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# Lee–Yang Zeros and Stokes Phenomenon in a Model with a Wetting Transition

**C. Pisani**[1] **and E. R. Smith**[1]

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We consider the statistical mechanics of a fluctuating string (1D solid-on-solid model) of $N$ columns with a contact energy term displaying a critical wetting transition. For this model we derive a contour integral representation for the finite-size partition function. From this representation we derive a polynomial representation and obtain the Lee–Yang zeros for $N \lesssim 100$. Through the asymptotic evaluation of the contour integral we evaluate the zeros for higher $N$. This asymptotic evaluation displays a Stokes phenomenon providing a different viewpoint of the mechanism by which a phase transition can arise, supplementing the picture of Lee and Yang. We also reproduce and extend somewhat the results of Smith for the finite-size scaling limit of the partition function.

**KEY WORDS:** Partition function zeros; Stokes phenomenon; wetting transition.

## 1. INTRODUCTION

The traditional Lee–Yang[1,2] picture characterizes a phase transition in the following way. The finite-size partition function has a representation as a polynomial in the coupling parameter, which has degree proportional to the size of the system. Singularities in the thermodynamic functions occur at the (complex) zeros of the polynomial and a phase transition can arise if, in the thermodynamic limit, the zeros condense onto lines which pinch the real coupling axis. This is a very appealing picture and this program has been carried out on a number of systems displaying a phase transition (see, e.g., ref. 3). This work has been primarily of a numerical nature because of the need to work with finite-size partition functions. Analytic

[1] Department of Mathematics, La Trobe University, Bundoora, Victoria 3083, Australia.



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techniques generally are only suited to the thermodynamic limit, the exception being the Ising model. Here the temperature zeros are known[4] and the magnetic field zeros, while not calculated, are known to lie on the imaginary axis as a result of the Lee–Yang circle theorem.[1,5]

There exists another viewpoint characterizing a phase transition. A phase transition is said to occur when the thermodynamic limit has different analytic forms in different regions of the coupling parameter space. The notion of a parameter-dependent asymptotic limit appears commonly in the theory of special functions and is nothing but the Stokes phenomenon.[6] Here, typically, the limit $|z| \to \infty$ is taken (being analogous to the $N \to \infty$ limit) and the asymptotic form differs, depending on which region $\arg z$ (being analogous to the coupling parameter) lies. There are many many examples of this and they can be pursued in the literature.[7,8] Indeed, recently there has been further progress in the study of Stokes phenomena by Berry and others.[9] The traditional view of Stokes phenomena is that the asymptotic expansion changes discontinuously across the so-called Stokes line. As the original functions are analytic, this discontinuity is an artifact. This recent work has obtained asymptotic approximations which are uniform (i.e., smooth but rapidly changing) across the Stokes lines.

While the Lee–Yang picture is very well known, the picture of a phase transition as a Stokes phenomenon is not so well known. In fact we only know of a few references in which it is in some way invoked. One is the paper of Itzykson *et al.*[10] which in its introduction describes Lee–Yang zeros "as falling on Stokes lines which separate different asymptotic behaviours of the partition function in the thermodynamic limit." (There is a confusion of terminology in the literature as to what constitutes a Stokes line and what constitutes an anti-Stokes line. We shall follow the mathematical literature. With this interpretation Lee–Yang zeros fall on anti-Stokes lines.) There has also been some recent work on the calculation of the zeros of the finite-size scaling limit of the partition function[11,12] and here Stokes phenomena play a role. As the Stokes phenomenon characterization of a phase transition is very natural, we suspect that it is, in some sense, well known in the literature. As far as we are aware, however, it has not been developed in full on a model with a phase transition.

In this paper we shall consider the model studied in Smith.[11] This model is simple enough to explicitly and (largely) analytically develop both the above viewpoints, yet complex enough to display a phase transition. The model which we study here is a variant of a much-studied model for the critical wetting transition (i.e., the transition at coexistance) (see, e.g., ref. 13). The model consists of $N$ heights $x_i$, where $x_i$ is a continuous variable taking values $-1 \leqslant x_i \leqslant 1$ (see Fig. 1). The endpoints of the string

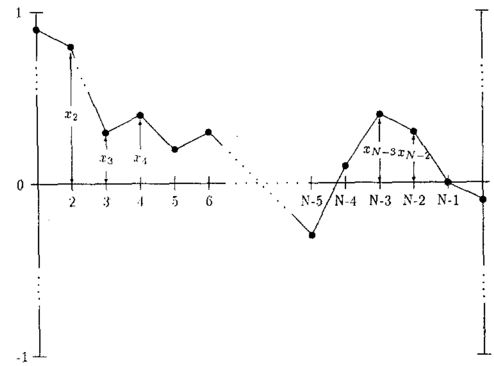

Fig. 1. A sample configuration of the continuous string. $x_1$ and $x_N$ are the ordinates of the first and last heights. We calculate the partition function for the case $x_1 = x_N = 1$.

