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Surface energy of integrable quantum spin chains

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Abstract. The surface energy of the antiferromagnetic spin-$\frac{1}{2}$ XXZ Heisenberg chain is derived in the region $\Delta < -1$ from the known Bethe ansatz solution for free boundaries with surface fields. The result gives the surface energy of related models satisfying the Temperley-Lieb algebra. The models discussed are the quantum Q-state Potts chain and a family of isotropic spin-s chains including the spin-1 biquadratic model.

1. Introduction

Bethe's ansatz [1], originally for the wavefunction of the isotropic spin-$\frac{1}{2}$ Heisenberg chain, together with its subsequent generalisation, has been seen to encapsulate the basic physics of all the exactly solved models (see, e.g., [2-5]). Traditionally, one imposes periodic boundary conditions. Typical is the one-dimensional Bose gas [6], where the particles occupy a circle and the boundary considerations turn into periodicity conditions on the wavefunction. However, when the system is enclosed in a 'box', the wavefunction must vanish at the two ends of the interval. In this case Gaudin [7] constructed the Bethe ansatz (BA) wavefunction by explicitly allowing for the superposition of waves reflecting from the ends. He then calculated the boundary or 'surface' energy of the Bose gas in its ground state. It was also Gaudin who gave the BA solution of the XXZ Heisenberg chain with free boundaries [4, 7].

A more general XXZ spin chain, with Hamiltonian,

$$H_{XXZ} = -\frac{1}{2}\left(\sum_{j=1}^{N-1} (\sigma_j^x\sigma_{j+1}^x + \sigma_j^y\sigma_{j+1}^y + \Delta\sigma_j^z\sigma_{j+1}^z) + p(\sigma_1^z - \sigma_N^z)\right) \tag{1.1}$$

was recently considered by Alcaraz *et al* [8, 9]. This model has also been discussed by Sklyanin in the framework of the quantum inverse method [10].

Here we define the surface energy, f, by

$$f = \lim_{N\to\infty} (E_0 - Ne_\infty) \tag{1.2}$$

where e_∞ is the ground-state energy per site, E_0/N, in the infinite-size limit. The surface energy of (1.1) was derived for $|\Delta| < 1$ by Hamer *et al* [11] using a systematic method proposed by de Vega and Woynarovich [12] for calculating finite-size corrections in BA systems.

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The values of the parameters Δ and p of particular interest [8, 9] are those satisfying

$$\Delta^2 - p^2 = 1. \tag{1.3}$$

For this case we have the result [11]

$$f(A) = \frac{\pi \sin\gamma}{2\gamma} - \frac{\cos\gamma}{2} - \frac{\sin\gamma}{4} \int_{-\infty}^{\infty} dx \left[1 - \coth\left(\frac{\pi x}{4}\right) \tanh\left(\frac{\gamma x}{2}\right)\right]. \tag{1.4}$$

Here $\Delta = -\cos\gamma$ and $p = \mathrm{i} \sin\gamma$, with $\gamma \in [0, \pi)$. Our result for $p = 0$ is

$$f(B) = \frac{\pi \sin\gamma}{2\gamma} - \frac{\cos\gamma}{2} - \frac{\sin\gamma}{4} \int_{-\infty}^{\infty} dx \left[1 - \tanh\left(\frac{\pi x}{4}\right) \tanh\left(\frac{\gamma x}{2}\right)\right]. \tag{1.5}$$

We have evaluated these integrals for a few values of γ, and give the corresponding values of f in table 1.

Table 1. Exact values of the surface energy integrals (1.4) and (1.5) for the *XXZ* Hamiltonian (1.1).

