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Finite-size scaling and universality in the spectrum of the quantum Ising chain: I. Periodic and antiperiodic boundary conditions

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Abstract. The spectrum of the quantum Ising chain is studied in the finite-size scaling limit for periodic and antiperiodic boundary conditions. The finite-size corrections are computed for all energy gaps. The results of our model are used to test the Privman-Fisher universality hypothesis and conformal theory.

At the critical point, it is shown how to build the spectrum from the irreducible representations of the Virasoro algebra. In addition, we find evidence for an unsuspected symmetry for systems both non-critical and of finite size.

1. Introduction

In Hamiltonian field theory, finite-size scaling (for a review see Barber (1983)) has been used to extract critical points and critical exponents from the two lowest eigenvalues of the Hamiltonian.

It is the object of this paper to study, in the finite-size scaling limit, the whole spectrum. This will be done for an exactly soluble model (Katsura 1962), defined on a chain with N sites:

$$H=-\frac{h}{2\gamma}\sum_{n=1}^{N}\sigma^z(n)-\frac{1}{4\gamma}\sum_{n=1}^{N}[(1+\gamma)\sigma^x(n+1)\sigma^x(n)+(1-\gamma)\sigma^y(n+1)\sigma^y(n)] \tag{1.1}$$

where σ^x, σ^y, σ^z are the Pauli matrices. We do not include terms of the form $b\,\Sigma_n\,\sigma^x(n)$, which give rise to a longitudinal magnetic field. The normalisation of H, which in principle is arbitrary, is fixed by the requirements of conformal theory (von Gehlen *et al* 1986). We shall first complete the definition of the problem and shall then explain what we want to do.

The phase diagram is well known (Barouch and McCoy 1971). For all γ $(0<\gamma\leqslant 1)$, there is a critical point at $h_c=1$, which falls into the 2D Ising universality class.

We specify the boundary conditions taking in (1.1):

$$\sigma(N+1)=(-1)^{\tilde{Q}}\sigma(1) \tag{1.2}$$

where σ stands for σ^x or σ^y and get the Hamiltonians $H^{(\tilde{Q})}$. Free boundary conditions will be studied in a separate paper. H commutes with the operator:

$$Q=\frac{1}{2}\left(1-\prod_{n=1}^{N}\sigma^z(n)\right) \tag{1.3}$$

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which has eigenvalues 0 and 1. The corresponding eigenspaces of Q are called sectors 0 and 1. We are thus left with the blocks $H_Q^{(\tilde{Q})}$, where Q labels the sectors 0 and 1. We can further prediagonalise $H_Q^{(\tilde{Q})}$ by using translational invariance, where the momentum P will be used to label the resulting submatrices.

The scaling variable z is defined as

$$z = N(h-1) \tag{1.4}$$

and we are interested in the finite-size scaling limit $N \to \infty$, $h \to 1$ and z fixed.

Since our Hamiltonian (1.1) is exactly soluble (Katsura 1962), it provides a fine laboratory for testing general ideas. In this work, we focus on the question of universality with respect to γ. We now state what we want to compute.

(i) Consider the case $z = 0$. Our first aim is to obtain the finite-size corrections to the ground-state energy E_0:

$$E_0/N = \varepsilon_0 + \varepsilon_2/N^2 + \varepsilon_4/N^4 + \mathrm{O}(N^{-6}). \tag{1.5}$$

We find that only ε_2 is a universal number. This confirms a result from conformal theory for periodic boundary conditions (Blöte *et al* 1986, Affleck 1986):

$$\varepsilon_2 = -\tfrac{1}{6}\pi c \tag{1.6}$$

where c is the central charge of the Virasoro algebra ($c = \frac{1}{2}$ for the Ising model (Belavin *et al* 1984))

$$[L_n, L_m] = (n-m)L_{n+m} + \tfrac{1}{12}c(n^3 - n)\delta_{n+m,0}. \tag{1.7}$$

Next, we turn to the scaled energy gaps $F_i = (N/2\pi)(E_i - E_0)$ of a level E_i of H with the ground state E_0 (see § 2 for a precise definition):

$$F_i = A_i + B_i(\gamma)N^{-2} + C_i(\gamma)N^{-4} + \mathrm{O}(N^{-6}) \tag{1.8}$$

where i is a label of the excited levels. The numbers A_i are universal and are given by the irreducible representations of a pair of Virasoro algebras with the same central charge c (Belavin *et al* 1984, Cardy 1986a, von Gehlen and Rittenberg 1986). We shall identify the irreducible representations which build the spectrum of the $H_Q^{(\tilde{Q})}$ at the critical point. The $B_i(\gamma)$ and the $C_i(\gamma)$ show a unique γ dependence for all levels.

The spectra of our $H_Q^{(\tilde{Q})}$ are in a one-to-one correspondence with the spectrum of the continuum field theoretic Majorana Hamiltonian (see, e.g., Bander and Itzkyson 1977) with prescribed boundary conditions. This connection will be shown in full detail.

(ii) We now take $z \neq 0$. For the energy gap, we obtain

$$F_i(z) = A_i(z/\gamma) + \mathrm{O}(N^{-1}) \tag{1.9}$$

and we shall compute the universal functions A_i exactly, for all energy levels. Our results include, as special cases, previous studies on the lowest excitations (Hamer and Barber (1981) and Burkhardt and Guim (1985) at $\gamma = 1$ and von Gehlen *et al* (1984) for γ arbitrary and $z = 0$).

Our result confirms, to leading order in $1/N$, the Privman–Fisher (1984) universality hypothesis, which states that the inverse correlation length ξ_i^{-1} should be

$$\xi_i^{-1} = N^{-1} Y_i(Dz) \tag{1.10}$$

where D is a non-universal system-dependent constant and Y_i is a universal function. We stress that, besides D, there is no further non-universal constant involved. To our knowledge, this is the first time that (1.10) is checked for the whole spectrum.

At this point, a few remarks are in order. The Hamiltonian H can be written as the sum of the critical point Hamiltonian H_c and a perturbation

$$H = H_c + \sum_j a_j(\gamma)\Phi_j \tag{1.11}$$

where the Φ_j are scaling fields from the irreducible representations of the Virasoro algebra and the $a_j(\gamma)$ are γ-dependent non-universal constants. As will be shown in detail by Reinicke (1986), the corrections to the critical point Hamiltonian in both z and $1/N$ can be obtained in terms of perturbation theory from (1.11) using the n-point correlation functions at the critical point.

