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Zeros of the Finite-Size Scaling Region Partition Function for a Model with a Wetting Transition

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We derive a finite-size scaling representation for the partition function for an Onsager–Temperley string model with a wetting transition, and analyze the zeros of this partition function in the complex scaled coupling parameter of relevance. The system models the one-dimensional interface between two phases in a rectangular two-dimensional region $\{(x, y) \in \mathbb{R}^2,\ -L \leqslant y \leqslant L, 0 \leqslant x \leqslant N\}$. The two phases are at coexistence. The string or interface has a surface tension $2KkT$ per unit length and an extra Boltzmann weight a per unit length if it touches the surfaces at $y = \pm L$. There is a critical value $a_c = 1/2K$ and for $a > a_c$ the string is confined to one of the surfaces, while for $a < a_c$ the string moves roughly in the rectangular region. The finite-size scaling parameters are $\alpha = a_c^2 N/L^2$ and $\zeta = L(a - a_c)/a_c^2$. We find that for $|\zeta|$ large, the zeros of the scaled partition function lie close to the lines $\arg(\zeta) = \pm\pi/4$ with $\mathrm{re}(\zeta) > 0$. We discuss the motion of all the zeros as α changes by both analytic and numerical arguments.

KEY WORDS: Wetting transition; finite-size scaling; partition function zeros.

1. INTRODUCTION

In a pair of famous papers, Yang and Lee[1,2] discussed the structure of the grand canonical partition function for a system in which the particles have a hard core, so that there is a maximum number density. For a finite system the grand canonical partition function is then a polynomial in the fugacity z. They showed how a phase transition can result in the thermodynamic limit if the zeros of this polynomial lie on lines in the complex z plane forming a finite density per unit length on the lines. The phase transition occurs when these arcs of zeros cut the positive real z axis in the

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thermodynamic limit. They also proved their famous circle theorem for ferromagnetic Ising lattice gases, illustrating their mechanism for phase transitions. Later, Penrose[3] extended these ideas to systems with particles whose short-ranged interaction was not necessarily hard core, but merely repulsive enough to allow the thermodynamic free energy density to exist. In magnetic lattice systems these ideas transfer with the variable $\exp(2H/kT)$ (H being the magnetic field) replacing z. The idea of studying the zeros has led to extending the Lee–Yang circle theorem to other systems, some of them quantum mechanical,[4,5] and to extensive numerical studies of the zeros of the partition function for a variety of Ising models. This work continues with, for example, a discussion of the motion of the first Lee–Yang zero for a d-dimensional ferromagnetic Ising model.[6]

Fisher[7] and Ono *et al.*[8] considered the zeros of the partition function as a function of complex $\beta = 1/kT$ and illustrated these ideas with the two-dimensional Ising model. Jones[9] developed a general theory for these complex temperature zeros. A more recent paper by Itzykson *et al.*[10] considered a general system of volume V and an external field h with an infinite-volume-limit phase transition with critical temperature T_c and critical field h_c. Developing ideas originally due to Fisher and Barber,[11] Itzykson *et al.* introduced finite-size scaling variables $t = (T - T_c)\, V^p$ and $v = (h - h_c)\, V^q$ and wrote the partition function $Z(V, T, h)$ in the form

$$F(t, v) = \lim_{V \to \infty} \frac{Z(V, T_c + tV^{-p}, h_c + vV^{-q})}{Z(V, T_c, h_c)} \tag{1.1}$$

They then considered the zeros of $F(t, v)$ as functions of complex t and v. Glasser *et al.*[12] identified $F(t, 0)$ for a system undergoing a classical mean field transition as proportional to a particular $K_{1/4}$ Bessel function and showed that the zeros of $F(t, 0)$ are on lines $\mathrm{re}(t) > 0$, $\arg(t) = \pm 3\pi/4$, verifying the theory developed by Itzykson *et al.* for the dependence of critical exponents on the angle at which lines of zeros approach the real axis. Later work by Glasser *et al.*[13] extended the ideas of Itzykson *et al.* and their own mean field work to describe the position of zeros in the scaled complex temperature plane of the finite-size scaling region partition function for general systems undergoing phase transitions. For zeros of large magnitude (i.e., far from the origin in the complex t plane), they develop asymptotic expansions for the zeros in terms of the parameters α and $A_\pm$ in the singular part of the free energy density

$$f^{(s)} \approx A_\pm\, |t|^{2-\alpha} \tag{1.2}$$

and the angle φ at which the lines of zeros cut the real temperature axis. Here the parameter $t = (T - T_c)/T_c$, so that large, positive t corresponds to weak coupling and large, negative t corresponds to strong coupling. They found, for large n,

$$t_n \approx \{2\pi n[A_+^2 + A_-^2 - 2A_+A_- \cos(\pi\alpha)]^{-1/2}/V\}^{1/(2-\alpha)} \exp[i(\pi - \phi)] \quad (1.3)$$

In this paper we implement these ideas on a model which shows a wetting transition, the Onsager–Temperley string.[14] We consider the string on a rectangular lattice to begin with, but later reduce it to a string with continuous heights, because the resulting technical problems are rather simpler. The initial system is considered as composed of $N+1$ columns, $0 \leqslant x \leqslant N$. In each of these there is to begin a discrete real height variable $y(x) = ln(x)$, where $n(x)$ is an integer on $-L' \leqslant n(x) \leqslant L'$ and also $-L \leqslant y(x) \leqslant L$. Thus, $L = lL'$. These height variables define a contour from $y(0) = L-1$ to $y(N) = L-1$ composed of "horizontal" pieces of length 1 from $(x-1/2, y(x))$ to $(x+1/2, y(x))$ for $1 \leqslant x \leqslant N-1$ [and of length 1/2 from $(0, L-1)$ to $(1/2, L-1)$ and $(N-1/2, L-1)$ to $(N, L-1)$] and "vertical" pieces from $(x-1/2, y(x-1))$ to $(x-1/2, y(x))$, $1 \leqslant x \leqslant N$. The length of this contour is

$$L = N + \sum_{x=0}^{N+1} |y(x+1) - y(x)| \quad (1.4)$$

As the contour changes shape, the horizontal part of this length, N, does not change, and so we ignore it below.

We consider the contour as the interface between two phases and assume it has a surface tension $2KkT$ per unit length. We also include an extra adsorption potential

$$V(ln) = -\varepsilon(\delta_{n,-L'} + \delta_{n,L'}) \quad (1.5)$$

which has $\varepsilon > 0$, so that the adsorption potential tries to stick the contour to either the upper or lower surface. If the contour lies entirely on one of these surfaces, then the system is filled with one phase or the other. The dominant phase "wets" the channel. This model was been studied extensively by Abraham and Smith[15,16] with the two bulk phases not in coexistence. This work relies heavily on their analysis of the general problem.

