - \theta(2\lambda_L(z))]\\ &\qquad + \frac{1}{2\pi}\int_{-(z_m+r/L)}^{z_m+r/L}\theta(\lambda_L(z) - \lambda_L(\bar{z}))\,\mathrm{d}\bar{z}\\ &\qquad + \frac{1}{4\pi L}[\theta(\lambda_L(z) + \lambda_L(z_m + r/L)) + \theta(\lambda_L(z) - \lambda_L(z + r/L))]\\ &\qquad + \frac{\lambda_L'(z_m + r/L)}{24\pi L^2}[\theta'(\lambda_L(z) + \lambda_L(z_m + r/L)) - \theta'(\lambda_L(z) - \lambda_L(z_m + r/L))]\\ &\quad = z\end{aligned} \tag{5.8}$$

where we introduced z_m:

$$z_m = N/L. \tag{5.9}$$

Expanding λ_L around $\pm z_m$ and making the following ansatz for $\lambda_L(z)$:

$$\lambda_L(z) = \lambda_\infty(z) + \frac{g_1(z)}{L} + \frac{g_2(z)}{L^2} + \mathrm{O}\left(\frac{1}{L^3}\right) \tag{5.10}$$

we find

$$\left(1 - \frac{\hat{K}}{2\pi}\right)\rho_\infty = \frac{1}{\pi} \tag{5.11}$$

$$\left(1 - \frac{\hat{K}}{2\pi}\right)\rho_\infty g_1 = \frac{1}{2\pi}[\theta(2\lambda) + \theta(\lambda) - \theta_+(\lambda) - \theta_-(\lambda)] - \frac{1+2r}{4\pi}[\theta(\lambda + q) + \theta(\lambda - q)] \tag{5.12}$$

$$\begin{aligned}\rho_\infty g_2 &= \tfrac{1}{2}(\rho_\infty g_1^2)' + \tfrac{1}{2}(M(\lambda, q) - M(\lambda, -q))\\ &\quad \times\left(\rho_\infty g_1^2(q) + (2r+1)g_1(q) + \frac{r^2 + r + \frac{1}{6}}{\rho_\infty(q)}\right)\end{aligned} \tag{5.13}$$

where

$$\rho_\infty(\lambda_\infty)=\frac{\mathrm{d}z(\lambda_\infty)}{\mathrm{d}\lambda_\infty} \tag{5.14}$$

$$q=\lambda_\infty(z_m) \tag{5.15}$$

and operators $\hat{K}$ and $\hat{M}$ were defined previously by formulae (2.14) and (2.15).

To obtain the finite-size corrections to the energy, we start with the exact expression

$$E_{\mathrm{gr}}^{r}=\sum_{j=1}^{N+r}\lambda_j^2-\mu_0(N+r) \tag{5.16}$$

where the λ_j are subject to the constraint (4.31). Performing manipulations similar to those described above, we get with the help of (5.11)-(5.13)

$$E_{\mathrm{gr}}^{r}=Le_\infty+f+\frac{\pi v_{\mathrm{s}}}{2L}\{[\varepsilon(q)+2(r+1)x_{\mathrm{p}}^{1/2}]^2-\tfrac{1}{12}\} \tag{5.17}$$

where

$$e_\infty=\tfrac{1}{2}\int_{-q}^{q}\lambda^2\rho_\infty(\lambda)\,\mathrm{d}\lambda \tag{5.18}$$

$$f=\tfrac{1}{2}q^2+\int_{-q}^{+q}\lambda(\varepsilon(\lambda)-\gamma(\lambda))\,\mathrm{d}\lambda \tag{5.19}$$

$$\varepsilon(\lambda)=\frac{1+\hat{M}}{2\pi}[\theta(2\lambda)+\theta(\lambda)-\theta_+(\lambda)-\theta_-(\lambda)] \tag{5.20}$$

$$\gamma(\lambda)=\frac{1+\hat{M}}{2\pi}[\theta(\lambda+q)+\theta(\lambda-q)]. \tag{5.21}$$

For the ground-state energy ($r=0$), we have

$$E_{\mathrm{gr}}=Le_\infty+f+\frac{\pi v_{\mathrm{s}}}{2L}\{[\varepsilon(q)+x_{\mathrm{p}}^{1/2}]^2-\tfrac{1}{12}\}. \tag{5.22}$$

The second term in the RHS of the last equation is the surface energy term and can be shown to be different from the one obtained in [16].