For our model, (1.9) tells us that the gaps depend on the unique variable z/γ. This means that there is a single scaling field Φ which describes, to leading order in $1/N$, the z dependence of the scaling function. The observed γ dependence of the argument of the scaling function comes from the amplitude $a(\gamma)$ of the scaling field Φ.

Next, we look at the corrections in $1/N$ to (1.9). We have

$$F_i(z) = A_i(z/\gamma) + N^{-1}B_i(z, \gamma) + \ldots\ldots \tag{1.12}$$

The leading corrections, given by the functions $B_i(z, \gamma)$, are not in agreement with the Privmann-Fisher hypothesis. This is probably not too surprising if more than one scaling field contributes. In this case, we have more than one $a_j(\gamma)$ (see (1.11)) and consequently a more complicated γ dependence.

(iii) Finally, we return to the spectra of the $H_Q^{(\tilde{Q})}$. At $z = 0$, the levels are highly degenerate. Most of these degeneracies are broken if one moves away from $z = 0$, but we also find a pattern of states which remain degenerate for arbitrary values of both z as well as $1/N$. This is an indication for the existence of a new, unexpected, symmetry in our model.

The paper is organised as follows. In § 2, we briefly review the diagonalisation of H and establish our notation. In § 3, we give the irreducible representations of the Virasoro algebra which build the spectrum. In addition, we give the explicit relation of the spectra of the continuum Majorana Hamiltonian with the $H_Q^{(\tilde{Q})}$. In § 4, we study the finite-size behaviour for $z = 0$.

The scaling functions are computed in § 5, where we shall also confirm the Privman-Fisher hypothesis. A list of the gaps of the lowest excitations corresponding to the primary fields of conformal theory is given in § 6. In § 7, we examine the spectrum away from the critical point. A summary of our results is presented in § 8.

In the appendix, we analyse the sums encountered in the finite-size scaling study.

2. Statement of the problem

In this section we outline the calculation of the spectrum of H. It is mainly intended to establish our notation.

We diagonalise the Hamiltonian of (1.1) by a Jordan-Wigner transformation followed by a canonical transformation (for details see Katsura 1962) and obtain

$$H = -\sum_m \Lambda(\varphi(m))(-\eta_m^+\eta_m + \tfrac{1}{2}) \tag{2.1}$$

where η_m^+, η_m are fermionic creation and annihilation operators and

$$\Lambda(\varphi) = \frac{1}{\gamma}\left((h-1)^2 + 4(h-1+\gamma^2)\sin^2\frac{\varphi}{2} - 4(\gamma^2-1)\sin^4\frac{\varphi}{2}\right)^{1/2}. \tag{2.2}$$

The function $\varphi(m)$ depends on the boundary conditions (Lieb *et al* 1961, see also Burkhardt and Guim 1985). We distinguish two cases (Hamiltonians $H^{(A)}$, $H^{(B)}$)

$$\text{(A)} \qquad \varphi(m)=\frac{2m+1}{N}\pi \qquad m=0,\ldots, \tag{2.3}$$

$$\text{(B)} \qquad \varphi(m)=\frac{2m}{N}\pi \qquad m=0,\ldots, \tag{2.4}$$

and $[x]$ is the largest integer less or equal to x. Case A corresponds to antiperiodic boundary conditions and case B corresponds to periodic boundary conditions in the fermions. The identification of the Hamiltonians $H^{(A)}$, $H^{(B)}$ with the Hamiltonians $H_Q^{(\tilde{Q})}$ is as follows.

The sector 0 in the space with an even number of fermionic excitations and the sector 1 is the space with an odd number of excitations. We can identify

$$\begin{aligned} H^{(A)}_{\text{even}} &= H_0^{(0)} \qquad & H^{(A)}_{\text{odd}} &= H_1^{(1)} \\ H^{(B)}_{\text{even}} &= H_0^{(1)} \qquad & H^{(B)}_{\text{odd}} &= H_1^{(0)}. \end{aligned} \tag{2.5}$$

For $z=0$, we have in addition $H_0^{(1)}=H_1^{(0)}$.

Let $E_0^{(0)}$ be the energy of the lowest state of $H_0^{(0)}$ and let $E_Q^{(\tilde{Q})}(P,r)$ be an eigenvalue of $H_Q^{(\tilde{Q})}$ with an eigenstate of momentum P. We are interested in the gaps

$$F_Q^{(\tilde{Q})}(P,r)=\frac{N}{2\pi}\left(E_Q^{(\tilde{Q})}(P,r)-E_0^{(0)}\right) \tag{2.6}$$

where $r=0$ denotes the lowest gap, $r=1$ the second gap (for a fixed momentum P) and so on. For two states, which use the same function $\varphi(m)$, the F are directly given by the $\Lambda(m)$. If two states use different functions $\varphi(m)$, the F will receive, besides the contribution of the $\Lambda(m)$, an additional contribution from the difference of the ground-state energies of the Hamiltonians $H_Q^{(\tilde{Q})}$ used.

In the following, the F will be computed as a function of the scaling variable

$$z=N(h-1) \tag{2.7}$$

in the limit $N\to\infty$, $h\to 1$ and z fixed.

3. Spectrum and Virasoro algebra

In this section we present, in the limit $N\to\infty$, the spectra of the $H_Q^{(\tilde{Q})}$ and give the representations of the Virasoro algebra which build the spectrum. In the next subsection, we briefly review (see Friedan *et al* 1984) the facts about the Virasoro algebra that we need for our purposes. In the following subsection, the representations building the spectra for the $H_Q^{(\tilde{Q})}$ are given. In § 3.3, we give the relation to the continuum Majorana Hamiltonian.

For this whole section, we take $z=0$.

3.1. The Virasoro algebra

The irreducible representations of the Virasoro algebra (1.7) can be characterised by their highest weight states $|\Delta\rangle$, which are defined by

$$\begin{aligned} L_0|\Delta\rangle &= \Delta|\Delta\rangle \\ L_n|\Delta\rangle &= 0 \qquad \text{if } n>0. \end{aligned} \tag{3.1}$$

These are just the primary fields known from conformal theory. They give the lowest lying states of our spectra. Excited states are, in principle, generated from the primary fields by

$$|\Delta+r\rangle = L_{-r_1}\ldots L_{-r_k}|\Delta\rangle \qquad r_i>0 \tag{3.2}$$

and $r=r_1+\ldots+r_k$ but not all of the states are independent. Let $d(\Delta, r)$ denote the degeneracy of the level $(\Delta+r)$.