The partition function for the system may be written, with $\omega = \varepsilon/kT$, as

$$\begin{aligned} &\mathbb{Z}_N(n(0), n(N), \omega) \\ &\quad = \sum_{n(1)=-L'}^{L'} \cdots \sum_{n(N)=-L'}^{L'} \exp\left\{-2Kl \sum_{x=0}^{N-1} |n(x+1) - n(x)| \right. \\ &\qquad \left. + \frac{\omega}{2} [\delta_{n(x),-L'} + \delta_{n(x-1),-L'} + \delta_{n(x),L'} + \delta_{n(x-1),L'}] \right\} \end{aligned} \quad (1.6)$$

We may write this partition function in terms of the real symmetric transfer matrix

$$\mathscr{T}(n, n') = \exp\left\{ -2Kl\,|n(x+1) - n(x)| + \frac{\omega}{2}\left[\delta_{n(x), -L'} + \delta_{n(x-1), -L'} + \delta_{n(x), L'} + \delta_{n(x-1), L'}\right]\right\} \tag{1.7}$$

This transfer matrix is real and symmetric, so that its eigenvalues are all real and its left and right eigenvectors are equal and may be written using real arithmetic only. The equation

$$\sum_{n'=-L'}^{L'} \mathscr{T}(n, n')\,\tilde{\varphi}_m(n') = \lambda_m \tilde{\varphi}_m(n) \tag{1.8}$$

may be rewritten as

$$\sum_{n'=-L'}^{L'} T(n, n'; \omega)\,\phi_m(n') = \lambda_m \phi_m(n) \tag{1.9}$$

where

$$T(n, n'; \omega) = \exp\{-2Kl\,|n(x+1) - n(x)| + \omega[\delta_{n(x), -L'} + \delta_{n(x), L'}]\} \tag{1.10}$$

and

$$\phi_m(n) = \tilde{\varphi}_m(n) \exp\left[-\frac{\omega}{2}(\delta_{n, -L'} + \delta_{n, L'})\right] \tag{1.11}$$

Since we may write the partition function in terms of the eigenvalues and eigenvectors of $\mathscr{T}$, we may also write them in terms of the eigenvalues and eigenvectors of T. Thus, we find

$$\mathbb{Z}_N(L'-1, L'-1; \omega) = \sum_{m=1}^{\infty} \lambda_m^N \phi_m^2(L'-1) \tag{1.12}$$

It turns out that it is convenient to define the parameter a by

$$a = l[\exp(\omega) - 1] \tag{1.13}$$

At any finite l, we can solve the problem of the partition function via the transfer matrix formalism, for we can find the eigenvalues and right eigenvectors of T. The details are more than a little complicated and it is easier to consider the limit $l \to 0$ with a and L fixed (so that $L' \to \infty$). We then find

$$\mathbb{Z}_N(L'-1, L'-1; \omega) = l^{-(N-1)} \mathbb{Q}_N(L\text{-}, L\text{-}; a) \tag{1.14}$$

where

$$\mathbb{Q}_N(y(0), y(N); a)$$
$$= \int_{-L}^{L} dy(1) \cdots \int_{-L}^{L} dy(N-1) \exp\left[-2K \sum_{x=1}^{N} |y(x) - y(x-1)|\right]$$
$$\times \prod_{x=1}^{N-1} [1 + a\delta(y(x) - L) + a\delta(y(x) + a)] \tag{1.15}$$

In (1.14), L- is a notation which represents the limit of $l(L'-1)$ as $l \to 0$ with L fixed. That is, the contour is pinned at the "top" of the rectangle, but just outside the adsorbing potential, which gives the delta functions in (1.15).

This partition function may be evaluated by the formula

$$\mathbb{Q}_N(L\text{-}, L\text{-}; a) = \sum_{m=1}^{\infty} \lambda_m \phi_m^2(L\text{-}) \tag{1.16}$$

where the λ_m and $\phi_m(y)$ are the eigenvalues and normalized eigenvectors of the transfer operator

$$(T_K(a; L)\,\phi)(y) = \int_{-L}^{L} dy'\, e^{-2K|y-y'|}\phi(y')\,dy'$$
$$+ ae^{-2K(L-y)}\phi(L) + ae^{-2K(L+y)}\phi(-L) \tag{1.17}$$

The function $\mathbb{Q}_N(y(0), y(N); a)$ is thus the partition function for a string with continuous heights $-L \leqslant y \leqslant L$ on discrete columns with an energy $2KkT$ per unit length of contour and with an extra Boltzmann factor if the contour is sticking either to the top or to the bottom of the rectangle. The embarassment, obvious in (1.14) as $l \to 0$, is simply avoided by always considering ratios of partition functions.

In Section 2 the necessary results for the nonsymmetric transfer operator $T_K(a; L)$ are reviewed. We note here that our derivation of this operator ensures that its eigenvalues are all real and that for $\mathbb{Q}_N(L\text{-}, L\text{-}; a)$ we only need the square of the normalized right eigenvectors $\phi_m^2(L\text{-})$. Further details may be found in ref. 16. In Section 3 we display the phase transition which occurs in the thermodynamic limit $N \to \infty$ and then $L \to \infty$, with critical coupling $a_c = 1/2K$. We also derive a finite-size scaling partition function ratio $F(\zeta, \alpha)$ [cf. (1.1)] with $N = \alpha L^2/a_c^2$ and $a = a_c(1 + a_c(1 + a_c\zeta/L)$ in the limit $L \to \infty$. This partition function ratio requires the solutions of a finite-size scaling eigenvalue relation which is discussed in Section 4. The zeros of the scaled partition function ratios are discussed in Section 5.