are fixed at $x_1 = x_N = 1$. The model can be viewed as a fluctuating string (or as a solid-on-solid model). The partition function is

$$Z_N^c(K_c, a_c, x_1, x_N) = \int_{-1}^{1} dx_2 \cdots \int_{-1}^{1} dx_{N-1} \exp\left( - \sum_{j=1}^{N-1} K_c \, |x_{j+1} - x_j| \right) \times \prod_{j=1}^{N} [1 + a_c \delta(x_j, 1) + a_c \delta(x_j, -1)] \tag{1.1}$$

Various quantities are labelled with $c$ (denoting continuous) to distinguish these from corresponding quantities in other cases which shall arise. The Boltzmann weight in (1.1) has a surface tension term which favors smooth configurations of the string over rough ones. There is also a contact energy (or adsorption potential) term which favors configurations where the string is pinned either to the top or to the bottom (in the solid-on-solid model interpretation this is a surface field). Usually one has only one surface to which the string can bind, in line with the wetting transition interpretation. In having two surfaces to which the string can be pinned we are following Smith.[11] The presence of a second surface is of no importance to our investigations here. We have included it with an eye to further investigations in which competition can be arranged between the string favoring the top or the bottom.

The partition function (1.1) does not have a phase transition as one takes the thermodynamic limit ($N \to \infty$). However, if one first takes $K_c \to \infty$, then the resulting partition function does have a phase transition in the thermodynamic limit. As $K_c$ is a surface tension parameter, it is far from clear as to why this limit should yield a phase transition. However, if one lets $x_i' = K_c x_i$ and

$$a = K_c a_c \tag{1.2}$$

then the configurations of the string are such that $-K_c \leqslant x_i' \leqslant K_c$ and one has unit surface tension. Thus, as $K_c \to \infty$, the string is allowed to fluctuate over an infinite channel. A phase transition did not arise in the original model because it was a one-dimensional model with short-range interactions (and thus phase transitions are forbidden via well-known theorems). This rescaling makes it clear that a phase transition arises in the $K_c \to \infty$ limit, because in this limit the model becomes essentially two dimensional. In this interpretation $K_c$ plays the role which $L$ plays in Smith's paper.[11] However, Smith did not present the surface tension interpretation.

In this paper we present a contour integral representation for (1.1) [see (4.3)] and its limit as $K_c \to \infty$ [see (4.4) and (4.5)] as a function of $a$. This representation is based on the use of a Green's function. Through standard techniques the partition function can be written in terms of an $(N-1)$-fold product of a transfer matrix $T$. The Green's function of $T$ is defined as

$$G = (z - T)^{-1} \tag{1.3}$$

where $z$ is a complex variable. One can then readily show that

$$T^{N-1}(x_1, x_N) = \frac{1}{2\pi i} \oint_C z^{N-1} G(x_1, x_N)\, dz \tag{1.4}$$

where we supress the coupling dependence. The integral is taken over a contour $C$ which goes anticlockwise around all the eigenvalues of $T$. Equation (1.4) is readily derived using the eigenfunction expansion of the Green's function

$$G(x_1, x_N) = \sum_\alpha \frac{\phi_\alpha(x_1)\, \phi_\alpha(x_N)}{z - \lambda_\alpha} \tag{1.5}$$

where $\phi_\alpha$ and $\lambda_\alpha$ are, respectively, the $\alpha$th eigenvector and corresponding eigenvalue of $T$. In this derivation, one first assumes that all the couplings are real and that the transfer matrix has been chosen to be symmetric. Then eigenvalues are real and the eigenvectors can be chosen real and the derivation follows. Having established (1.4) and then having obtained $G$, one can then define the partition function for complex couplings via analytic continuation.

There are thus two steps in the procedure: (i) evaluating the Green's function and (ii) evaluating the resulting contour integral. This approach was originally chosen to avoid the eigenvalue summations in the evaluation of the finite-size scaled partition function. It turned out that this approach was also useful for the study of the finite-size partition function.

In Section 2 we derive a somewhat more general version of (1.1) from a discrete version of the model. In Section 3 we evaluate the Green's function for the more general model. In Section 4 we obtain the contour integral representation for (1.1) and take the limit $K_c \to \infty$. For finite $N$ we then derive a polynomial representation for the partition function and evaluate the zeros (for $N \lesssim 100$) in $a$ of this polynomial for various values of $N$ (see Fig. 2). This gives, of course, the Lee–Yang viewpoint of the phase transition. In Section 5 we perform an asymptotic evaluation of the contour integral, present the Stokes phenomenon viewpoint, and make contact with the Lee–Yang viewpoint. In Section 6 we use the asymptotic expansion to evaluate the large-$N$ expression for the Lee–Yang zeros. In Section 7 we recover, and go somewhat beyond, the finite-size scaling limit results of Smith.[11] In Section 8 we conclude with some discussion.

This paper arose as a continuation of the work of Smith and related papers and uses techniques learnt in previous study by one of the authors (C.P) on the calculation of quantum virial coefficients using the techniques of quantum scattering theory (see, e.g., refs. 14).