For the Ising model, the central charge (see (1.7)) is $\frac{1}{2}$ and Δ can only take the values 0, $\frac{1}{16}$ and $\frac{1}{2}$ (Friedan *et al* 1984). Using the character formula of Rocha-Caridi (1984), Altschüler and Lacki (1985) have computed the values of $d(\Delta, r)$ which are listed in table 1. The $d(\Delta, r)$ are the numbers which will be compared with our spectra in the next section.

Table 1. The function $d(\Delta, r)$ representing the degeneracies of the level $(\Delta+r)$ of the irreducible representation with the lowest weight Δ.

	r										
Δ	0	1	2	3	4	5	6	7	8	9	10
0	1	0	1	1	2	2	3	3	5	5	7
$\frac{1}{2}$	1	1	1	1	2	2	3	4	5	6	8
$\frac{1}{16}$	1	1	1	2	2	3	4	5	6	8	10

3.2. *Identification of the irreducible representations*

Recall that the spectra are given by two commuting Virasoro algebras with the same central charge. The spectra are thus given by pairs of irreducible representations. The primary fields are characterised by two numbers Δ and $\bar{\Delta}$, where $x=\Delta+\bar{\Delta}$ is the scaling dimension and $s=\Delta-\bar{\Delta}$ is the spin of the primary field $(\Delta, \bar{\Delta})$. In the spectrum built from this field one gets the levels

$$\begin{aligned} F(P) &= (\Delta+r)+(\bar{\Delta}+\bar{r}) \\ P &= (\Delta+r)-(\bar{\Delta}+\bar{r})+\tfrac{1}{2}\tilde{Q} \end{aligned} \tag{3.3}$$

($r, \bar{r}=0, 1, 2, \ldots$) with degeneracy $d(\Delta, r)\cdot d(\bar{\Delta}, \bar{r})$.

Returning to our model (1.1), we take the $F_Q^{(\tilde{Q})}(P)$ from (2.6). The momentum operator is

$$P=\sum_m p(m)\eta_m^+\eta_m \tag{3.4}$$

where

$$p(m)=\begin{cases} m+\frac{1}{2} & \text{case A, equation (2.3)} \\ m & \text{case B, equation (2.4).} \end{cases} \tag{3.5}$$

The spectra are shown, for $z=0$, in figures 1-3. From (3.3) and table 1 we see that the spectrum of $H_0^{(0)}$ is generated from (0, 0) and $(\frac{1}{2}, \frac{1}{2})$, $H_1^{(1)}$ is generated from $(\frac{1}{2}, 0)$ and $(0, \frac{1}{2})$ and $H_0^{(1)}$ and $H_1^{(0)}$, which have the same spectrum, are generated from $(\frac{1}{16}, \frac{1}{16})$.

After we had finished this calculation, we received a paper by Cardy (1986b), where the same identification of the primary fields with the spectra was obtained.

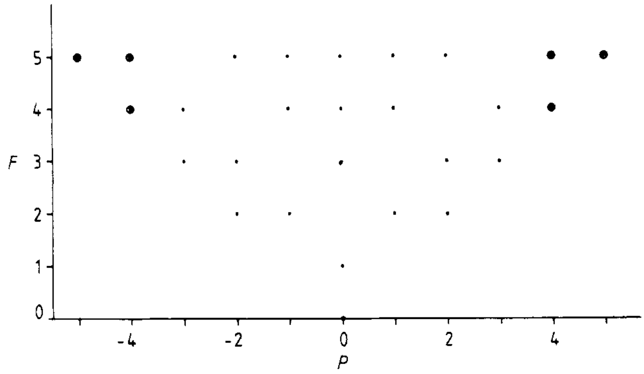

Figure 1. Spectrum of $H_0^{(0)}$ at $z = 0$ and $N \to \infty$. The symbol ⊙ denotes a twofold degenerate state.

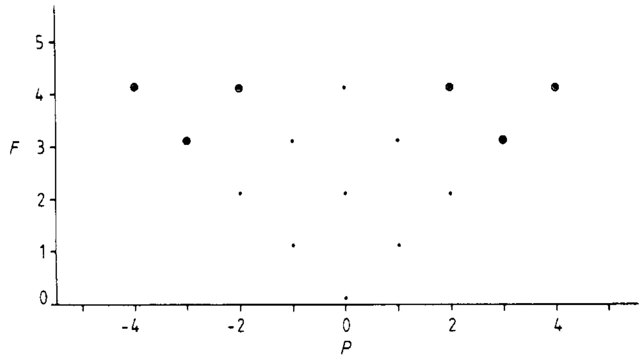

Figure 2. Spectrum of $H_1^{(0)}$ and $H_0^{(1)}$ at $z = 0$ and $N \to \infty$. The zero of energy is chosen to be the ground state of $H_0^{(0)}$.

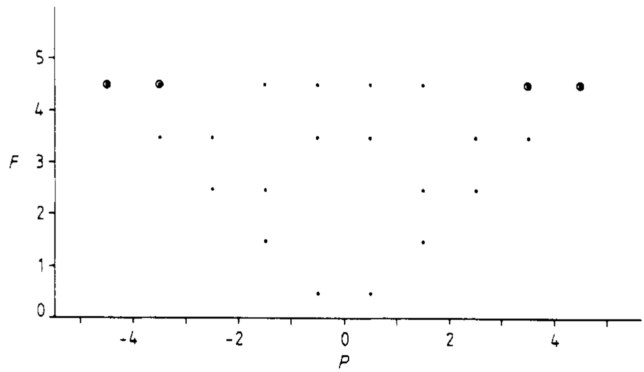

Figure 3. Spectrum of $H_1^{(1)}$ at $z = 0$ and $N \to \infty$. The zero of energy is the ground state of $H_0^{(0)}$.

3.3. *Relation to the Majorana Hamiltonian*

We now give the relation between the Hamiltonians $H_Q^{(\tilde{Q})}$ and the continuum Majorana (e.g. Bander and Itzkyson 1977, see also von Gehlen *et al* 1986) Hamiltonian with definite boundary conditions.

Begin with case A (equation (2.3)). This corresponds to antiperiodic boundary conditions for the Majorana spinor. The sector 0 is given by $H_0^{(0)}$ and sector 1 by $H_1^{(1)}$. Case B (equation (2.4)) corresponds to periodic boundary conditions for the Majorana spinors. The spectrum is given by $H_0^{(1)}$ and $H_1^{(0)}$.