2. THE PARTITION FUNCTION FOR THE STRING

In (1.16) the eigenvectors and eigenvalues obey

$$(T_K(a; L)\,\phi_m)(y) = \lambda_m \phi_m \tag{2.1}$$

where $T_K(a; L)$ is given by (1.17) and the eigenvalues λ_m are all real, as discussed above. The normalization of the eigenvectors comes from the ordinary normalization of the $\tilde{\varphi}_m(n)$, the transformation (1.11), and the taking of the limit $l \to 0$. The normalization is then

$$\int_{-L}^{L} \phi_m(y)\,\phi_n(y)\,dy + a[\phi_m(L)\,\phi_n(L) + \phi_m(-L)\,\phi_n(-L)] = \delta_{m,n} \tag{2.2}$$

With the representation (1.17) for $T_K(a; L)$, (2.1) my be differentiated twice to give

$$\phi_m''(y) - \frac{1}{4L^2}\left(1 - \frac{1}{K\lambda_m}\right)\phi_m(y) = 0 \tag{2.3}$$

on $-L < y < L$ together with the boundary conditions

$$\phi_m'(L) = -2K\left(1 - \frac{2a}{\lambda_m}\right)\phi_m(L) \tag{2.4}$$

and

$$\phi_m'(-L) = 2K\left(1 - \frac{2a}{\lambda_m}\right)\phi_m(-L) \tag{2.5}$$

We define

$$a_c = 1/2K \tag{2.6}$$

and then

$$\mu_n^2 = -(1 - 2a_c/\lambda_m) \Rightarrow \lambda_m = 2a_c/(1 + \mu_m^2) \tag{2.7}$$

There are then two classes of eigenfunction, one class odd in y and the other even in y.

The even eigenfunctions are

$$\phi_{em}(y) = A_m \cos(\mu_m y/a_c) \tag{2.8a}$$

where the μ_m are solutions of

$$\frac{\mu_m L}{a_c}\sin\left(\frac{\mu_m L}{a_c}\right) + \left[\frac{L}{a_c}\left(\frac{a}{a_c} - 1\right) + \frac{a}{L}\left(\frac{\mu_m L}{a_c}\right)^2\right]\cos\left(\frac{\mu_m L}{a_c}\right) = 0 \tag{2.9a}$$

and the normalization constants are

$$A_m = \left\{ L\left[1 + \frac{a_c}{2\mu_m L}\sin\left(\frac{2\mu_m L}{a_c}\right)\right] + 2a\cos^2\left(\frac{\mu_m L}{a_c}\right)\right\}^{-1/2} \tag{2.10a}$$

The odd eigenfunctions are

$$\phi_{om}(y) = B_m \sin(\mu'_m y/a_c) \tag{2.8b}$$

where the μ'_m are solutions of

$$\frac{\mu'_m L}{a_c}\cos\left(\frac{\mu'_m L}{a_c}\right) - \left[\frac{L}{a_c}\left(\frac{a}{a_c} - 1\right) + \frac{a}{L}\left(\frac{\mu'_m L}{a_c}\right)^2\right]\sin\left(\frac{\mu'_m L}{a_c}\right) = 0 \tag{2.9b}$$

and the normalization constants are

$$B_m = \left\{ L\left[1 - \frac{a_c}{2\mu'_m L}\sin\left(\frac{2\mu'_m L}{a_c}\right)\right] + 2a\sin^2\left(\frac{\mu'_m L}{a_c}\right)\right\}^{-1/2} \tag{2.10b}$$

If we write $r_m = \mu_m L/a_c$ and $r'_m = \mu'_m L/a_c$, then the eigenvalue equations may be rewritten

$$r_m \tan(r_m) = -[(L/a_c^2)(a - a_c) + ar_m^2/L] \tag{2.9c}$$

and

$$r'_m \cot(r'_m) = [(L/a_c^2)(a - a_c) + ar'^2_m/L] \tag{2.9d}$$

Since on $(n - 1/2)\pi < r < (n + 1/2)\pi$, $r\tan(r)$ is continuous, monotonic, and spans $(-\infty, \infty)$, there is exactly one root r_n on this subinterval of r for all $n \geqslant 1$. There are other similar solutions for $n \leqslant -1$, but these give the same eigenvalues λ_n. Similarly, there is exactly one root r'_n on $n\pi < r < (n+1)\pi$ for all $n \geqslant 1$ (and $n \leqslant -1$, again giving the same eigenvalues). There is also a solution r_0 of (2.11a) on $0 \leqslant r < \pi/2$ provided $a \leqslant a_c$ and a solution r'_0 of (2.11b) on $0 < r < \pi$ provided $a < \bar{a}_c = a_c + a_c^2/L$. If $a > a_c$, the solution r_0 becomes $r_0 = is_0$ with s_0 satisfying

$$s_0 \tanh(s_0) = (L/a_c^2)(a - a_c) - as_0^2/L \tag{2.9e}$$

which has exactly one solution for $a > a_c$. The associated eigenfunction is then

$$\phi_{e0}(y) = A_0 \cosh(s_0 y/L) \tag{2.8c}$$

with

$$A_0 = \left\{ L\left[1 + \frac{1}{2s_0}\sinh(2s_0)\right] + 2a\cosh^2(s_0)\right\}^{-1/2} \tag{2.10c}$$

If $a > \bar{a}_c$, then the solution r_0' becomes $r_0' = is_0'$ with s_0' satisfying

$$s_0' \coth(s_0') = (L/a_c^2)(a - a_c) - a s_0'^2/L \tag{2.9f}$$

which has exactly one solution for $a > \bar{a}_c$. The associated eigenfunction is then

$$\phi_{o0}(y) = B_0 \sinh(s_0' y/L) \tag{2.8d}$$

with

$$B_0 = \left\{ L\left[1 - \frac{1}{2s_0'} \sinh(2s_0')\right] - 2a \sinh^2(s_0') \right\}^{-1/2} \tag{2.10d}$$

For real μ_m (or μ_m') we have $\mu_m < \mu_{m+1}$ (or $\mu_m' < \mu_{m+1}'$) and so $\lambda_{e,m} > \lambda_{e,m+1}$ (or $\lambda_{o,n} > \lambda_{o,n+1}$). Also, $\mu_m < \mu_m'$ and so $\lambda_{e,m} > \lambda_{o,m}$. Also, if $\mu_0 = iv_0$, we have $\lambda_{e,0} > \lambda_{e,n}$, $n \geqslant 1$, and similarly if $\mu_0' = iv_0'$, we have $\lambda_{o,0} > \lambda_{o,n}$, $n \geqslant 1$. Finally, $\lambda_{e,0} > \lambda_{o,0}$ whether μ_0 and μ_0' are real or imaginary. The largest eigenvalue is thus always $\lambda_{e,0}$. These facts complete the description of the partition function $\mathbb{Q}_N(L\text{-}, L\text{-}, a)$.