## 2. MODEL VIA A CONTINUUM LIMIT

One could apply the calculational procedure outlined above directly to the partition function (1.1). However, our experience has shown that this is somewhat awkward. More importantly, we attempted this procedure with a similar model with a magnetic field and found that our original continuum model was somewhat ill defined. As a result we instead prefer to derive the partition function via a careful continuum limit of a discrete model. We present this derivation for a somewhat more general model than that considered by Smith. We do this both because the extra effort involved is small and with an eye to possible future investigations.

We begin with a discrete string whose configuration is given by $N$ heights $\{n_1, n_2,..., n_N\}$, where $n_i \in (-L,..., L)$ and $L$ is some fixed integer. The energy of the configuration is given by

$$\begin{aligned}
&\beta E\{K_d, t_d, b_d, h_d; n_1, n_2,..., n_N\} \\
&\quad = \sum_{j=1}^{N-1} K_d\,|n_{j+1} - n_j| \\
&\qquad - \sum_{j=1}^{N} [2t_d \delta(n_i, L) + 2b_d \delta(n_i, -L)] + \sum_{j=1}^{N} 2h_d n_j
\end{aligned} \tag{2.1}$$

where the $d$ label, denoting discrete, is to distinguish this model from its continuum limit. $\delta(a, b)$ is the usual Kronecker delta. The first term favors smooth configurations over rough ones. The second term gives an extra weight to those configurations in which the string is adsorbed to the top or the bottom. The third term is a symmetry-breaking (magnetic field) term.

The partition function for this model is

$$Z_N^d(L, K_d, t_d, b_d, h_d; n_1, n_N) = \sum_{n_2=-L}^{L} \sum_{n_3=-L}^{L} \cdots \sum_{n_{N-1}=-L}^{L} e^{\beta E\{K_d, t_d, b_d, h_d; n_1, n_2, \ldots, n_N\}} \tag{2.2}$$

It is essential in order for our methods to work to keep the boundary conditions on the string, i.e., $n_1, n_N$, fixed. They may nonetheless take arbitrary values.

Using standard techniques,[2] we write the partition function in terms of a transfer matrix

$$\begin{aligned} Z_N^d(L, K_d, t_d, b_d, h_d; n_1, n_N) &= e^{-h_d(n_1+n_N)} e^{t_d[\delta(n_1, L)+\delta(n_N, L)]} \\ &\quad \times e^{b_d[\delta(n_1, -L)+\delta(n_N, -L)]} T_d^N(L, K_d, t_d, b_d, h_d; n_1, n_N) \end{aligned} \tag{2.3}$$

where $T_d$ is the $(2L+1)\times(2L+1)$ transfer matrix

$$\begin{aligned} T_d(L, K_d, t_d, b_d, h_d; n_j, n_{j+1}) &= e^{-K_d|n_{j+1}-n_j| - h_d(n_{j+1}+n_j)} \\ &\quad \times e^{t_d[\delta(n_{j+1}, L)+\delta(n_j, L)] + b_d[\delta(n_{j+1}, -L)+\delta(n_j, -L)]} \end{aligned} \tag{2.4}$$

We obtain boundary terms in (2.3) because we have chosen to work with a symmetric transfer matrix.

The Green's function satisfies

$$z_d G_d(n_1, n_N) - \sum_{n_k=-L}^{L} T_d(n_1, n_k)\, G_d(n_k, n_N) = \delta(n_1, n_N) \tag{2.5}$$

The most convenient way to perform the continuum limit is via the equation defining the Green's function. We thus consider the continuum limit of (2.5). Of course once this is done one can apply the scalings [see (2.11) below] directly to the discrete partition function and take the continuum limit for a more direct view of the continuum model. (1.1) can of course be derived in this way.

In deriving (1.4) it is convenient to work with a symmetric transfer matrix. Having obtained (1.4), a symmetric transfer matrix is no longer required. In fact, retaining a symmetric transfer matrix is quite inconvenient in the continuum limit because the Kronecker deltas in the transfer matrix are quite awkward to handle. These Kronecker deltas can be removed by performing a similarity transformation

$$G_d(n_1, n_N) = e^{-h_d n_1} e^{t_d \delta(n_1, L) + b_d \delta(n_1, -L)} \tilde{G}_d(n_1, n_N) \times e^{h_d n_N} e^{-t_d \delta(n_N, L) - b_d \delta(n_N, -L)} \tag{2.6}$$

Using the identity

$$e^{a\delta(n_k, L)} = 1 + (e^a - 1)\, \delta(n_k, L) \tag{2.7}$$

as well as defining

$$\tilde{t}_d = e^{2t_d} - 1, \qquad \tilde{b}_d = e^{2b_d} - 1 \tag{2.8}$$

we find that (2.5) becomes

$$\begin{aligned} z_d \tilde{G}_d(n_1, n_N) &- \sum_{n_k = -L}^{L} e^{-K_d |n_1 - n_k| - 2h_d n_k} \tilde{G}_d(n_k, n_N) \\ &- \tilde{t}_d e^{-K_d |n_1 - L| - 2h_d L} \tilde{G}_d(L, n_N) - \tilde{b}_d e^{-K_d |n_1 + L| + 2h_d L} \tilde{G}_d(-L, n_N) \\ &= \delta(n_1, n_N) \end{aligned} \tag{2.9}$$