γ	$f(A)$	$f(B)$
$\pi/2$	1	$1-2/\pi$
$\pi/3$	$\frac{3}{4}$	$\frac{1}{4}(6\sqrt{3}-9)$
$\pi/4$	$(3\pi-4)/2\sqrt{2}\pi$	$1/2\sqrt{2}$
$\pi/6$	$(6\sqrt{3}-7)/4\sqrt{3}$	$(3\pi-2)/2\pi - 17/12\sqrt{3}$
0	$\frac{1}{2}(\pi-1)-\log 2$	$\frac{1}{2}(\pi-1)+\log 2$

The Hamiltonian (1.1) for case (B) (i.e. for $p=0$) is directly related [8, 13] to the quantum Hamiltonian of the critical Ashkin–Teller model [13] with free boundary conditions. In this way the surface energy of the Ashkin–Teller chain follows from $f(B)$. On the other hand, for case (A) (i.e. for p satisfying (1.3)) (1.1) is related [8, 14] to the quantum Hamiltonian of the critical Q-state Potts model [14, 15]. In this case the surface energy of the free Potts chain for $Q \leq 4$ is related to $f(A)$. The surface energy of the critical two-dimensional Potts model and the corresponding six-vertex model have recently been calculated by Owczarek and Baxter [16].

In this paper we extend our calculations for the spin chain into the region $\Delta < -1$. The analogous result for $f(A)$ is derived in section 2. Then in section 3 we use the result for $f(A)$ to write down the surface energy of the Potts chain, now for $Q > 4$. In section 4 we use our results to give the surface energy of a family of integrable isotropic spin-s chains which are related to the Potts and *XXZ* chains via the Temperley–Lieb algebra [17, 18]. A discussion of the results is given in section 5.

2. Surface energy of the *XXZ* chain

In order to derive the surface energy, we begin by following our earlier treatment for $|\Delta| < 1$ [11] (see also [16]). However, because the system is massive, the treatment is more akin to the earlier calculations of de Vega and Woynarovich [12] for periodic boundary conditions. In particular, Fourier integrals for the massless case are to be replaced by Fourier series.

For $\Delta < -1$, we set

$$\Delta = -\cosh\theta \tag{2.1}$$

with $p = \sinh\theta$. The BA equations [9, 10] can then be written

$$2N\phi(\alpha_j, \theta) = 2\pi I_j + \sum_{k=1,k\neq j}^{n} [\phi(\alpha_j - \alpha_k, 2\theta) + \phi(\alpha_j + \alpha_k, 2\theta)] \tag{2.2}$$

for $j = 1, \ldots, n$, where

$$\phi(\alpha, \theta) = 2\tan^{-1}[\coth(\theta/2)\tan(\alpha/2)] \qquad 0 < \alpha < \pi \tag{2.3}$$

and n is the number of down spins in the σ^z basis—a good quantum number. The I_j are integers with

$$I_j = j \qquad \text{for} \qquad j = 1, \ldots, n \tag{2.4}$$

for the lowest eigenvalue for given n [4, 7, 9]. The ground state occurs in the largest sector, where $n = N/2$. For convenience we assume that N is even.

The eigenvalues of H_{XXZ} are independent of the parameter p and given by [9]

$$E_N = \tfrac{1}{2}(N-1)\cosh\theta - 2\sinh\theta \sum_{j=1}^{n} \phi'(\alpha_j, \theta) \tag{2.5}$$

where

$$\phi'(\alpha, \theta) = \frac{\sinh\theta}{\cosh\theta - \cos\alpha}. \tag{2.6}$$

In order to proceed, we set $\alpha_{-k} = -\alpha_k$ with $\alpha_0 = 0$. Then following [12] we define

$$Z_N(\alpha) = \frac{1}{\pi}\phi(\alpha, \theta) + \frac{1}{2\pi N}[\phi(\alpha, 2\theta) + \phi(2\alpha, 2\theta)] - \frac{1}{2\pi N}\sum_{k=-n}^{n} \phi(\alpha - \alpha_k, 2\theta) \tag{2.7}$$

so that

$$Z_N(\alpha_j) = I_j/N. \tag{2.8}$$

The derivative

$$\sigma_N(\alpha) = \frac{dZ_N}{d\alpha} \tag{2.9}$$

is related to the root density. In the asymptotic limit, we have

$$\sigma_\infty(\alpha) = \frac{1}{\pi}\phi'(\alpha, \theta) - \int_{-\pi}^{\pi} \frac{d\beta}{2\pi}\sigma_\infty(\beta)\phi'(\alpha - \beta, 2\theta). \tag{2.10}$$