3. THE PARTITION FUNCTION AND FINITE-SIZE SCALING

We may now evaluate the free energy per column in the thermodynamic limit for the continuous variable contour. This is

$$\frac{\psi(a; L)}{kT} = \lim_{N \to \infty} \frac{1}{N} \log \mathbb{Q}_N(L\text{-}, L\text{-}; a) \tag{3.1}$$

We may also consider L large and so we may take $N \to \infty$ in (3.1) first and then $L \to \infty$, or we may take $L \to \infty$ first and then $N \to \infty$. We may also take $L \to \infty$ and $N \to \infty$ together, with some fixed relation between L and N. If we define

$$\psi_1(a) = \lim_{L \to \infty} \psi(a; L) \tag{3.2}$$

then

$$\psi_1(a) = -kT \lim_{L \to \infty} \log(\lambda_{e,0}) \tag{3.3}$$

We also define

$$\psi_2(a) = -kT \lim_{N \to \infty} \lim_{L \to \infty} \frac{1}{N} \log \mathbb{Q}_N(L\text{-}, L\text{-}; a) \tag{3.4}$$

For $a > a_c$ we have $\lambda_{e,0} = 2a_c/(1 - v_0^2)$, where v_0 is the solution of

$$\left(\frac{v_0}{a_c}\right)^2 + 2\left(\frac{v_0}{a_c}\right)\frac{1}{2a}\tanh\left(\frac{v_0}{a_c}\right) - \frac{1}{aa_c^2}(a - a_c) = 0 \tag{3.5}$$

In the limit $L \to \infty$, the hyperbolic tangent is 1, and so

$$v_0 = \frac{a - a_c}{a} \tag{3.6}$$

Thus, for $a > a_c$ we have

$$\psi_1(a)/kT = \log[1 - (1 - a_c/a)^2] - \log(2a_c) \tag{3.7}$$

For $a < a_c$ we have $\lambda_{e,0} = 2a_c/(1 + \mu_0^2)$, where μ_0 is the solution on $0 \leqslant \mu_0 \leqslant \pi a_c/2L$ of

$$\mu_0 \tan\left(\frac{\mu_0 L}{a_c}\right) = \frac{a_c - a}{a_c} - \frac{a}{a_c}\mu_0^2 \tag{3.8}$$

Thus, as $L \to \infty$, $\lambda_{e,0} \to 2a_c$ and we have

$$\psi_1(a)/kT = -\log(2a_c) \tag{3.9}$$

The system has a phase transition. If we study the height–height correlation function, we find that for $a > a_c$, this correlation function decays exponentially with column separation and the height distribution function is localized close to the surface at $y = L$. For $a < a_c$ the correlation decays polynomially in column separation and the height distribution function is no longer localized. Interpreted as an interface, the contour becomes rough for $a < a_c$ and one phase can wet the surface at $y = L$. For $a > a_c$ the contour is smooth and there is no wetting of the surface.

If we take the limit $L \to \infty$ first, we see that for $a < a_c$ the μ_n become uniformly distributed on the real line and we may replace the sum over eigenvalues by a Riemann integral. We find

$$\lim_{L \to \infty} \mathbb{Q}_N(L\text{-}, L\text{-}; a)$$

$$= \frac{2}{\pi a_c}(2a_c)^N \int_0^\infty \frac{x^2}{x^2 + (a/a_c - 1 + ax^2/a_c)^2}(1 + x^2)^{-N}\,dx \tag{3.10a}$$

for $a < a_c$. If we consider $a > a_c$, there are two eigenvalues split off from the band of eigenvalues on $0 \leqslant \lambda \leqslant a_c$ and when we include their contribution we find

$$\lim_{L\to\infty} \mathbb{Q}_N(L\text{-}, L\text{-}; a)$$
$$= (2a_c)^N \left\{ \frac{a-a_c}{a(a-a_c/2)} \left[1 - \left(\frac{a-a_c}{a}\right)^2 \right]^{-N} + \frac{2}{\pi a_c} \int_0^\infty \frac{x^2}{x^2 + (a/a_c - 1 + ax^2/a_c)^2} (1+x^2)^{-N}\, dx \right\} \tag{3.10b}$$

for $a > a_c$. If we evaluate the integrals in (3.10a), (3.10b), we find

$$\psi_1(a)/kT = \psi_2(a)/kT \tag{3.11}$$

We may now consider finite-size scaling effects for both of the above limiting processes. If we consider $N \to \infty$ first, then the structure of the partition function for $a = a_c(1+\Delta)$, $\Delta > 0$, will be dominated by $(2a_c)^N (1 - v_0^2)^{-N}$, which will have an interesting limit when $v_0^2 = O(1/N)$. The equation for v_0 is

$$v_0 \tanh(v_0 L/a_c) = (a - a_c)/a - av_0^2/a_c \tag{2.9g}$$

If $v_0 = \alpha N^{-1/2}$, we find

$$\alpha^2 L/a_c = \kappa - a\alpha^2/a_c \tag{3.12}$$

with

$$\kappa = N(a - a_c)/a_c \tag{3.13}$$

Thus we find

$$G_1(\kappa) = \lim_{N\to\infty} \frac{\mathbb{Q}_N(L\text{-}, L\text{-}; a_c(1+\kappa/N))}{\mathbb{Q}_N(L\text{-}, L\text{-}; a_c)} = \exp \frac{a_c \kappa}{L} \tag{3.14}$$

The limit of this ratio as $L \to \infty$ is 1. The same result also holds for $a = a_c(1-\Delta)$, $\Delta > 0$.

On the other hand, we may consider the limit $L \to \infty$ and then $N \to \infty$. In that case we may define

$$\xi = N^{1/2}(a - a_c)/a_c \tag{3.15}$$

and consider

$$G_2(\xi) = \lim_{N\to\infty} \lim_{L\to\infty} \frac{\mathbb{Q}_N(L\text{-}, L\text{-}; a_c(1+\xi/\sqrt{N}))}{\mathbb{Q}_N(L\text{-}, L\text{-}; a_c)} \tag{3.16}$$

using (3.10a), (3.10b) directly. An asymptotic expansion of the integrals then gives

$$G_2(\xi)=\begin{cases} 2\sqrt{\pi}\left(\xi e^{\xi^2}+\dfrac{1}{\pi}\displaystyle\int_0^\infty \frac{x^2e^{-x^2}}{x^2+\xi^2}\,dx\right) & \text{for} \quad \xi>0 \\ \dfrac{2}{\sqrt{\pi}}\displaystyle\int_0^\infty \frac{x^2e^{-x^2}}{x^2+\xi^2}\,dx & \text{for} \quad \xi>0 \end{cases} \tag{3.17}$$

We may evaluate the integral here to give

$$G_2(\xi)=\sqrt{\pi}\,\xi e^{\xi^2}[1+\operatorname{erf}(\xi)]+1 \tag{3.18}$$

which is expression valid for all ξ.