One now has

$$\begin{aligned} Z_N^d(L, K_d, t_d, b_d, h_d; n_1, n_N) &= e^{-2h_d n_1} e^{2t_d \delta(n_1, L) + 2b_d \delta(n_1, L)} \\ &\times \frac{1}{2\pi i} \oint_C dz_d\, z_d^{N-1} \tilde{G}_d(L, K_d, t_d, b_d, h_d; n_1, n_N) \end{aligned} \tag{2.10}$$

Note that the $n_1 \leftrightarrow n_N$ symmetry in the partition function is no longer manifest.

We next perform some scalings. Let

$$\begin{gathered} K_c = K_d L, \quad h_c = h_d L, \quad n_1 = x_1 L, \quad n_N = x_N L, \quad n_k = yL \\ L^2 \tilde{G}_d(n_k, n_N) = G_c(y, x_N), \quad \tilde{t}_d = t_c L, \quad \tilde{b}_d = b_c L, \quad z_d = \frac{2}{K_c} z_c L \end{gathered} \tag{2.11}$$

The subscripts $c$ now denote the couplings for the continuum model. The extra factor in the $z_d$ scaling has nothing to do with the continuum limit, but is for later convenience. These scalings are uniquely determined by the requirement that they lead to a nontrivial continuum limit for (2.9).

One can now take the continuum limit, $L \to \infty$. In this limit we use the identification for the sole remaining Kronecker delta

$$\lim_{L \to \infty} L\delta(x_1 L, x_N L) = \delta(x_1 - x_N) \tag{2.12}$$

where the right-hand side is a Dirac delta function. This identification seems natural, as

$$1 = \frac{1}{L} \sum_{n_k = -L}^{L} L\delta(x_k L, x_N L) = \int_{-1}^{1} \delta(y - x_N)\, dy \tag{2.13}$$

Identifying the continuum partition function $Z_N^c$ via

$$\begin{aligned} &Z_N^c(K_c, t_c, b_c, h_c; x_1, x_N) \\ &\quad = \lim_{L \to \infty} \frac{1}{L^{N-2}} Z_N^d\left(L, \frac{K_c}{L}, \frac{1}{2}\log(1 + t_c L), \frac{1}{2}\log(1 + b_c L), \frac{h_c}{L}; x_1 L, x_N L\right) \end{aligned} \tag{2.14}$$

and finally taking $L \to \infty$ in (2.9) and (2.10), one obtains the partition function for the continuum string model,

$$\begin{aligned} &Z_N^c(K_c, t_c, b_c, h_c; x_1, x_N) \\ &\quad = \left(\frac{2}{K_c}\right)^N e^{-h_c x_1} \frac{1}{2\pi i} \oint_C z_c^{N-1} G_c(K_c, t_c, b_c, h_c; x_1, x_N)\, dz_c \end{aligned} \tag{2.15}$$

where $G_c$ satisfies the inhomogenous integral equation

$$\begin{aligned} &\int_{-1}^{1} dy\, e^{-K_c|x_1 - y| - 2h_c y} G_c(y, x_N) + t_c e^{-K_c(1 - x_1) - 2h_c} G_c(1, x_N) \\ &\quad + b_c e^{-K_c(x_1 + 1) + 2h_c} G_c(-1, x_N) - \frac{2z_c}{K_c} G_c(x_1, x_N) = -\delta(x_1 - x_N) \end{aligned} \tag{2.16}$$

This derivation has been formal. In order to perform a more satisfactory derivation, one could try to make the above argument more rigorous. A more satisfactory procedure would be to obtain the discrete partition function directly and take the continuum limit for this expression. We have been able to do this in the case $t_d = b_d$, $h_d = 0$. We found that the resulting partition function for the continuum model was equal to that obtained by solving the continuum integral equation derived above only if $x_1$ or

$x_N \neq \pm 1$, $\pm(1-1/L)$, or $\pm(1-2/L)$. Viewing $Z_N^c$ as a function of $(x_1, x_N)$, we thus find a boundary layer around the edges of the domain $\{(x_1, x_N)\colon -1 \leqslant x_1 \leqslant 1, -1 \leqslant x_N \leqslant 1\}$. Because of this we shall restrict our considerations to $\{(x_1, x_N)\colon -1 < x_1 < 1, \ -1 < x_N < 1\}$. It will transpire that the partition function obtained is well defined as $x_1, x_N \to \pm 1$. We shall thus define the partition function on the boundaries of the boundary configuration space via this limit.