The most general excited state can be produced, by creating particle-hole pairs, labelled by an integer s, in the r-particle sector. Let $p(s)$ and $h(s)$ be positions of particles and holes, correspondingly. Then, the energy of this state up to order $1/L$ is

$$E_{r,\{s\}}^{\mathrm{ex}}=Le_\infty+f+\frac{\pi v_{\mathrm{s}}}{L}\left(-\tfrac{1}{24}+\tfrac{1}{2}[\varepsilon(q)+(2r+1)x_{\mathrm{p}}^{1/2}]^2+\sum_s(p(s)-h(s))\right). \tag{5.23}$$

In the presence of the boundary, conformal transformations must be restricted to those that leave the surface invariant. Conformally transforming the strip of size L into the upper half-plane ($\mathrm{Im}\, z\geqslant 0$), we conclude that for the boundary conditions (4.2) with†

$$\alpha_+=-\alpha_-^{\ 1} \tag{5.24}$$

† Note that boundary conditions (5.24) include free and fixed boundary conditions as a special case.

these transformations must map the upper half-plane into itself. Making use of the formula [10]

$$E_{\mathrm{gr}}(L)=Le_{\infty}+f-\frac{\pi v_{\mathrm{s}}}{24L}c \tag{5.25}$$

and equation (5.22), one might conclude at first glance that c is given by

$$c=1-12[\varepsilon(q)+x_{\mathrm{p}}^{1/2}]^{2}<1. \tag{5.26}$$

However this conclusion is obviously in direct contradiction with the Hermiticity of the Hamiltonian (4.1).

This paradox can be explained if we regard the ground state as a defected vacuum of the theory. Indeed, we can minimise the energy still further, subtracting a fractional number of particles r_0†:

$$r_0=\frac{1}{2}+\frac{\varepsilon(q)}{2\sqrt{x_{\mathrm{p}}}}. \tag{5.27}$$

This situation is somewhat analogous to that of the XXZ chain on an odd number of sites where the defected ground state contains half of a particle (kink).

If we now switch to the true vacuum, we readily derive for the conformal anomaly

$$c=1. \tag{5.28}$$

We now turn to the surface exponents of the model. Associated with the lowest energy E^{r}_{gr} in each r-particle sector we have the surface exponent x^{r}_{s}, which may be estimated from the following formula [19]:

$$x^{r}_{\mathrm{s}}=(E^{r}_{\mathrm{gr}}-E^{0}_{\mathrm{gr}})L/\pi v_{\mathrm{s}}. \tag{5.29}$$

With the help of formulae (5.17) and (5.29) we will obtain

$$x^{r}_{\mathrm{s}}=2(r+r_0)^2x_{\mathrm{p}}-2r_0^2x_{\mathrm{p}}. \tag{5.30}$$

Thus, we see that all surface exponents are corrected by the presence of the r_0 particles in the ground state. Because the surface breaks translational invariance, correlation functions have a more complicated dependence than in the bulk. However, at the bulk critical point, the one-point function of a scaling operator ϕ_i is restricted by the scaling and translational invariance along the real axis to the form [20]:

$$\langle\phi_i(y)\rangle=A/y^{x_i} \tag{5.31}$$

where y is the distance measured from the surface and x_i is the bulk scaling dimension of ϕ_i. In particular, for the current operator $\psi^{+}(y)\psi(y)$ we have

$$\langle\psi^{+}(y)\psi(y)\rangle=\frac{A}{y}+B\frac{\cos(2\pi Dy)}{y^{1/4x_{\mathrm{p}}}}\qquad 1/q\ll y\ll L \tag{5.32}$$

where use of equation (1.8) was made.