We may also let N and L become large together. A string in two dimensions pinned at (0, 0) and (0, N) has fluctuations that are $O(\sqrt{N})$. Further, the spin-up, spin-down interface in the two-dimensional Ising model can exhibit similar scale fluctuations.[17] Thus, we may expect that when $L=O(\sqrt{N})$, the contour will fluctuate over the whole of $-L\leqslant y\leqslant L$. Thus, we define α and ζ by

$$N=\alpha L^2/a_c^2 \tag{3.19}$$

and

$$\zeta=L(a-a_c)/a_c^2 \tag{3.20}$$

We then consider [again cf. (1.1)]

$$F(\zeta,\alpha)=\lim_{L\to\infty}\frac{\mathbb{Q}_{\alpha L^2/a_c^2}(L\text{-},L\text{-};a_c(1+a_c\zeta/L))}{\mathbb{Q}_{\alpha L^2/a_c^2}(L\text{-},L\text{-};a_c)} \tag{3.21}$$

If we consider $\alpha\to 0$, then we should expect the behavior of $F(\zeta,\alpha)$ to resemble that of $G_2(\zeta)$. We may expect the $\alpha\to\infty$ limit to be rather singular, since it should resemble the function $G_1(\kappa)=1$. In this finite-size scaling limit $L\to\infty$, the eigenvalue equations become

$$r_n\tan(r_n)=-\zeta-r_n^2/L \tag{2.9h}$$

and

$$r'_n\cot(r'_n)=\zeta+r_n'^2/L \tag{2.9i}$$

The quantities $\lambda_{e,n}^N$ in the partition function $\mathbb{Q}$ are then

$$\lambda_{e,n}^N=(2a_c)^N(1+\alpha r_n^2/N)^{-N}\approx(2a_c)^N\exp(-\alpha r_n^2) \tag{3.22}$$

with a similar formula for $\lambda_{0,n}^N$. The normalization of the eigenfunctions gives

$$\psi_{e,n}^2(L) = \left\{ L\left[1 + \tan^2(r_n) + \frac{1}{r_n}\tan(r_n)\right] + 2a \right\}^{-1} \tag{3.23}$$

and another similar formula for $\psi_{0,n}^2(L)$. If we now let L become large, we obtain

$$\begin{aligned}
&\mathbb{Q}_{\alpha L^2/a_c^2}\left(L\text{-}, L\text{-}; a_c\left(\frac{1+a_c\zeta}{L}\right)\right) \\
&\quad = \frac{1}{2L}(2a_c)^{\alpha L^2/a_c^2}\left\{\sum_{n=-\infty}^{\infty}\left[\frac{p_n^2\exp(-\alpha p_n^2)}{p_n^2+\zeta^2-\zeta} + \frac{q_n^2\exp(-\alpha q_n^2)}{q_n^2+\zeta^2-\zeta}\right]\right\} \\
&\quad \times\left(1 + O\left(\frac{1}{L}\right)\right)
\end{aligned} \tag{3.24}$$

where the p_n are all the solutions of

$$p_n \sin(p_n) + \zeta\cos(p_n) = 0 \tag{2.9j}$$

and the q_n are all the solutions of

$$q_n \sin(q_n) - \zeta\cos(q_n) = 0 \tag{2.9k}$$

When $\zeta = 0$ we have $p_n = n\pi$, $n \neq 0$, and $q_n = (n+1/2)\pi$, for all $n \in \mathbb{Z}$. Further, $p_0^2 \sim -\zeta$ for small ζ. Thus, we have

$$\begin{aligned}
&\mathbb{Q}_{\alpha L^2/a_c^2}(L\text{-}, L\text{-}; a_c) \\
&\quad = \frac{1}{2L}(2a_c)^N \sum_{n=-\infty}^{\infty} \exp\left(\frac{-n^{2\pi^2}}{4}\right)\left[1 + O\left(\frac{1}{L}\right)\right] \\
&\quad = \frac{1}{2L}(2a_c)^N \vartheta_3\left(0, \exp\left(\frac{-\alpha\pi^2}{4}\right)\right)\left(1 + O\left(\frac{1}{L}\right)\right)
\end{aligned} \tag{3.25}$$

where we have used the Bateman manuscript definition of the Jacobi theta functions.[18] We thus have

$$F(\zeta, \alpha) = \sum_{n=-\infty}^{\infty}\left[\frac{p_n^2\exp(-\alpha p_n^2)}{p_n^2+\zeta^2-\zeta} + \frac{q_n^2\exp(-\alpha q_n^2)}{q_n^2+\zeta^2-\zeta}\right]\left[\vartheta_3\left(0, \exp\left(\frac{-\alpha\pi^2}{4}\right)\right)\right]^{-1} \tag{3.26}$$

Later we describe the zeros in ζ of $F(\zeta, \alpha)$ and compare them with those of $G_2(\xi)$. We are particularly interested in the motion of the zeros as α varies.

4. SOLUTIONS OF THE ASYMPTOTIC EIGENVALUE EQUATIONS AND FINITE-SIZE SCALING FORM FOR THE FREE ENERGY

We consider the two eigenvalue equations

$$p_n \sin(p_n) + \zeta \cos(p_n) = 0 \tag{2.9j}$$

and

$$q_n \sin(q_n) - \zeta \cos(q_n) = 0 \tag{2.9k}$$

To understand the structure of the solutions, we construct asymptotic expansions for $p_n(\zeta)$ and $q_n(\zeta)$ for small and large $|\zeta|$ and then describe the numerical behavior of the solutions.

Suppose first that $|\zeta|$ is small. The first solution is p_0 and we have

$$p_0(\zeta) = [\zeta \exp(i\pi)]^{1/2}\,[1 + \zeta/6 + 11\zeta^2/360 + O(\zeta^3)] \tag{4.1}$$

There is another solution at $-p_0(\zeta)$. The other solutions are close to $p_n = n\pi$ and we find

$$p_n(\zeta) = n\pi[1 - \zeta/(n\pi)^2 - \zeta^2/(n\pi)^4 + O(\zeta^3)], \qquad |n| \geqslant 1 \tag{4.2}$$

There are also solutions $q_n(\zeta)$ close to $(n + 1/2)\,\pi$ and we find

$$q_n(\zeta) = \left(n + \frac{1}{2}\right)\pi \left\{1 - \zeta\Big/\left[\left(n+\frac{1}{2}\right)\pi\right]^2 - \zeta^2\Big/\left[\left(n+\frac{1}{2}\right)\pi\right]^4 + O(\zeta^3)\right\}, \quad \forall n \tag{4.3}$$

If we consider $\zeta = \beta \exp(i\gamma)$ with β small, then as γ varies from $-\pi$ to π, the solutions of Eqs. (2.9j), (2.9k) describe loops clockwise about $n\pi$ or $(n + 1/2)\,\pi$. The size of these loops decreases as n increases.