## 3. THE GREEN'S FUNCTION

The integral equation (2.16) can be readily converted to the following boundary value problem:

$$\begin{aligned}\frac{\partial^2 G_c}{\partial x_1^2} &- K_c^2\left(1 - \frac{1}{z_c} e^{-h_c x_1}\right) G_c(x_1, x_N)\\ &= \frac{K_c}{2z_c}\left[\frac{\partial^2 \delta(x_1 - x_N)}{\partial x_1^2} - K_c^2 \delta(x_1 - x_N)\right]\\ &= \frac{K_c}{2z_c}\left(\frac{\partial^2}{\partial x_N^2} - K_c^2\right)\delta(x_1 - x_N)\end{aligned} \tag{3.1}$$

where the boundary conditions are

$$\frac{\partial G_c}{\partial x_1}(1, x_N) = K_c\left(\frac{K_c t_c}{z_c} e^{-h_c} - 1\right) G_c(1, x_N) \tag{3.2a}$$

$$\frac{\partial G_c}{\partial x_1}(-1, x_N) = K_c\left(1 - \frac{K_c b_c}{z_c} e^{h_c}\right) G_c(-1, x_N) \tag{3.2b}$$

To obtain (3.1), one divides the integration range in (2.16) into $\int_{-1}^{x_1} + \int_{x_1}^{1}$, differentiates twice with respect to $x_1$, and uses (2.16) in the resulting expression. To obtain the first (second) boundary condition one differentiates (2.16) and adds (subtracts) to (from) it $K_c \times (2.16)$. One then takes $x_1 \to (-)1$ in the resulting expression. The delta functions that appear in the boundary conditions do not contribute, since we are only considering $-1 < x_1, x_N < 1$ according to the strategy for handling the boundary layer outlined in the previous section.

Here we note an advantage of the Green's function method. The eigenvalue problem for the transfer matrix would have been identical to the above boundary value problem except that the inhomogenity in (3.1) would be absent. The eigenfunction series for the partition function [obtained by substituting (1.5) into (1.4) and evaluating the contour integral by residues] requires normalized eigenfunctions. The Green's function evaluation, which is only marginally more complicated than the eigenvalue problem, allows one to avoid calculating normalization integrals.

If one defines a new function $\tilde{G}_c$ as

$$G_c(x_1, x_N) = \frac{K_c}{2z_c}\left(\frac{\partial^2}{\partial x_N^2} - K_c^2\right)\tilde{G}_c(x_1, x_N) \tag{3.3}$$

then the boundary value problem for $\tilde{G}_c$ becomes a special case of the general boundary value problem for the Sturm–Liouville Green's function on $[a, b]$,

$$\frac{d}{dx}\left[p(x)\frac{du}{dx}\right] + q^2(x)\,u(x) = \delta(x-y) \tag{3.4}$$

$$\left(\frac{du}{dx} - \gamma_a u\right)\bigg|_{x=a} = 0 \tag{3.5a}$$

$$\left(\frac{du}{dx} - \gamma_b u\right)\bigg|_{x=b} = 0 \tag{3.5b}$$

whose solution, obtained by standard methods (see, e.g., ref. 7), is

$$u(x, y) = \frac{1}{p(y)\,W\{u_1(x), u_2(x)\}_y\,(F^< - F^>)}\begin{cases} u^<(y)\,u^>(x) & y < x < b \\ u^>(y)\,u^<(x) & a < x < y \end{cases} \tag{3.6}$$

where

$$\begin{aligned} u^<(x) &= u_1(x) - F^< u_2(x) \\ u^>(x) &= u_1(x) - F^> u_2(x) \\ F^< &= \frac{u_1'(a) - \gamma_a u_1(a)}{u_2'(a) - \gamma_a u_2(a)} \\ F^> &= \frac{u_1'(b) - \gamma_b u_1(b)}{u_2'(b) - \gamma_b u_2(b)} \end{aligned} \tag{3.7}$$

and where $u_1(x)$ and $u_2(x)$ are linearly independent solutions of the homogeneous differential equation.

Once $\tilde{G}_c$ is obtained, $G_c$ is readily obtained from (3.3) by using the fact that $\tilde{G}_c$ also satisfies the differential equation as a function of $x_N$. In fact, the differential operator in (3.3) is equivalent to multiplication by a simple factor. Some simple algebraic manipulation then gives us the general solution for the partition function.