4. Finite-size corrections at $z=0$

In this section, we study the finite-size corrections to the ground-state energy and to the energy gaps at $z=0$.

4.1. *Ground-state energy*

The lowest lying level of the $H_Q^{(\tilde{Q})}$ is the $E_0^{(0)}$ defined in § 2. From equations (2.1)-(2.3) we have

$$E_0^{(0)}=-\sum_{k=0}^{N-1}\left[\sin^2\left(\frac{\pi(k+\frac{1}{2})}{N}\right)-\frac{\gamma^2-1}{\gamma^2}\sin^4\left(\frac{\pi(k+\frac{1}{2})}{N}\right)\right]^{1/2}. \tag{4.1}$$

This sum is analysed in the appendix, with the result (equation (A13)):

$$\frac{E_0^{(0)}}{N}=-\frac{1}{2}T_1(\gamma)-\frac{\pi}{12N^2}+\frac{7\pi^3}{960N^4}\left(\frac{1}{\gamma^2}-\frac{4}{3}\right)+\mathrm{O}(N^{-6}) \tag{4.2}$$

where $T_1(\gamma)$ is defined in equation (A12).

We can now compare our results with conformal theory. The leading correction in $1/N$ to the ground-state energy per spin, which is of the order of $1/N^2$, is seen from (4.2) to be a universal number. This is in agreement with a formula by Blöte *et al* (1986) and Affleck (1986) already mentioned in the introduction (equation (1.6)) which provides a relation with the central charge c. For the numerical value of c we find $c=\frac{1}{2}$, in agreement with the result of Belavin *et al* (1984).

4.2. *Energy gaps*

Before we give the general result, we look at an example. Consider $F_1^{(0)}(0,0)$ which receives contributions from the ground-state energies of both $H_0^{(0)}$ and $H_1^{(0)}$, since the first state is in sector 1. The gap is thus given by the difference of the zero-point energies of $H_0^{(0)}$ and $H_1^{(0)}$, which use different froms of $\varphi(m)$ (see equations (2.3) and (2.4)):

$$F_1^{(0)}(0,0)=\frac{N}{4\pi}\sum_m[\Lambda(\varphi_{\mathrm{B}}(m))-\Lambda(\varphi_{\mathrm{A}}(m))] \tag{4.3}$$

$$=\frac{N}{2\pi}(S_{2N}-2S_N) \tag{4.4}$$

$$=\frac{1}{8}-\frac{\pi^2}{128}\left(\frac{1}{\gamma^2}-\frac{4}{3}\right)N^{-2}+\mathrm{O}(N^{-4}) \tag{4.5}$$

where S_N is taken from the appendix (A17). Other gaps are obtained along the lines given in § 2.

If both states use the same function $\varphi(m)$, the gaps are given by $\Lambda(m)$, which we write down here for case A:

$$\Lambda(m)=\frac{2\pi}{N}\left\{|m+\tfrac{1}{2}|+|m+\tfrac{1}{2}|^3\frac{\pi^2}{2}\left(\frac{1}{\gamma^2}-\frac{4}{3}\right)N^{-2}\right.$$
$$\left.-|m+\tfrac{1}{2}|^5\left[\frac{\pi^4}{8}\left(\frac{1}{\gamma^2}-\frac{4}{3}\right)^2+\frac{4\pi^4}{3}\left(\frac{1}{\gamma^2}-\frac{16}{15}\right)\right]N^{-4}+\mathrm{O}(N^{-6})\right\}. \tag{4.6}$$

To obtain case B, replace $m+\frac{1}{2}$ by m.

If different functions $\varphi(m)$ are used by both states, then in addition to the contribution of the $\Lambda(m)$, the gap gets a contribution as the one in (4.5).

To summarise: the next-to-leading term, which is of the order of $1/N^2$, shows the same γ dependence for all gaps. For the next-to-leading correction, of order $1/N^4$, we first observe from (4.6) that again all gaps show the same γ dependence. Its γ dependent factor contains two terms. The first one can be thought of as a second-order effect from the leading correction, while the second term introduces a new contribution.

In terms of scaling fields (see (1.11)) this means that the leading correction, of order $1/N^2$, is generated from a single scaling field Φ_1, while the next-to-leading correction, of order $1/N^4$, has contributions from Φ_1 and at least one more field Φ_2.

5. Finite-size scaling functions

In this section, we obtain the exact scaling functions for the whole energy spectrum. In addition, we study corrections to scaling.

A major topic of this section is to find out to what extent the Privman–Fisher (1984) universality hypothesis is valid. We expect for our normalised gaps $F_i(z)$

$$F_i(z)=Y_i(Dz) \tag{5.1}$$

where i labels the specific gap, D is a model-dependent non-universal constant and Y_i is a universal function. Besides D, there is no further non-universal constant involved.

We now present the scaling functions. As in § 4.2, we begin with the gap $F_1^{(0)}(0,0)$, which is given by

$$F_1^{(0)}(0,0)=\frac{N}{2\pi}\left(\frac{z}{N\gamma}+\frac{1}{2}S_{2N}(2z)-S_N(z)\right) \tag{5.2}$$

where $S_N(z)$ is analysed in the appendix (A28). We have

$$F_1^{(0)}(0,0)=\frac{1}{8}+\frac{1}{4\pi}\frac{|z|}{\gamma}+\frac{\ln 2}{4\pi^2}\frac{z^2}{\gamma^2}+\tfrac{1}{2}R_{1\frac{1}{2},0}\left(\frac{z^2}{4\pi^2\gamma^2}\right)-\frac{1}{8}R_{1\frac{1}{2},0}\left(\frac{z^2}{\pi^2\gamma^2}\right)+\mathrm{O}(N^{-1}) \tag{5.3}$$

where

$$R_{1\frac{1}{2},0}(x)=-4\sum_{r=1}^{\infty}\left((r^2+x)^{1/2}-r-\frac{x}{2r}\right) \tag{5.4}$$

is a remnant function (Fisher and Barber 1972), of which we need the property

$$R_{1\frac{1}{2},0}(x)=\mathrm{O}(x^2) \qquad \text{if } x\to 0. \tag{5.5}$$

Equation (5.3) gives, to leading order in $1/N$, the exact scaling function. For $\gamma=1$, this result was already obtained by Hamer and Barber (1981)†.