This equation is readily solved by Fourier series (our definitions and some appropriate formulae are summarised in appendix 1), with the result

$$\sigma_\infty(\alpha) = \frac{1}{\pi}\left(\frac{1}{2} + \sum_{n=1}^{\infty} \frac{\cos n\alpha}{\cosh n\theta}\right). \tag{2.11}$$

To obtain the ground-state energy per site as $N \to \infty$, we first rewrite (2.5) as

$$e_N = \tfrac{1}{2}\cosh\theta + \frac{1}{N}(\sinh\theta\phi'(\alpha, \theta) - \tfrac{1}{2}\cosh\theta) - \frac{\sinh\theta}{N}\sum_{j=-n}^{n} \phi'(\alpha_j, \theta) \tag{2.12}$$

from which we can establish the result

$$e_\infty=\tfrac{1}{2}\cosh\theta-\sinh\theta\int_{-\pi}^{\pi}\mathrm{d}\alpha\,\sigma_\infty(\alpha)\phi'(\alpha,\theta). \tag{2.13}$$

This expression can alternatively be written

$$e_\infty=\tfrac{1}{2}\cosh\theta-\sinh\theta\left(1+4\sum_{n=1}^{\infty}\frac{1}{1+\mathrm{e}^{2n\theta}}\right) \tag{2.14}$$

as originally obtained for periodic boundary conditions by Orbach and Walker [19, 20] (see also Yang and Yang [21] and des Cloizeaux and Gaudin [22]).

In order to get at the finite-size corrections, we turn to the difference between the finite and the infinite systems [12]. From (2.9) and (2.10) we have

$$\begin{aligned}\sigma_N(\alpha)-\sigma_\infty(\alpha)=&\frac{1}{2\pi N}[\phi'(\alpha,2\theta)+\phi'(2\alpha,2\theta)]-\int_{-\pi}^{\pi}\frac{\mathrm{d}\beta}{2\pi}\phi'(\alpha-\beta,2\theta)S_N(\beta)\\&-\int_{-\pi}^{\pi}\frac{\mathrm{d}\beta}{2\pi}\phi'(\alpha-\beta,2\theta)[\sigma_N(\beta)-\sigma_\infty(\beta)]\end{aligned} \tag{2.15}$$

for the root density. And from (2.12) and (2.13)

$$\begin{aligned}e_N-e_\infty=&\frac{1}{N}[\sinh\theta\,\phi'(\alpha,\theta)-\tfrac{1}{2}\cosh\theta]-\sinh\theta\int_{-\pi}^{\pi}\mathrm{d}\alpha\,\phi'(\alpha,\theta)S_N(\alpha)\\&-\sinh\theta\int_{-\pi}^{\pi}\mathrm{d}\alpha\,\phi'(\alpha,\theta)[\sigma_N(\alpha)-\sigma_\infty(\alpha)]\end{aligned} \tag{2.16}$$

for the energy per site. In both equations

$$S_N(\alpha)=\frac{1}{N}\sum_{j=-n}^{n}\delta(\alpha-\alpha_j)-\sigma_N(\alpha). \tag{2.17}$$