$$\begin{aligned} &Z_N^c(K_c, t_c, b_c, h_c; x_1, x_N) \\ &\quad = -4\left(\frac{2}{K_c}\right)^{N-3} e^{-h_c(x_1 + x_N)}\,\frac{1}{2\pi i}\oint_C dz_c\, z_c^{N-3} G_c(K_c, t_c, b_c, h_c; x_1, x_N) \end{aligned} \tag{3.8}$$

where

$$G_c(x_1, x_N) = \frac{1}{W\{u_1(x), u_2(x)\}} \left\{ \frac{u_1(x_1)\, u_1(x_N)}{F^< - F^>} + \frac{F^< F^>}{F^< - F^<} u_2(x_1)\, u_2(x_N) \right.$$
$$- \frac{u_1(x_1)\, u_2(x_N) + u_2(x_1)\, u_1(x_N)}{2} \frac{F^< + F^>}{F^< - F^>}$$
$$\left. \mp \frac{u_1(x_1)\, u_2(x_N) - u_2(x_1)\, u_1(x_N)}{2} \right\} \tag{3.9}$$

where the upper sign is for $x_1 > x_N$ and the lower sign is for $x_N > x_1$ [for our purposes this form of the Green's function is clearer that the usual form (3.6)]. The general solution displays the following properties: (i) $x_1 \leftrightarrow x_N$ symmetry is once again manifest; (ii) $u_1 \leftrightarrow u_2$ symmetry (i.e., labeling of the linearly independent solutions); and (iii) $u_i \to \mu u_i$ symmetry (i.e., the result is independent of the normalization chosen for the linearly independent solutions).

One can solve (3.1) subject to (3.2) in terms of Bessel functions leaving $Z_N^c$ in the form of a contour integral. The analysis of the resulting contour integral is quite difficult. In this paper we shall limit ourselves to Smith's model, which involves the much simpler case $h_c = 0$. The $h_c \neq 0$ case is the subject of current investigations.

## 4. FINITE-SIZE PARTITION FUNCTION AND LEE–YANG POLYNOMIALS

When $h_c = 0$ the homogeneous analog of (3.1) is readily solvable. We choose, as linearly independent solutions, $u_1(x) = \cosh qx$ and $u_2(x) = \sinh qx$, where $q = K_c(1 - 1/z)^{1/2}$. The principal branch of the square root function is taken (i.e., $\sqrt{z} \equiv |z|^{1/2} e^{i\theta/2}$, where $z = |z|\, e^{i\theta}$ with $-\pi < \arg z \leqslant \pi$). Using the general formula (3.9), we find that

$$Z_N^c(K_c, t_c, b_c, 0; x_1, x_N) = 2\left(\frac{2}{K_c}\right)^{N-3} \frac{1}{2\pi i} \oint_c dz\, z^{N-3} \left(\frac{A + B + C}{\Delta} + D\right) \tag{4.1}$$

where

$$\begin{aligned} \Delta &= \{q^2(\gamma_{-1} - \gamma_1) \cosh 2q + (q^2 - \gamma_{-1}\gamma_1)\, q \sinh 2q\} \\ A &= (q^2 + \gamma_{-1}\gamma_1) \cosh q(x_1 + x_N) \\ B &= q(\gamma_1 + \gamma_{-1}) \sinh q(x_1 + x_N) \\ C &= \cosh q(x_1 - x_N)\{(q^2 - \gamma_1\gamma_{-1}) \cosh 2q + q(\gamma_{-1} - \gamma_1) \sinh 2q\} \\ D &= \mp \frac{\sinh q(x_1 - x_N)}{q} \end{aligned} \tag{4.2}$$

The integrand, despite the appearance of the square roots, is manifestly meromorphic, as required by (1.5). This would not have been so obvious had we used $u_1(x)=e^{qx}$ and $u_2(x)=e^{-qx}$. While we can, in principle, consider the case of different couplings to the top and the bottom, as well as vary the (fixed) endpoints of the string, we shall now restrict ourselves to Smith's case, i.e., $b_c=t_c=a_c$, $x_1=x_N=1$. The more general case is the subject of current investigations.

In Smith's case the partition function simplifies to

$$Z_N^c(K_c, a_c, a_c, 0; 1, 1)$$
$$= 2\left(\frac{2}{K_c}\right)^{N-2} \frac{1}{2\pi i}\oint_c dz\, z^{N-3} \frac{(q+\gamma)\, e^{2K_c q} + (q-\gamma)\, e^{-2K_c q}}{(q+\gamma)^2\, e^{2K_c q} - (q-\gamma)^2\, e^{-2K_c q}} \tag{4.3}$$

where $q=(1-1/z)^{1/2}$, $\gamma=1-a/z$, and $a=a_c/a_c^{\text{crit}}=K_c a_c$. As we discussed in the introduction, the model, as it stands, does not display a phase transition. One can now see why from a mathematical point of view. The integrand above is meromorphic and thus the contour integral can be done as a sum of poles. The positions of the poles, in particular the position of the largest pole (which dominates in the thermodynamic limit in the usual way), are analytic functions of the coupling $a$. However, when one takes $K_c \to \infty$ one obtains a much simpler object (it is here and in subsequent manipulations where the contour integral representation is much more flexible than the eigenfunction representation). We define the partition function in this limit as

$$Z_N(a) = \lim_{K_c \to \infty} K_c^{N-2} Z_N^c(K_c, a_c, a_c, 0; 1, 1) = 2^{N-1} f_N(a) \tag{4.4}$$

Then

$$f_N(a) = \frac{1}{2\pi i}\oint_c dz\, z^{N-3} \frac{1}{(1-1/z)^{1/2}+1-a/z} \tag{4.5}$$

It is clear that the eigenvalue spectrum, being essentially that of a Schrödinger operator on an unbounded domain, condenses to form a cut together with, for large coupling, a bound state. As the (real) coupling $a$ decreases past the critical value, the bound state "sticks" to the leading edge of the continuum. The nonanalytic behavior of the leading eigenvalue is the mechanism of the phase transition. We will have more to say about this mechanism in Section 5.