To obtain the other gaps, we have to compute the $\Lambda(m)$. We find, after a tedious calculation

$$\Lambda(m)=\frac{2\pi}{N}\left(A_0+\sum_{r=1}^{4}\left[A_0A_r(A_0^2N)^{-r}\right]\right)+O(N^{-6}) \tag{5.6}$$

where (for case A)

$$A_0=\left((m+\tfrac{1}{2})^2+\frac{1}{4\pi^2}\frac{z^2}{\gamma^2}\right)^{1/2} \tag{5.7}$$

$$A_1=\frac{1}{2}\left(m+\frac{1}{2}\right)^2\frac{z}{\gamma^2} \tag{5.8}$$

$$A_2=\left(m+\frac{1}{2}\right)^6\frac{\pi^2}{6}\left(\frac{1}{\gamma^2}-\frac{4}{3}\right)-\left(m+\frac{1}{2}\right)^4\frac{1}{6}\frac{z^2}{\gamma^2} \tag{5.9}$$

$$A_3=-\left(m+\frac{1}{2}\right)^8\frac{\pi^4}{4}\left(\frac{1}{\gamma^2}-\frac{2}{3}\right)\frac{z}{\gamma^2}-\frac{1}{96\pi^2}\left(m+\frac{1}{2}\right)^4\frac{z^5}{\gamma^6} \tag{5.10}$$

$$A_4=-\left(m+\frac{1}{2}\right)^{12}\frac{\pi^4}{8}\left(\frac{1}{\gamma^4}-\frac{16}{15}\right)+\left(m+\frac{1}{2}\right)^{10}\frac{\pi^2}{8}\left(\frac{1}{\gamma^4}-\frac{2}{\gamma^2}+\frac{56}{45}\right)\frac{z^2}{\gamma^2}$$
$$-\left(m+\frac{1}{2}\right)^8\frac{1}{16}\left(\frac{1}{\gamma^2}-\frac{38}{45}\right)\frac{z^4}{\gamma^4}+\frac{1}{180\pi^2}\left(m+\frac{1}{2}\right)^6\frac{z^6}{\gamma^6}. \tag{5.11}$$

Case B is obtained by replacing $m+\frac{1}{2}$ by m.

To leading order in $1/N$, the scaling functions of any desired gap can be obtained by combining (5.3), (5.6) and (5.7).

We point out that, to the order in $1/N$ specified, these equations give the exact scaling functions.

We now look at the leading terms in $1/N$. From (5.3), (5.6) and (5.7) we see that the scaling function of an arbitrary gap depends only on the variable z/γ, but not on z or γ alone. This is just what is stated by (5.1). To leading order in $1/N$, we have thus verified for all gaps the Privman–Fisher universality hypothesis.

Next, we consider corrections to scaling. It is sufficient to consider only gaps of states which belong to $H_0^{(0)}$, so that we only have to deal with $\Lambda(m)$ from (5.6)–(5.11). Consider the leading correction, which is of order $1/N$. From (5.8), we see that A_1 contains, besides the factor z/γ, an additional factor of $1/\gamma$, which is not accommodated by (5.1). The second correction, of order $1/N^2$, shows an entirely different γ dependence. We also note that the γ-dependence of the leading correction is different from the one found for $z=0$. We conclude that, for $z\neq 0$, already the leading corrections to scaling do not satisfy the Privman–Fisher hypothesis. This argment can be extended to the other $H_Q^{(\hat{Q})}$. As already mentioned in the introduction, the confirmation of the Privman–Fisher hypothesis means that the corrections in z are generated by a single scaling field. The correction in $1/N$ contain contributions from more than one field. In (5.8)–(5.11) we note the appearance of new fields with increasing order of $1/N$. In principle, one can obtain from these expressions the $a_j(\gamma)$ for the scaling fields Φ_j of (1.11).

† The formula of Hamer and Barber (1981, equation (4.8)) contains two minor errors.

We conclude with a remark on the leading contribution. Consider (5.7). The amplitude gives the gaps for the $H_0^{(0)}$, whose states are generated by *pairs* of fermionic excitations. From (3.4) and (3.5) we recall that the $m+\frac{1}{2}$ is a momentum eigenvalue. Consequently, the leading term gives an energy-momentum relation $F=(p^2+\mu_B^2)^{1/2}$ which is the same as for a bosonic particle with mass $\mu_B=(1/4\pi)z/\gamma$.

On the other hand, for the $H_1^{(0)}$, whose states are generated by an *odd* number of fermionic excitations, we have a linear energy-momentum relation as shown in figure 5. The lowest gap in this sector is $F=(1/4\pi)z/\gamma+O(z^2)$. This characterises a Dirac particle with mass $\mu_F=(1/4\pi)z/\gamma$. Since we have from (5.3) that $\mu_B<2\mu_F$, the Hamiltonian H (1.1) has a bosonic bound state.

6. Gaps of the primary fields

In this section, we collect the inverse spin-spin and energy-energy correlation lengths, which are just the gaps of the primary fields mentioned in § 3 for the purpose of easy reference (see Reinicke 1986).

Begin with $z=0$. The gaps of the primary fields are given by $F_Q^{(\tilde{Q})}(P,0)$ (see § 2) where the momentum P is $P=0$ for $H_0^{(0)}$, $P=\pm 1$ for $H_0^{(1)}$ and $P=\pm\frac{1}{2}$ for $H_1^{(1)}$. Introduce the parametrisation

$$F_Q^{(\tilde{Q})}(P,0)=F^{(0)}+\frac{\pi^2}{N^2}\left(\frac{1}{\gamma^2}-\frac{4}{3}\right)F^{(2)}+O(N^{-4}). \tag{6.1}$$

The numbers $F^{(0)}$ and $F^{(2)}$ are given in table 2. Note that for $\tilde{Q}=1$, there are two states which give the same gap (see § 3). For comparison, we also give in table 2 the scaling dimensions Δ and $\bar{\Delta}$.

Now, let z be arbitrary. We take the parameterisation

$$F_Q^{(\tilde{Q})}(P,0;z)=F^{(0)}+\frac{1}{4\pi}\frac{z}{\gamma}F^{(1)}+\frac{1}{(4\pi)^2}\frac{z^2}{\gamma^2}F^{(2)}+\dots. \tag{6.2}$$

The numbers $F^{(0)}$, $F^{(1)}$ and $F^{(2)}$ are given in table 3.

We now give a qualitative description. In the limit $N\to\infty$, the corrections in z are given by the perturbations of the energy operator

$$\varepsilon=\frac{1}{2\gamma}(h-1)\sum_{n=1}^{N}\sigma^z(n). \tag{6.3}$$

From table 3, we immediately see that the one-fermion gap $F_1^{(0)}$ gets a first-order correction whereas the leading correction for the bosonic gap $F_0^{(0)}$ is a second-order contribution of the same term.