Equation (2.15) can be solved by Fourier series, with the result

$$\sigma_N(\alpha)-\sigma_\infty(\alpha)=\frac{1}{2\pi N}[p(\alpha)+p_2(\alpha)]-\int_{-\pi}^{\pi}\frac{\mathrm{d}\beta}{2\pi}p(\alpha-\beta)S_N(\beta) \tag{2.18}$$

where

$$p(\alpha)=\frac{1}{2}+\sum_{n=1}^{\infty}\frac{2\cos n\alpha}{1+\mathrm{e}^{2n\theta}}, \tag{2.19}$$

$$p_2(\alpha)=1+\sum_{n=1}^{\infty}\frac{2\cos 2n\alpha}{\cosh 2n\theta}. \tag{2.20}$$

Inserting (2.18) into (2.16) gives

$$e_N-e_\infty=\frac{g}{N}-\pi\sinh\theta\,I_N \tag{2.21}$$

where

$$I_N=\int_{-\pi}^{\pi}\mathrm{d}\alpha\sigma_\infty(\alpha)S_N(\alpha) \tag{2.22}$$

and g is the collection of terms with an explicit $1/N$ dependence:

$$g = -\tfrac{1}{2}\cosh\theta + \pi\sinh\theta\,\sigma_\infty(0) - \sinh\theta\left(1 + 4\sum_{n=1}^{\infty}\frac{1}{1+e^{4n\theta}}\right). \tag{2.23}$$

For periodic boundary conditions, de Vega and Woynarovich [12] have shown that the integral I_N decreases exponentially with N. So, at first glance one might conclude that the surface energy is simply given by the factor g (this is indeed the case for $|\Delta|<1$ [11]). However, for the present boundary conditions we establish in appendix 2 that, to leading order,

$$I_N \sim -\frac{1}{2\pi N}\prod_{n=1}^{\infty}\left(\frac{1-q^n}{1+q^n}\right)^2 \qquad \text{as } N\to\infty \tag{2.24}$$

where $q = e^{-\theta}$. Thus from the definition (1.2) and (2.21) the surface energy is given by

$$f = g - \tfrac{1}{4}\Lambda_{XXZ} \tag{2.25}$$

where Λ_{XXZ} is the known gap in the eigenspectrum of the periodic XXZ chain [22, 23]:

$$\Lambda_{XXZ} = 2\sinh\theta\prod_{n=1}^{\infty}\left(\frac{1-q^n}{1+q^n}\right)^2 \tag{2.26}$$

$$= 2\sinh\theta\left(1 + 4\sum_{n=1}^{\infty}\frac{(-1)^n q^n}{1+q^n}\right). \tag{2.27}$$

The fact that Λ_{XXZ} appears in the result for the surface energy is somewhat surprising. Explicitly, we have the ground-state energy behaving as

$$E_N \sim Ne_\infty + g - \tfrac{1}{4}\Lambda_{XXZ} \qquad \text{as } N\to\infty. \tag{2.28}$$

In appendix 2 we have also examined the asymptotic behaviour of the integral I_N for the lowest eigenvalue in each of the remaining sectors of the Hamiltonian. Labelling the sectors by

$$n = \frac{N}{2} - r \qquad r = 0, 1, \ldots \tag{2.29}$$

we find

$$I_N^{(r)} \sim (1+4r) I_N \qquad \text{as } N\to\infty \tag{2.30}$$

so that

$$E_N^{(r)} - E_N^{(0)} \sim r\Lambda_{XXZ} \tag{2.31}$$

i.e., we do indeed see the gap of the periodic XXZ chain in the eigenspectrum.

3. The quantum Potts chain

The Q-state Potts model has a long history [5, 24]. The Hamiltonian of the (1+1)-dimensional quantum version [14, 15] on a chain of L sites with free ends can be written as

$$H_Q = -\frac{1}{\sqrt{Q}}\left(\sum_{l=1}^{L}\sum_{k=0}^{Q-1} X_l^k + \sum_{l=1}^{L-1}\sum_{k=0}^{Q-1} Z_l^k Z_{l+1}^{Q-k}\right). \tag{3.1}$$

The operators X_l and Z_l at site l obey a $Z(Q)$ algebra

$$X_lZ_l=\omega^{-1}Z_lX_l \qquad X_lZ_l^\dagger=\omega Z_l^\dagger X_l \qquad X_l^Q=Z_l^Q=1 \tag{3.2}$$

with $\omega=\mathrm{e}^{2\pi\mathrm{i}/Q}$. In the low-temperature representation, we have, e.g., $X=\sigma^x$ and $Z=\sigma^z$, the usual Pauli matrices, when $Q=2$.