We may also consider $|\zeta| = \beta$ large. For (2.9j), either $|p_n|$ is large or $|\cos(p_n)|$ is small. There are two solutions for $|p_n|$ large, namely

$$p_{0\pm} = \pm i\zeta\{1 + O(\exp[-2\,\mathrm{re}(\zeta)])\} \tag{4.4}$$

This expansion is valid when $\mathrm{re}(\zeta) > 0$, that is, for $-\pi/2 < \phi < \pi/2$ in $\zeta = \beta \exp(i\gamma)$. There are also two-large modulus solutions to (2.9k),

$$q_{0\pm} = \pm i\zeta\{1 + O(\exp[-2\,\mathrm{re}(\zeta)])\} \tag{4.5}$$

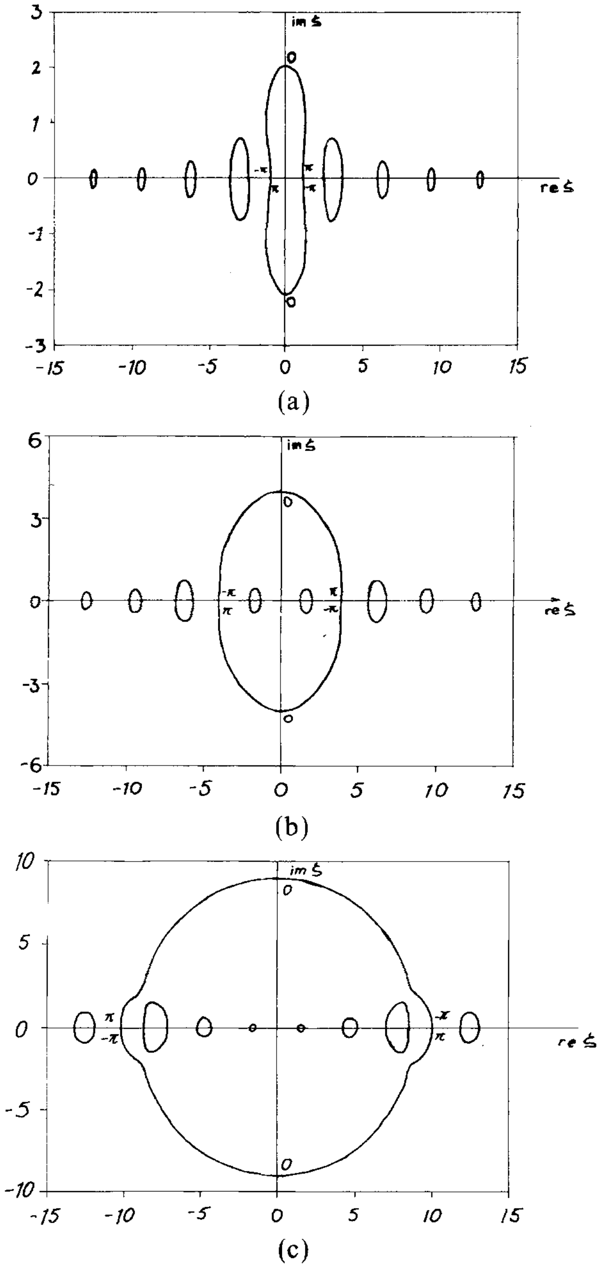
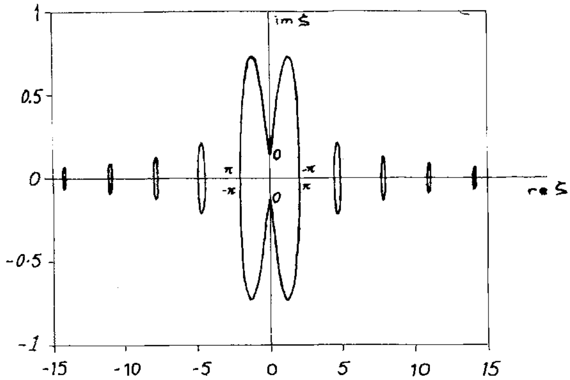
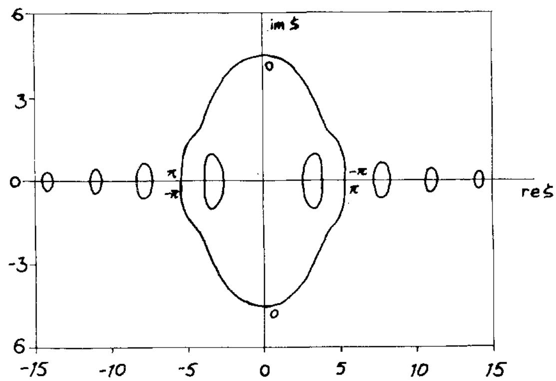


Fig. 1. Motion of the eigenvalues p_n and q_n as functions of $\zeta = \beta \exp(i\gamma)$ as γ varies from 0 to 2π. Marks on the curves refer to values of γ. (a) The p_n for $\beta = 2$. (b) The p_n for $\beta = 4$. (c) The p_n for $\beta = 9$. (d) The q_n for $\beta = 1.05$. (e) The q_n for $\beta = 4.5$.



(d)



(e)

Fig. 1. (*Continued*)

for $-\pi/2 < \gamma < \pi/2$. If $|\cos(p_n)|$ is to be small, then p_n must be close to $(n + 1/2)\,\pi$ and we then find

$$p_n(\zeta) = \left(n + \frac{1}{2}\right)\pi \left[1 + \zeta^{-1} + \zeta^{-2} - \frac{1}{3}\left[\left(n + \frac{1}{2}\right)\pi\zeta^{-1}\right]^3 \times \left\{1 - 3\Big/\left[\left(n + \frac{1}{2}\right)\pi\right]^2\right\} + O(\zeta^{-4})\right] \tag{4.6}$$

Similarly, there will be solutions to (2.9k) with $|\sin(q_n)|$ small. These solutions will be close to $n\pi$ and

$$q_n(\zeta) = n\pi\left\{1 + \zeta^{-1} + \zeta^{-2} - \frac{1}{3}(n\pi\zeta^{-1})^3\,[1 - 3/(n\pi)^2] + O(\zeta^{-4})\right\} \tag{4.7}$$

As γ varies from $-\pi$ to π, these solutions also describe clockwise loops about $(n+1/2)\pi$ or $n\pi$ and the size of the loops increases as n increases. The remainder of the large-$|p_n|$ or large-$|q_n|$ trajectories for $\pi/2<\gamma<3\pi/2$ form half loops interleaving the loops along the real axis. The large-$|p_n|$ and large-$|q_n|$ trajectories are thus roughly circular with indentations or bumps close to the real axis. In Figs. 1a–1e we present some representative trajectories at fixed β with $-\pi<\gamma<\pi$. The trajectories reflect the conclusions we can draw from the asymptotic expansions.