Table 2. Numerical value for the inverse spin-spin and energy-energy correlation lengths at $z=0$.

Q	$\tilde{Q}$	$F^{(0)}$	$F^{(2)}$	Δ	$\bar{\Delta}$
0	0	1	$\frac{1}{8}$	$\frac{1}{2}$	$\frac{1}{2}$
1	1	$\frac{1}{2}$	$\frac{1}{16}$	$\frac{1}{16}$	$\frac{1}{16}$
1	0	$\frac{1}{8}$	$-\frac{1}{128}$	$\begin{cases}0\\ \frac{1}{2}\end{cases}$	$\frac{1}{2}$ 0

Table 3. Numerical values for the inverse spin-spin and energy-energy correlation lengths to leading order in $1/N$. The scaling dimensions Δ and $\bar{\Delta}$ are the same as in table 2.

Q	$\tilde{Q}$	$F^{(0)}$	$F^{(1)}$	$F^{(2)}$
0	0	1	0	8
1	1	$\frac{1}{2}$	0	4
1	0	$\frac{1}{8}$	1	$4 \ln 2$

The numbers given in tables 2 and 3 and the role of the energy operator are reproduced by the perturbation method of Reinicke (1986).

7. Degeneracies in the spectrum for $z \neq 0$

Having computed the scaling functions in the limit $N \to \infty$ and their leading corrections, we return to the spectra of the $H_Q^{(\tilde{Q})}$. At $z=0$, as we saw in § 3, the levels are highly degenerate. Most of the states, which were degenerate at $z=0$, are non-degenerate for $z \neq 0$. However, there are groups of states which remain degenerate, even if $z \neq 0$ and on finite chains. This is much more profound than the trivial degeneracy of states with opposite momenta P and $-P$.

In order to illustrate what can happen, we compute the spectra of the $H_Q^{(\tilde{Q})}$ for $N=100$ and $z=4$. In figure 4, we show the spectrum of $H_0^{(0)}$. We observe, for example, a group of four states with $F \simeq 2.5$ (they have $F=2$ at $z=0$) which remain degenerate. Further sets of four degenerate states each can be found at $F \simeq 3.5$, 4.3, 4.4, 5.3, 5.4 and 5.9. Up to $F=6$, we have thus seen seven sets of degenerate levels.

Since the *exact* gaps are obtained by combining (2.2) and (2.3), it is easy to see that this degeneracy holds true for all z and for all values of N (provided the chain is long enough to guarantee the existence of the higher levels).

We also note that states which have the same F and P at $z=0$ always split for $z \neq 0$.

The same phenomenon is observed for the spectrum of $H_1^{(0)}$, where we find two sets of four states at $F \simeq 4$ and 5 (see figure 5). The spectrum of $H_0^{(1)}$ is related to the

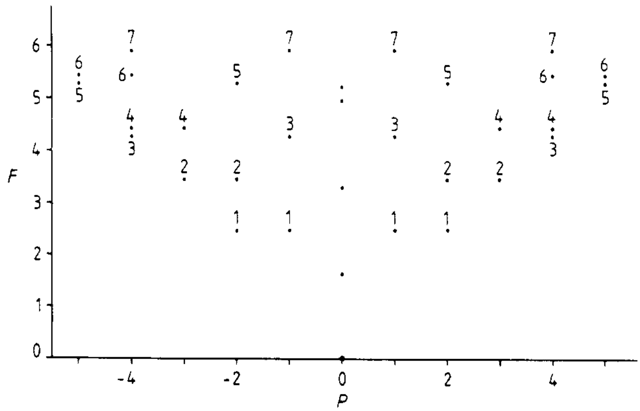

Figure 4. Spectrum of $H_0^{(0)}$ at $z=4$ and $N=100$. The numbers label the sets of degenerate states.

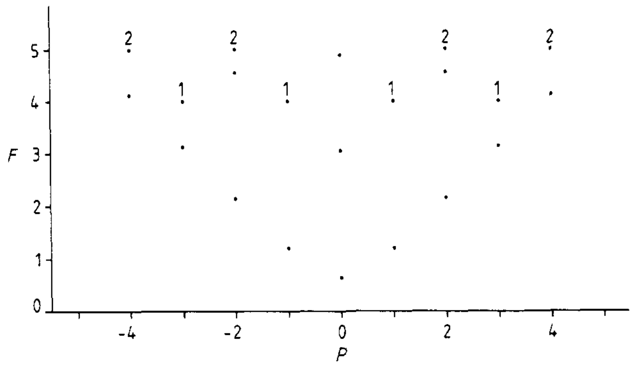

Figure 5. Spectrum of $H_1^{(0)}$ at $z=4$ and $N=100$. The zero of energy is the ground state of $H_0^{(0)}$. The numbers label the sets of degenerate states.

spectrum of $H_1^{(0)}$ via

$$F_0^{(1)}(z)=F_1^{(0)}(z)+z/2\pi\gamma \tag{7.1}$$

and does not contain independent information.

Finally, we have the same effect for $H_1^{(1)}$ (figure 6), where at $F \simeq 5.1$ we have a set of eight degenerate states.

To conclude, we have seen a regular pattern of degenerate states with remains degenerate if either $z \neq 0$ or N finite. This means that there exists an unsuspected symmetry in the model which becomes apparent if either

(i) the thermodynamic limit is approached via a sequence of non-critical ($z \neq 0$) models, or

(ii) the system is kept at finite size.

At the time of writing, the nature of this additional symmetry remains unknown. This is an open problem under investigation.

Finally, we mention that a similar effect has shown up for the Z_3 quantum chain (von Gehlen and Rittenberg 1986).

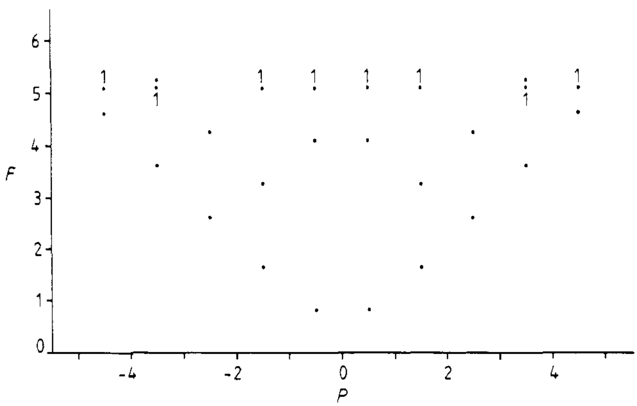

Figure 6. Spectrum of $H_1^{(1)}$ at $z=4$ and $N=100$. The zero of energy is the ground state of $H_0^{(0)}$. The numbers label the sets of degenerate states.