† Formula (5.25) holds true for conformally invariant theories, where the interpretation of the spectrum in terms of particles may be inconsistent.

The two-point correlation function $\langle\phi_i\phi_i\rangle$ in the surface geometry is constrained by the small conformal group to the form [21]

$$\langle\phi_i(y_2, t_2)\phi_i(y_1, t_1)\rangle = \frac{1}{(y_1 y_2)^{x_i}}\,\phi(\chi) \tag{5.33}$$

where

$$\chi = \frac{(t_2 - t_1)^2 + y_1^2 + y_2^2}{y_1 y_2} \tag{5.34}$$

and $\phi(\chi)$ is some undetermined function, which falls off like χ^{-x_s} as its argument $\chi \to \infty$. If y_1 is located near the boundary, i.e.

$$y_1 \approx 1/q \tag{5.35}$$

and

$$1/q \ll y_2 \ll L \qquad 1/q \ll t_2 \ll L \tag{5.36}$$

then one can obtain

$$\langle\phi_i(y_2, t_2)\phi_i(y_1, t_1)\rangle \sim \frac{1}{[y_2^2 + (t_2 - t_1)^2]^{x_s^i}(y_2^{x_i - x_s^i})}. \tag{5.37}$$

The field operator $\psi(y, t)$ is associated with the ground state in the one-particle sector

$$x_\psi = x_{\mathrm{p}} \qquad x_{\mathrm{s}}^{\psi} = 2(2r_0 + 1)x_{\mathrm{p}}. \tag{5.38}$$

Making use of (4.37) and (4.38), we finally have for the two-point field correlator

$$\langle\psi^+(y, t)\psi(0, 0)\rangle \sim \frac{1}{[y^2 - v_{\mathrm{s}}^2 t^2]^{(4r_0+2)x_{\mathrm{p}}} y^{-(4r_0+1)x_{\mathrm{p}}}}. \tag{5.39}$$

The last expression is valid for the class of boundary conditions (4.2) and (5.24) and shows no dependence on α.

In the infinite coupling limit $g \to \infty$ the two-point field correlator becomes particularly simple:

$$\lim_{g\to\infty} \langle\psi^+(y, t)\psi(0, 0)\rangle \sim \frac{y^{3/4}}{(y^2 - v_{\mathrm{s}}^2 t^2)}. \tag{5.40}$$

We hope to verify this prediction of conformal invariance by exact calculations in future publications.

6. Summary and conclusions

Let us briefly summarise the main new results. All exactly integrable models for which finite-size corrections have been obtained in the past have possessed inversion formulae, giving the density of Bethe ansatz roots $\rho(\lambda)$ as an explicit function of λ. We have extended the technique to a situation where it is impossible to obtain $\rho(\lambda)$ in closed form.

We have obtained the surface energy for the case of reflecting wall boundary conditions. In particular, we correct a previous calculation [16] for the special case of fixed boundary conditions.

We have extended standard predictions of conformal invariance to include oscillating terms in the Green functions.

Known exact results have been previously confined to a few operators only [14]. We have obtained all possible operator scaling dimensions, which indicate that the NLS model belongs to the Gaussian model universality class. This result is consistent with the analysis of the XXZ model [22]. There is, however, an important distinction. In the latter case vortex excitations correspond to the string configurations of Bethe ansatz roots, while for the NLS model they are created by the shift of the Fermi band as a whole. The results obtained in this paper for twisted and reflecting wall boundary conditions are completely new. It is important to point out that twist (unlike reflecting walls) affects bulk critical behaviour.

Let us further note that, since the scaling dimensions obtained in this paper are known exactly for all values of the coupling constant g, our results offer the possibility of systematically resumming $1/g$ expansions for the long-distance behaviour of the Green functions.

The technique we have used can be extended systematically to obtain all higher-order corrections. These give us information about coefficients in the operator product expansion and irrelevant operators in the critical Hamiltonian. In the NLS model all the higher-order corrections are integer powers of L and the critical Hamiltonian is not spinless with respect to the fixed-point Hamiltonian as is usually the case.

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