One point which can be seen from the shapes of these trajectories of $p_n(\beta\exp(i\gamma))$ and $q_n(\beta\exp(i\gamma))$ with γ is that there is a sequence of numbers ζ_m at which $f_p(z)=z\sin(z)+\zeta_m\cos(z)$ has a double root. There is also another sequence ζ'_m at which $f_q(z)=z\cos(z)-\zeta'_m\sin(z)$ has a double root. At such points the denominators in the two sums in the partition function can be zero. However, there are four terms in each sum with zero denominators for each m and the residues cancel. Examination shows that at such values ζ_m or ζ'_m of ζ, the function $F(\zeta,\alpha)$ is in fact analytic.

For large $|\zeta|$, we may use the leading order terms in the asymptotic expansions for the eigenvalues to obtain, for the singular part of the free energy,

$$F^s(\zeta,\alpha)\sim\left[4\zeta e^{\alpha\zeta^2}-\zeta^{-2}\frac{\partial}{\partial\alpha}\vartheta_3\left(0,\exp\left(\frac{-\alpha\pi^2}{4}\right)\right)\right]\Big/\vartheta_3\left(0,\exp\left(\frac{-\alpha\pi^2}{4}\right)\right) \tag{4.8}$$

The singular part of the free energy density may be obtained from (3.7) and (3.9) and may be written

$$\psi_1^{(s)}(\tau)\sim A_\pm\tau^2 \tag{4.9}$$

with $\tau=(a-a_c)/a_c$, $A_+=-1$, and $A_-=0$. This makes contact with the phenomenological description of scaling region partition function zeros due to Glasser *et al.*[13] Here the Glasser *et al.* parameter α is not the "shape" parameter α used in this paper, but takes the value 0, as may be seen by comparing (4.9) with (1.2). In this description $\tau>0$ corresponds to strong coupling and $\tau<0$ corresponds to weak coupling, so that scaling region partition function zeros should be -1 times those derived from the formulas of Glasser *et al.* Their formula [given in (1.3)] requires the angle ϕ, which in this system is $\pi/4$. Changing the Glasser *et al.*[13] formula into our notation, the prediction of Glasser *et al.* is that there should be zeros of $F(\zeta,\alpha)$ for large n at

$$\zeta_{n\pm}\sim(2\pi n/\alpha)^{1/2}e^{\pm i\pi/4} \tag{4.10}$$

While it would naturally be of interest to pursue the detailed structure of the scaling partition function and the corrections to scaling, we do not do so here, turning now to the distribution of the zeros of $F(\zeta, \alpha)$.

5. LOCATION OF THE PARTITION FUNCTION ZEROS

We consider first the function $G_2(\xi)$. For $\mathrm{re}(\xi) < 0$ we use the representation

$$G_2(\xi) = 1 - \sqrt{\pi}\, \xi e^{\xi^2} \operatorname{erfc}(-\xi) \tag{5.1}$$

This function is analytic in the finite part of the complex ξ plane. We now construct a contour $C_\delta(R)$ going in a straight line from 0 to $R \exp[-i(\pi/2 - \delta)]$, then via a semicircular arc $R \exp(i\theta)$, $-(\pi/2 - \delta) \leqslant \theta \leqslant (\pi/2 - \delta)$, to $R \exp[i(\pi/2 - \delta)]$, and then via a straight line back to zero. We then consider the integral

$$I(R, \delta) = \frac{1}{2\pi i} \int_{C_\delta(R)} \frac{h'(\xi)}{h(\xi)}\, d\xi \tag{5.2}$$

Here $h(\xi) = G_2(-\xi)$. We may then use the asymptotic representation[19]

$$\operatorname{erfc}(\xi) = \frac{e^{-\xi^2}}{\xi \sqrt{\pi}} \left[1 - \frac{\xi^{-2}}{2} + \frac{3A(\xi)}{4\beta^4 \cos(\gamma)} \right] \tag{5.3}$$

for $\xi = \beta \exp(i\gamma)$, with $|A(\xi)| < 1$. The contribution from the semicircular part of the contour is then $-(1 - 2\delta/\pi)[1 + B/R^2 \sin(\delta)]$, where $|B|$ is bounded. The contribution from the straight-line parts of the contour is

$$-\frac{1}{2\pi i} \log \left[\frac{h(R \exp[i(\pi/2 - \delta)])}{h(R \exp[-i(\pi/2 - \delta)])} \right] = \left(\frac{1 - 2\delta}{\pi} \right) \left(\frac{1 + \bar{B}}{R^2 \sin(\delta)} \right)$$

where $|\bar{B}|$ is bounded. The integral $I(R, \delta)$ is then $C/R^2\delta$, where $|C|$ is bounded. We may then take $\delta = 1/R$ and then see that the integral $I(R, 1/R) \to 0$ as $R \to \infty$. Thus, there are no zeros of $G_2(\xi)$ for $\mathrm{re}(\xi) < 0$.

Further,

$$G_2(i\zeta) = 1 - 2\zeta e^{-\zeta^2} \int_0^\zeta e^{u^2}\, du + \sqrt{\pi}\, i\zeta e^{-\zeta^2} \tag{5.4}$$

so that if ζ be real, the imaginary part of $G_2(i\zeta)$ is nonzero unless $\zeta = 0$, which is not a zero of $G_2(i\zeta)$. Thus, there are no zeros of $G_2(\xi)$ for $\mathrm{re}(\xi) \leqslant 0$.