As normalised here, the Hamiltonian (3.1) is a direct sum

$$H_Q=-\sum_{l=1}^{L}U_{2l-1}-\sum_{l=1}^{L-1}U_{2l} \tag{3.3}$$

of Temperley-Lieb operators [25]

$$U_{2l-1}=\frac{1}{\sqrt{Q}}\sum_{k=0}^{Q-1}X_l^k \tag{3.4}$$

$$U_{2l}=\frac{1}{\sqrt{Q}}\sum_{k=0}^{Q-1}Z_l^kZ_{l+1}^{Q-k} \tag{3.5}$$

which obey the ubiquitous Temperley-Lieb algebra [5, 26]:

$$\begin{aligned} &U_l^2=\sqrt{Q}\,U_l && U_lU_{l\pm1}U_l=U_l \\ &U_kU_l=U_lU_k && \text{for } |k-l|>1. \end{aligned} \tag{3.6}$$

In order to make contact with the XXZ chain [8], we use the Temperley-Lieb representation in terms of Pauli spin operators [26]:

$$U_l=\tfrac{1}{2}(\sigma_l^x\sigma_{l+1}^x+\sigma_l^y\sigma_{l+1}^y)+\tfrac{1}{2}\cosh\theta(1-\sigma_l^z\sigma_{l+1}^z)+\tfrac{1}{2}\sinh\theta(\sigma_{l+1}^z-\sigma_l^z) \tag{3.7}$$

where

$$\sqrt{Q}=2\cosh\theta. \tag{3.8}$$

Substitution of (3.7) in (3.3) yields the operator equivalence

$$H_Q\Leftrightarrow H_{XXZ}(2L)-\tfrac{1}{2}(2L-1)\cosh\theta \tag{3.9}$$

where $H_{XXZ}(2L)$ is the Hamiltonian (1.1) defined on a chain of $2L$ sites. From (3.9), the ground-state energy per site of H_Q is related to that of H_{XXZ} by

$$e_L(Q)=2e_{2L}^{(0)}-\left(1-\frac{1}{2L}\right)\cosh\theta. \tag{3.10}$$

Thus for the infinite chain, we have the result

$$e_\infty(Q)=2e_\infty-\cosh\theta \tag{3.11}$$

with e_∞ given in (2.14). The surface energy of the Potts model is simply

$$f_Q=f+\tfrac{1}{2}\cosh\theta \tag{3.12}$$

with f as given in (2.25). Some results for $e_\infty(Q)$ and f_Q as functions of Q are shown in table 2. Also indicated for comparison are the exact values† for $Q\leqslant 4$.

† The exact expressions for $e_\infty(Q)$ are from the tabulated results of [8]; the corresponding values of f_Q follow from the equivalence, $f_Q=f(A)+\frac{1}{2}\cos\gamma$, with $f(A)$ as in table 1 and $\sqrt{Q}=2\cos\gamma$.

Table 2. Numerical values of the ground state and surface energy of the Q-state Potts model (3.1).