8. Summary

We now collect our results.

We have studied, in the finite-size scaling limit, the spectrum of the Hamiltonian (1.1) for periodic and antiperiodic boundary conditions. By the introduction of a parameter γ we could study different models in the same universality class. We computed the scaling functions of all gaps and examined corrections to scaling.

We obtained the following results.

(1) At the critical point, the spectrum of the Hamiltonian is given by the irreducible representation of a pair of commuting Virasoro algebras with the same central charge.

(2) The spectrum of the continuum Majorana Hamiltonian with periodic and antiperiodic boundary conditions is given by the spectra of the $H_Q^{(\tilde{Q})}$.

(3) At the critical point, the leading correction in $1/N$ to the ground-state energy per spin, which is of order $1/N^2$, is universal. Its numerical value is in agreement with a result from conformal theory which gives a relation to the central charge c.

(4) To leading order in $1/N$, the exactly known scaling functions for all gaps and periodic and antiperiodic boundary conditions were found to be universal functions of the variable z/γ. We have thus verified for our model that the Privman–Fisher (1984) hypothesis is valid for the whole spectrum.

(5) Corrections to scaling are in general non-universal. This was seen for $z \neq 0$, where already the leading correction was non-universal in the Privman–Fisher sense. For $z=0$, however, we found that each order is $1/N$ shows the same γ dependence for all gaps.

(6) For $z \neq 0$, we observed in the spectra of the $H_Q^{(\tilde{Q})}$ groups of states which remain degenerate for all z and for all values of $1/N$. This indicates the existence of an unsuspected symmetry.

In a subsequent paper, we shall study this model for free boundary conditions.

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Appendix

We analyse the sums arising in the finite-size scaling analysis of §§ 4 and 5.

We begin with

$$P_N = \sum_{k=0}^{N-1} \left[\sin^2\left(\frac{\pi(k+\frac{1}{2})}{N}\right) - \frac{\gamma^2-1}{\gamma^2}\sin^4\left(\frac{\pi(k+\frac{1}{2})}{N}\right)\right]^{1/2} \tag{A1}$$

$$= \left[\sin^2\left(\frac{\pi}{2N}\right) - \frac{\gamma^2-1}{\gamma^2}\sin^4\left(\frac{\pi}{2N}\right)\right]^{1/2}$$

$$+ \sum_{k=1}^{N-1} \sin\left(\frac{\pi(k+\frac{1}{2})}{N}\right)\left[1 - \frac{\gamma^2-1}{\gamma^2}\sin^2\left(\frac{\pi(k+\frac{1}{2})}{N}\right)\right]^{1/2} \tag{A2}$$

$$= G_1 + G_2. \tag{A3}$$

For G_1, we have immediately

$$G_1 = \frac{\pi}{2N} + \frac{\pi^3}{16N^3}\left(\frac{1}{\gamma^2} - \frac{4}{3}\right) + O(N^{-5}). \tag{A4}$$

G_2 is expanded by the binomial theorem:

$$G_2 = \sum_{l=0}^{\infty} (-1)^l \binom{\frac{1}{2}}{l} \left(1 - \frac{1}{\gamma^2}\right)^l \sum_{k=1}^{N-1}{}' \left(\sin \frac{\pi(k+\frac{1}{2})}{N}\right)^{2l+1}. \tag{A5}$$

From Hansen (1975), equation (15.1.1) we have

$$\sum_{k=1}^{N-1}{}' \left(\sin \frac{\pi(k+\frac{1}{2})}{N}\right)^{2l+1}$$

$$= (-1)^l 4^{-l} \sum_{k=0}^{l} (-1)^k \binom{2l+1}{k} \cos\left((l+\tfrac{1}{2}-k)\frac{\pi}{N}\right) \cot\left((l+\tfrac{1}{2}-k)\frac{\pi}{N}\right). \tag{A6}$$

To obtain an expansion in $1/N$, we can expand the trigonometric functions of the right-hand side of (A6). In the following, we shall use three other identities:

$$\sum_{k=0}^{l} (-1)^k \binom{2l+1}{k} \frac{1}{2l+1-2k} = (-1)^l 2^{4l} \frac{(l!)^2}{(2l+1)!} \tag{A7}$$

(Hansen (1975), equation (6.6.32))

$$\sum_{k=0}^{l} (-1)^k \binom{2l+1}{k} (2l+1-2k) = 0 \qquad \text{if } l \geq 1 \tag{A8}$$

$$\sum_{k=0}^{l} (-1)^k \binom{2l+1}{k} (2l+1-2k)^3 = 0 \qquad \text{if } l \geq 2. \tag{A9}$$

Equations (A5) and (A6) follow directly from Hansen's (1975) equation (6.7.2).

Returning to (A6), the leading term, which is of order N, is obtained by using (A7):

$$\sum_{k=1}^{N-1}{}' \left(\sin \frac{\pi(k+\frac{1}{2})}{N}\right)^{2l+1} = \frac{N}{\pi} 2^{2l+1} \frac{(l!)^2}{(2l+1)!} + O(N^{-1}). \tag{A10}$$

For the contributions of order $1/N$, we see from (A8) that we only have to take into account the term with $l=0$. Similarly, for the contributions of order $1/N^3$, the only non-vanishing terms are those with $l=0, 1$. Finally, collecting terms, we have

$$G_2 = \frac{N}{2} T_1(\gamma) - \frac{5\pi}{12N} - \frac{67\pi^3}{960N^3}\left(\frac{1}{\gamma^2} - \frac{4}{3}\right) + O(N^{-5}) \tag{A11}$$

where

$$T_1(\gamma) = \sum_{l=0}^{\infty} (-1)^l \binom{\frac{1}{2}}{l} \frac{2^{2l+2}(l!)^2}{(2l+1)!\,\pi} \left(1 - \frac{1}{\gamma^2}\right)^l = \frac{2}{\pi}\left(1 + \frac{\cos^{-1}\gamma}{\gamma(1-\gamma^2)^{1/2}}\right). \tag{A12}$$