One also has a polynomial representation

$$f_N(a) = \sum_{n=0}^{N-2} b_n^N a^n \tag{4.6}$$

where

$$b_n^N = \left(\frac{1}{2}\right)^{N-n-2} \binom{2N-n-3}{N} \frac{n+1}{2N-n-3} \tag{4.7}$$

Equations (4.6) and (4.7) are derived as follows: using the identity for $\sum_{n=0}^{N} x^n$, one can derive

$$\frac{1}{(1-1/z)^{1/2}+1-a/z} = \frac{1}{(1-1/z)^{1/2}+1} \left\{ \sum_{n=0}^{M-1} \frac{a^n}{z^n[(1-1/z)^{1/2}+1]^n} \right\} + \frac{a^M}{z^M[(1-1/z)^{1/2}+1]^M} \frac{1}{(1-1/z)^{1/2}+1-a/z} \tag{4.8}$$

Substitute this identity into the integrand of (4.5) and then choose a circular contour of radius $R$. The last term of (4.8) gives a contribution to the integrand of (4.5) which behaves as $z^{N-M-3}$ as $z \to \infty$. Choose the radius $R$ so that the contour is in the region where the Laurent expansion of this contribution converges. Then, if $M \geqslant N-1$, evaluation of the contour integral gives zero, thus yielding that the partition function is a polynomial in $a$. One also has that

$$b_n^N = \frac{1}{2\pi i} \oint_c dz\, z^{N-n-3} \frac{1}{[(1-1/z)^{1/2}+1]^{n+1}} \tag{4.9}$$

This integral can be evaluated in the same manner as the remainder term, except that now the Laurent expansion of the integrand has a $1/z$ term, thus yielding a nonzero result. To obtain the Laurent expansion we use the result [see ref. 15, 2.8(6), p. 101]

$$\left[1+\left(1-\frac{1}{z}\right)^{1/2}\right]^{-n-1} = \left(\frac{1}{2}\right)^{n+1} F\left(\left(\frac{n}{2}+\frac{1}{2}\right), \left(\frac{n}{2}+1\right); n+2; \frac{1}{z}\right) \tag{4.10}$$

where $F$ is Gauss' hypergeometric function. The standard power series representation for this function yields, after some simplification, (4.7).

A polynomial representation for the finite-size partition function is of course the classic Lee–Yang description. It provides a wonderfully intuitive way of describing how the phase transition can arise. However, for large $N$ it is not a good representation for the purposes of calculating the zeros. We have found that it is possible to evaluate the zeros of the polynomial numerically up to $N \approx 100$ using `NSolve` in *Mathematica*.[16] In fact we were pleasantly surprised that we were able to go this far with relative ease. The zeros are shown in Fig. 2. To evaluate the zeros for higher $N$, one must use a more convenient representation of the $f_N(a)$. In fact, it is convienient to use the integral representation (4.5) directly. This is done in Section 5.

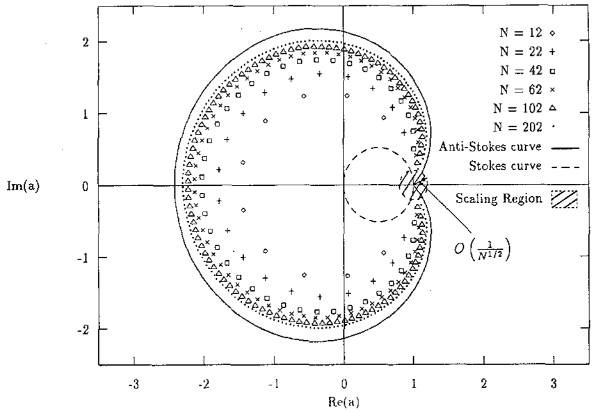


Fig. 2. Features of the partition function (1.1) as $K_c \to \infty$, as a function of the complex variable $a = K_c a_c$. The points are Lee–Yang zeros for various values of $N$.