Q	$-e_\infty(Q)$	f_Q
0	$4/\pi = 1.2732\ldots$	1
1	2	1
2	$\sqrt{2}(1+2/\pi) = 2.3145\ldots$	$\sqrt{2}(1-1/\pi) = 0.9640\ldots$
3	$(10\sqrt{3})/9+2/\pi = 2.5611\ldots$	$\frac{3}{2}-1/\sqrt{3} = 0.9266\ldots$
4	$4\log 2 = 2.7725\ldots$	$\frac{1}{2}\pi - \log 2 = 0.8776\ldots$
9	$3.5937\ldots$	$0.6550\ldots$
16	$4.4688\ldots$	$0.4976\ldots$
25	$5.3840\ldots$	$0.3992\ldots$
64	$8.2460\ldots$	$0.2499\ldots$
∞	∞	0

4. The isotropic spin-s chains

There has been a recent interest in constructing higher-spin representations of the Temperley-Lieb algebra [17, 18, 27-29]. The easiest representations to write down are those with isotropic interactions [17, 18]. Specifically,

$$U_n = (-1)^{2s}\left(\frac{2^s}{(2s)!}\right)^2 \prod_{k=1}^{2s} [\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1} + s(s+1) - \tfrac{1}{2}k(k+1)] \tag{4.1}$$

where $\boldsymbol{S}_n$ is a spin-s operator acting at site n. The corresponding spin Hamiltonians, defined on a chain of N sites with free ends, are sums of the Temperley-Lieb operators,

$$H_s = -\sum_{n=1}^{N-1} U_n \tag{4.2}$$

and are thus seen to be polynomials in the interactions $\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1}$.

The Temperley-Lieb algebra, (3.6), is satisfied for

$$\sqrt{Q} = 2s+1. \tag{4.3}$$

For spin-$\frac{1}{2}$ the representation (3.7) is recovered with $\theta = 0$, i.e. $Q = 4$. On the other hand for spin-1

$$U_n = (\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1})^2 - 1 \tag{4.4}$$

and $H_{s=1}$ is directly related [28] to the Hamiltonian of the biquadratic spin chain [30, 31]

$$H_{bQ} = -\sum_{n=1}^{N-1} (\boldsymbol{S}_n \cdot \boldsymbol{S}_{n+1})^2. \tag{4.5}$$

In this case the equivalence is with the nine-state Potts model [28, 32].

Substitution of (3.7) in (4.2) yields

$$H_s \Leftrightarrow H_{XXZ} - \tfrac{1}{2}(N-1)\cosh\theta \tag{4.6}$$

where both Hamiltonians are defined on N-site chains and

$$s + \tfrac{1}{2} = \cosh\theta. \tag{4.7}$$

From this equivalence, the ground-state energies of the two models are related by

$$e_N(s)=e_N^{(0)}-\frac{1}{2}\left(1-\frac{1}{N}\right)\cosh\theta. \tag{4.8}$$

Hence we obtain

$$e_\infty(s)=e_\infty-\tfrac{1}{2}\cosh\theta \tag{4.9}$$

$$f_s=f+\tfrac{1}{2}\cosh\theta \tag{4.10}$$

so that we also have the identifications, $e_\infty(s)=\frac{1}{2}e_\infty(Q)$ and $f_s=f_Q$, subject to (4.3).

The surface energy of the biquadratic Hamiltonian (4.5) is

$$f_{bQ}=f+\tfrac{7}{4} \tag{4.11}$$

with $\cosh\theta=\frac{3}{2}$ in (2.25). A numerical evaluation of the sums gives $f_{bQ}=1.655\,009\ldots$, in precise agreement with the estimate obtained from the finite-size BA data of [28].

5. Discussion

We have derived the surface energy for models related via the Temperley-Lieb equivalence from the Bethe ansatz solution of the corresponding *XXZ* chain. The matrix representations of the models considered here are of size $2^{2L}\times 2^{2L}$ for H_{XXZ}, $Q^L\times Q^L$ for H_Q and $(2s+1)^{2L}\times(2s+1)^{2L}$ for H_s. For all of the cases examined to date, there has been a one-to-one correspondence between the ground-state energies of the models. We also expect this faithfulness of the various representations to extend to the gaps in the excitation spectra. In this regard, a direct calculation of the gap of H_{bQ} via the corresponding three-state vertex model [31] directly confirms the result obtained from the *XXZ* chain via the Temperley-Lieb algebra [28]. We would thus expect the *XXZ* result (2.31) to apply to the Potts and spin-s chains. Our results should also be directly applicable to the anisotropic spin-1 Hamiltonian which satisfies the Temperley-Lieb algebra for all values of Q [29].