For $\mathrm{re}(\xi) > 0$ we use the expansion (5.3) again to obtain

$$G_2(\xi) = 2\sqrt{\pi}\,\xi e^{\xi^2} + B(\xi)/2\beta^2\cos(\gamma) \tag{5.5}$$

for $\xi = \beta\exp(i\gamma)$, with $|B(\xi)| < 1$. Hence, there can be no zeros of $G_2(\beta\exp(i\gamma))$ in $-\pi/4 \leqslant \gamma \leqslant \pi/4$ for $\beta > (4\sqrt{\pi})^{-1/3} \simeq 0.5$. For $|\xi|$ large, the zeros satisfy

$$\xi^3 e^{\xi^2} = -\frac{1}{4\sqrt{\pi}}\left[\frac{1 - C(\xi)}{\beta^2\cos(\gamma)}\right] \tag{5.6}$$

with $|C(\xi)|$ bounded. We then find that for large $|\xi|$ the zeros of $G_2(\xi)$ are close to the lines $\xi = \beta\exp(\pm i\pi/4)$. We find the expansions for the zeros

$$\xi_{n\pm} \sim \left[2\left(n + \frac{1}{8}\right)\pi\right]^{1/2}\exp\left\{\pm i\left[\frac{\pi}{4} + \frac{3}{(8n+1)\,\pi}\log\left(\frac{\pi(8n+1)}{2}\right)\right]\right\} \tag{5.7}$$

We may now turn to the zeros of $F(\zeta, \alpha)$. First we consider $|\zeta|$ large, when there are eigenvalues $p_0 = \pm i\zeta\{1 + O(\exp[-2\,\mathrm{re}(\zeta)]\}$, similar q_0 eigenvalues, and further eigenvalues given approximately by (4.6), (4.7). For α not too small (e.g., $\alpha \geqslant 1$) the terms in the sum on n for $|n| > 1$ may be ignored. To leading order in ζ, the equation for $F(\zeta, \alpha)$ may then be reduced to

$$\zeta^3 e^{\alpha\zeta^3} = -(\pi^2/8)\,e^{-\alpha\pi^2/4} \tag{5.8}$$

We may find zeros of large magnitude as with (5.6) and find that the zeros lie close to the lines $\zeta = \beta\exp(\pm i\pi/4)$. These zeros have the expansion

$$\zeta_{n\pm} \sim \alpha^{-1/2}\left[2\left(n + \frac{1}{2}\right)\pi\right]^{1/2}\exp\left\{\pm i\left[\frac{\pi}{4} + \frac{\pi\alpha}{16n+2} + \frac{3}{(8n+1)\,\pi} \times\log\left(\frac{8n+1}{\alpha\pi^{1/3}}\right)\right]\right\} \tag{5.9}$$

We notice that as α becomes large, these zeros coalesce and collapse into the origin, giving an essential singularity at $\zeta = 0$ of $F(\zeta, \infty)$. This reflects the singular nature of the free energy when we take the limit $N \to \infty$ first and then $L \to \infty$.

If α is small, the zeros spread out and move off any part of the ζ plane as $\alpha \to 0$. Indeed, for small α the sum over eigenvalues $n \neq 0$ in $F(\zeta, \alpha)$ may be approximated by an integral and the equation $F(\zeta, \alpha) = 0$ reduces to

$$\alpha^{3/2}\zeta^3 e^{\alpha\zeta^2} = -1/4\sqrt{\pi} \tag{5.10}$$

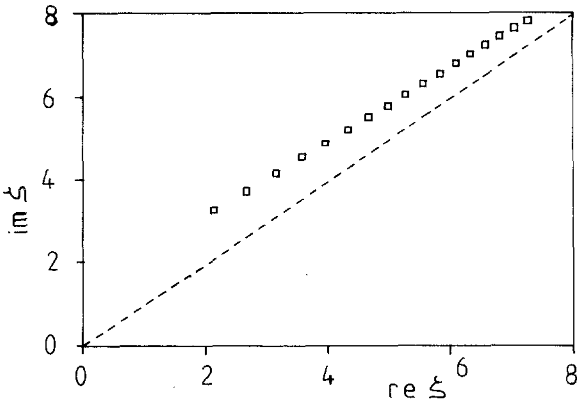


Fig. 2. Plot of the zeros ζ_{n+} of $F(\zeta, 1)$ for $\mathrm{im}(\zeta) > 0$. If ζ_{n+} is a zero, then $\zeta_{n-} = \zeta_{n+}^*$ is also a zero.

so that as $\alpha \to 0$, $\sqrt{\alpha}\,\zeta = \xi$, and we have the asymptotic zero equation for $G_2(\xi)$ again, namely (5.6). Thus, as $\alpha \to 0$, we retreive the structure of $G_2(\xi)$ from $F(\zeta, \alpha)$.

In Fig. 2 we plot the zeros ζ_{n+} of $F(\zeta, 1)$. They correspond to the sequence ζ_{n+} of Eq. (5.8) for $n \geqslant 2$. There do not appear to be further zeros in the sequence for $n < 2$. Numerical integration of $\{\partial F(\zeta, \alpha)/\partial\zeta\}/F(\zeta, \alpha)$ around appropriate contours in the complex ζ plane gives results less than 0.05 in magnitude unless the contour encloses one or more of the plotted zeros, when we obtain the correct zero count for the contour. As $\alpha \to 0$, the zeros move off the complex ζ plane according to $\zeta_n(\alpha) \sim \zeta_n(1)\,\alpha^{-1/2}$, while as $\alpha \to \infty$, the zeros collapse to the origin, giving the singular scaled free energy in the limit $N \to \infty$ first and then $L \to \infty$.

We may now consider the large-n behavior of these zeros to leading order. From (5.8) we have

$$\zeta_{n\pm} \sim (2n\pi/\alpha)^{1/2} \exp(\pm i\pi/4) \tag{5.11}$$

which is exactly the Glasser *et al.*[13] prediction for our system [cf. (1.3) and (4.10)]. This means that the phenomenological derivation of Glasser *et al.*[13] gives the correct asymptotic description of the scaling region partition function zeros for the wetting transition in the contour system studied in this paper.

It is of some interest to ask what happens if we study this whole problem with the partition function for the system with integer heights, as we used in Section 1 to derive the continuous height model. The differential equation for the eigenfunctions becomes a second-order constant-coefficient difference equation with similar boundary conditions. If for simplicity we choose $l = 1$ and set

$$a' = \exp(\varepsilon/kT) - 1 \tag{5.12}$$

then we find a critical value $a'_c = e^{-K}/(e^K - e^{-K})$, where $2K$ is again the contour energy per unit length. The calculations are rather more complicated than in the continuum height case, but their structure is identical. We obtain a partition function ratio in the finite-size scaling limit using

$$\zeta' = L(a - a_c)/a_c(1 + a_c) \tag{5.13}$$

and

$$N = \alpha' L^2/a_c(1 + a_c) \tag{5.14}$$

and the partition function ratio is then exactly $F(\zeta', \alpha')$. The description of the zeros in the ζ' plane is then identical to that in the continuous height case in the ζ plane. This correspondence is of some interest since we might expect some correspondence between these zeros and those of a two-dimensional Ising model with a boundary field H in the limit $K \to 0$. As Abraham and De Coninck[20] have shown, those zeros are on the line $\mathrm{re}(H) = 0$, which is emphatically not the case here. It is clear only that any connection between the two-dimensional Ising-model edge field zeros and those of the contour problem considered here is rather more subtle than the simple considerations of this paper will uncover.

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