So we obtain

$$P_N = \frac{N}{2} T_1(\gamma) + \frac{\pi}{12N} - \frac{7\pi^3}{960N^3}\left(\frac{1}{\gamma^2} - \frac{4}{3}\right) + O(N^{-5}). \tag{A13}$$

Next, we study

$$S_N = \sum_{k=0}^{N-1} \left[\sin^2\left(\frac{\pi k}{N}\right) - \frac{\gamma^2 - 1}{\gamma^2} \sin^4\left(\frac{\pi k}{N}\right) \right]^{1/2} \tag{A14}$$

$$= \sum_{l=0}^{\infty} (-1)^l \binom{\frac{1}{2}}{l} \left(1 - \frac{1}{\gamma^2}\right)^l \sum_{k=1}^{N-1} \left(\sin \frac{\pi k}{N}\right)^{2l+1}. \tag{A15}$$

From Hansen (1975), equation (15.1.1), we have

$$\sum_{k=1}^{N-1} \left(\sin \frac{\pi k}{N}\right)^{2l+1} = (-1)^l 4^{-l} \sum_{k=0}^{l} (-1)^k \binom{2l+1}{k} \cot\left((l + \tfrac{1}{2} - k) \frac{\pi}{N}\right). \tag{A16}$$

Now, the analysis is parallel to the one of G_2 (A5). Expanding the cotangent and collecting terms we obtain

$$S_N = \frac{N}{2} T_1(\gamma) - \frac{\pi}{6N} + \frac{\pi^3}{120 N^3} \left(\frac{1}{\gamma^2} - \frac{4}{3}\right) + O(N^{-5}). \tag{A17}$$

Finally, we study

$$S_N(z) = \frac{1}{\gamma} \sum_{k=0}^{N-1} \left[\frac{z^2}{N^2} + 4\gamma^2 \sin^2\left(\frac{\pi k}{N}\right) - 4(\gamma^2 - 1) \sin^4\left(\frac{\pi k}{N}\right) \right]^{1/2}. \tag{A18}$$

We follow the same route as Hamer and Barber (1981). We separate off the term with $k = 0$ and use the decomposition

$$(u^2 + v^2)^{1/2} = v\left[\left(1 + \frac{u^2}{v^2}\right)^{1/2} - 1 - \frac{u^2}{2v^2}\right] + v + \frac{u^2}{2v} \tag{A19}$$

where

$$u = \frac{z}{N} \qquad v = 4\gamma^2 \sin^2\left(\frac{\pi k}{N}\right)\left(1 - \frac{\gamma^2 - 1}{\gamma^2} \sin^2 \frac{\pi k}{N}\right). \tag{A20}$$

Thus

$$S_N(z) = z/N\gamma + g_1 + g_2 + g_3$$

where g_2 is given (A14), up to a constant factor, and for g_3 we have

$$g_3 = \frac{z^2}{4\gamma^2 N^2} \sum_{k=1}^{N-1} \left[\sin\left(\frac{\pi k}{N}\right)\left(1 - \frac{\gamma^2 - 1}{\gamma^2} \sin^2 \frac{\pi k}{N}\right)^{1/2} \right]^{-1} \tag{A21}$$

$$= \frac{z^2}{4\gamma^2 N^2} \sum_{l=0}^{\infty} (-1)^l \binom{-\frac{1}{2}}{l} \left(1 - \frac{1}{\gamma^2}\right)^l \sum_{k=1}^{N-1} \left(\sin \frac{\pi k}{N}\right)^{2l-1} \tag{A22}$$

and this can be analysed as above.

For $l = 0$, we have from Hamer and Barber (1981):

$$g_3^{(l=0)} = \frac{z^2}{2\pi\gamma^2 N} \left[\ln\left(\frac{2N}{\pi}\right) + C_{\mathrm{E}} \right] + O(N^{-2}) \tag{A23}$$

where $C_{\mathrm{E}} = 0.577\ldots$ is Euler's constant. The case $l = 1$ corresponds to $l = 0$ in (A5) and we have

$$g_3 = g_3^{(l=0)} + \frac{z^2}{4\gamma^2 N} T_2(\gamma) + O(N^{-2}) \tag{A24}$$

where

$$T_2(\gamma) = -\sum_{l=1}^{\infty} (-1)^l \binom{-\frac{1}{2}}{l} \frac{2^{2l-1}[(l-1)!]^2}{(2l-1)!\,\pi} \left(1-\frac{1}{\gamma^2}\right)^l = -\frac{2}{\pi} \ln \gamma. \qquad \text{(A25)}$$

Finally, we look at g_1:

$$g_1 = 4 \sum_{k=1}^{[\frac{1}{2}N]} \left(\sin\frac{\pi k}{N}\right)\left[1-\frac{\gamma^2-1}{\gamma^2}\sin^2\left(\frac{\pi k}{N}\right)\right]^{1/2}$$
$$\times\left(\left[1+\frac{z^2}{4\gamma^2N^2}\left\{\sin^2\left(\frac{\pi k}{N}\right)\left[1-\frac{\gamma^2-1}{\gamma^2}\sin^2\left(\frac{\pi k}{N}\right)\right]\right\}^{-1}\right]^{1/2}-1\right.$$
$$\left.-\frac{z^2}{8\gamma^2N^2}\left\{\sin^2\left(\frac{\pi k}{N}\right)\left[1-\frac{\gamma^2-1}{\gamma^2}\sin^2\left(\frac{\pi k}{N}\right)\right]\right\}^{-1}\right). \qquad \text{(A26)}$$

Following Hamer and Barber (1981), in this sum we can ignore everything but the lowest order in k and extend the sum to infinity. This introduces an error of the size $O(z^2/N^2)$. Consequently, with (5.4), we can write g_1 as a remnant function:

$$g_1 = -\frac{\pi}{N} R_{1\frac{1}{2},0}\left(\frac{z^2}{4\pi^2\gamma^2}\right) + O\left(\frac{z^2}{N^2}\right). \qquad \text{(A27)}$$

Collecting everything, we have

$$S_N(z) = \frac{1}{N}\left\{\frac{z}{\gamma}-\frac{\pi}{3}+\frac{z^2}{2\pi\gamma^2}\left[\ln\left(\frac{2N}{\pi}\right)+C_E\right]-\pi R_{1\frac{1}{2},0}\left(\frac{z^2}{4\pi^2\gamma^2}\right)\right\}$$
$$+NT_1(\gamma)+\frac{z^2}{4\gamma^2N}T_2(\gamma)+O(N^{-2}). \qquad \text{(A28)}$$

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