Note added in proof. The spin-s Hamiltonians defined in (4.1) and (4.2) have also been discussed by Klümper [34] who has identified the corresponding $(2s+1)$-state vertex models. The direct calculations confirm that the chains are massive with a gap in the eigenspectrum related to Λ_{XXZ}, in agreement with the findings of [17, 18].

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Appendix 1. Fourier series

We use the Fourier series pair defined by

$$f(\alpha)=\sum_{n=-\infty}^{\infty} f_n\,\mathrm{e}^{\mathrm{i}n\alpha} \tag{A1.1}$$

$$f_n=\frac{1}{2\pi}\int_{-\pi}^{\pi}\mathrm{d}\alpha\, f(\alpha)\,\mathrm{e}^{-\mathrm{i}n\alpha}. \tag{A1.2}$$

A useful result is the convolution formula

$$\int_{-\pi}^{\pi}\mathrm{d}\beta\, f(\alpha-\beta)g(\beta)=2\pi\sum_{n=-\infty}^{\infty} f_n g_n\,\mathrm{e}^{\mathrm{i}n\alpha}. \tag{A1.3}$$

We also make use of the identity

$$\int_{-\pi}^{\pi} \frac{d\alpha}{2\pi} p(\beta-\alpha)\phi'(\alpha, \theta) = \phi'(\beta, \theta) - \pi\sigma_\infty(\beta). \tag{A1.4}$$

Appendix 2. Analysis of the integral I_N

Here we examine the asymptotic behaviour of the integral (2.22) as $N \to \infty$. We begin by writing the root density (2.11) as

$$\sigma_\infty(\alpha) = \frac{K}{\pi^2} \mathrm{d}n(K\alpha/\pi, k) \tag{A2.1}$$

where K and $\mathrm{dn}(z, k)$ are elliptic functions of modulus k [33] with $K'/K = \theta/\pi$ and so with elliptic nome $q = \mathrm{e}^{-\theta}$. From the definition (2.9) we then have

$$\begin{aligned} Z_\infty(\alpha) &= \int_0^\alpha d\beta\, \sigma_\infty(\beta) \\ &= \frac{1}{\pi} \sin^{-1}[\mathrm{sn}(K\alpha/\pi, k)] \end{aligned} \tag{A2.2}$$

and therefore

$$\sigma_\infty(\alpha) = \frac{K}{\pi^2} [1 - k^2 \sin^2(\pi Z)]^{1/2}. \tag{A2.3}$$

To get the correct leading-order behaviour, it suffices to approximate $\sigma_N(\alpha)$ by $\sigma_\infty(\alpha)$ in I_N. Changing variables from α to Z and using (A2.3) then gives

$$I_N \simeq \frac{K}{\pi^2} \int_{-1/2-1/N}^{1/2+1/N} dZ[1 - k^2 \sin^2(\pi Z)]^{1/2} \left[\frac{1}{N} \sum_{i=-n}^{n} \delta\left(Z - \frac{i}{N}\right) - 1\right]. \tag{A2.4}$$

In obtaining the limits of integration we used the sum rule

$$\int_{-\pi}^{\pi} d\alpha\, \sigma_N(\alpha) = 1 + \frac{2}{N} \tag{A2.5}$$

which follows from the definition (2.9). The result (A2.4) can be broken into three pieces:

$$I_N = \frac{K}{\pi^2} (P_\mathrm{I} + P_\mathrm{II} + P_\mathrm{III}) \tag{A2.6}$$

where

$$P_\mathrm{I} = -\left(\int_{1/2}^{1/2+1/N} dZ + \int_{-1/2-1/N}^{-1/2} dZ\right)[1 - k^2 \sin^2(\pi Z)]^{1/2} \tag{A2.7}$$

$$P_\mathrm{II} = \frac{1}{N}\left[1 - k^2 \sin^2\left(\frac{\pi}{2}\right)\right]^{1/2} \tag{A2.8}$$

$$P_\mathrm{III} = \int_{-1/2}^{1/2} dZ[1 - k^2 \sin^2(\pi Z)^{1/2} \left[\frac{1}{N} \sum_{i=-n}^{n}{}' \delta\left(Z - \frac{i}{N}\right) - 1\right] \tag{A2.9}$$

with

$$\sum_{i=-n}^{n}{}' f_i \equiv \tfrac{1}{2}f_{-n} + f_{-n+1} + \ldots + f_{n-1} + \tfrac{1}{2}f_n. \tag{A2.10}$$

The Euler–Maclaurin formula (see e.g. [7]) then tells us that $P_{\rm III}$ is $o(1/N)$; in fact a saddle-point treatment following [12] shows that it decreases exponentially with N. For the remaining terms, we have

$$P_{\rm II} = \frac{k'}{N} \tag{A2.11}$$

where $k' = \sqrt{1-k^2}$ is the modulus conjugate to k; and finally

$$P_{\rm I} = -2\int_0^{1/N} {\rm d}Z[1-k^2\cos^2(\pi Z)]^{1/2} \tag{A2.12}$$

$$= -\frac{2k'}{N} + O\left(\frac{1}{N^2}\right). \tag{A2.13}$$

Collecting these results, we have

$$I_N = -\frac{Kk'}{\pi^2 N} + \text{higher-order terms}. \tag{A2.14}$$

Use of the relation [33]

$$\frac{2Kk'}{\pi} = \prod_{n=0}^{\infty}\left(\frac{1-q^n}{1+q^n}\right)^2 \tag{A2.15}$$

then leads to (2.24).

For the lowest state in each of the remaining sectors, the sum rule (A2.5) is replaced by

$$\int_{-\pi}^{\pi} {\rm d}\alpha\, \sigma_N(\alpha) = 1 + \frac{2(1+r)}{N} \tag{A2.16}$$

with r as defined in (2.29). Then

$$I_N^{(r)} = \frac{K}{\pi^2}(P_{\rm I}^{(r)} + P_{\rm II}^{(r)} + P_{\rm III}^{(r)}) \tag{A2.17}$$

where

$$P_{\rm I}^{(r)} = -\left(\int_{1/2-r/N}^{1/2+(1+r)/N} {\rm d}Z + \int_{-1/2-(1+r)/N}^{-1/2+r/N} {\rm d}Z\right)[1-k^2\sin^2(\pi Z)]^{1/2} \tag{A2.18}$$

$$P_{\rm II}^{(r)} = \frac{1}{N}\left[1-k^2\sin^2\left(\frac{\pi}{2}-\frac{r\pi}{N}\right)\right]^{1/2} \tag{A2.19}$$

$$P_{\rm III}^{(r)} = \int_{-1/2+r/N}^{1/2-r/N} {\rm d}Z[1-k^2\sin^2(\pi Z)]^{1/2}\left[\frac{1}{N}\sum_{i=-n}^{n}{}' \delta\left(Z-\frac{i}{N}\right)-1\right]. \tag{A2.20}$$

As $N\to\infty$, we find

$$P_{\rm I}^{(r)} \sim -\frac{2(1+2r)k'}{N} \tag{A2.21}$$

$$P_{\rm II}^{(r)} \sim \frac{k'}{N} \tag{A2.22}$$

with $P_{\rm III}^{(r)}$ decreasing exponentially with N. Inserting these results in (A2.17) gives (2.30).

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