In closing this section, we remark that there are in fact very many representations which can be derived from (4.5). By rationalizing the denominator of the integrand and evaluating a pole term (when present; see Section 5), one can show that

$$\begin{aligned}\left(\frac{1}{2}\right)^{N-1} & (2a-1) f_N(a) \\ &= \left(\frac{1}{a}-1\right)\left(\frac{a^2}{2a-1}\right)^{N-1} + \frac{1}{2\pi i}\oint_c dz\, z^{N-1} \frac{(1-1/z)^{1/2}}{z-a^2/(2a-1)} \\ &= \left(\frac{1}{a}-1\right)\left(\frac{a^2}{2a-1}\right)^{N-1} \\ &\quad + (-1)^{N-1}\binom{1/2}{N-1} F\left(-N+1, 1; \frac{3}{2}-N+1; \frac{a^2}{2a-1}\right) \end{aligned} \tag{4.11}$$

Once again the contour integral is evaluated via Laurent expansion of the integrand. One obtains a finite sum, corresponding to the truncated binomial series which can be expressed in terms of a hypergeometric function [see ref. 15, 2.8(8), p. 101]. Using the myriad transformations of the hypergeometric function, one can derive many, many different representations. One can also derive the representation

$$f_N(a) = -\frac{1}{\pi}\left(\frac{a^2}{2a-1}\right)^{N-1} \sum_{n=1}^{N-2} \left(\frac{2a-1}{a^2}\right)^n \frac{B(n+1/2, 3/2)}{a^2} + \frac{1}{2}\left(\frac{a^2}{2a-1}\right)^{N-2} \tag{4.12}$$

where $B(a, b)$ is the beta function, by noting that $f_N(a)$ satisfies a linear first-order inhomogeneous difference equation in $N$ and solving this equation using standard techniques (see ref. 7, p. 39). It is not immediately clear whether any of these representations have any special utility, either conceptually or numerically. While it may be possible that there are indeed useful representations hidden among the large collection derivable from (4.11), we choose to take a more direct approach, which we now describe.

## 5. THERMODYNAMIC LIMIT AND STOKES PHENOMENON VIEWPOINT

In order to observe the phase transition as arising from a Stokes phenomenon and to obtain the Lee–Yang zeros for $N > 100$, we now consider the asymptotic evaluation of the partition function as $N \to \infty$, i.e., the thermodynamic limit. In the contour integral representation

$$\frac{1}{2\pi i} \oint_c dz\, z^{N-1} \frac{(1-1/z)^{1/2} - (1-a/z)}{(2a-1)\, z - a^2} \tag{5.1}$$

the analytic structure of the integrand is clear. There is a pole at $z = a^2/(2a-1)$ and a branch cut from 0 to 1. Because of the $z^{N-1}$ factor, it is clear that as $N \to \infty$, the part of the integrand near $z = 1$ will dominate asymptotically. Thus the asymptotic expansion can be done by collapsing the contour onto the cut and evaluating the resulting (ordinary) integral via Watson's lemma (though this is not the approach we will be taking). The important point is the contribution of the pole. The numerator of the fraction in the integrand of (5.1) evaluated at the pole is

$$\left[\left(\frac{a-1}{a}\right)^2\right]^{1/2} + \frac{a-1}{a} = \begin{cases} 2\dfrac{a-1}{a}, & \operatorname{Re}\left(\dfrac{a-1}{a}\right) > 0 \\ 0, & \operatorname{Re}\left(\dfrac{a-1}{a}\right) < 0 \end{cases} \tag{5.2}$$

where care needs to be taken in evaluating the square root. $\operatorname{Re}((a-1)/a) = 0$ is a circle in the complex $a$ plane of radius 1/2 centered at (1/2, 0). If the complex coupling $a$ lies inside the circle, the asymptotic evaluation yields only the integral around the cut. If $a$ lies outside the circle, then one picks up the pole term as well. Since the pole contribution is "born" on crossing this circle, we will refer to it as a "Stokes curve." We shall elaborate on this terminology later. It is convenient to perform a conformal transformation of the coupling plane,

$$b = 1 - 1/a \tag{5.3}$$

In the complex $b$ plane the Stokes curve becomes a Stokes line, $\mathrm{Re}(b)=0$. It is also convenient to change the variable of integration to $w=1-1/z$. This maps the cut onto the usual square root branch cut. One obtains

$$a^2 f_N(a)=\frac{1}{2\pi i}\oint_c \frac{dw}{(1-w)^N}\frac{\sqrt{w-1+a(1-w)}}{w-b^2} \tag{5.4}$$

After collapsing the contour onto the cut, one obtains

$$a^2 f_N(a)=\frac{2b\Theta(\mathrm{Re}(b))}{(1-b^2)^N}+\frac{1}{\pi}\int_0^\infty \frac{dt}{(1+t)^N}\frac{\sqrt{t}}{t+b^2} \tag{5.5}$$

where $\Theta(x)$ is the usual Heaviside function. One can evaluate the integral in terms of the hypergeometric function [see ref. 15, 2.12(5), p. 115] to obtain another representation, no doubt related to Eq. (4.11).

By setting $t=x/N$, the $N\to\infty$ limit of (5.5) becomes

$$a^2 f_N(a)=\begin{cases}\dfrac{2b}{(1-b^2)^N}+\dfrac{1}{(\pi N)^{1/2}}\,[1-W(b\sqrt{N})]\left[1+O\left(\dfrac{1}{N}\right)\right], & \mathrm{Re}(b)>0\\[2ex] \dfrac{1}{(\pi N)^{1/2}}\,[1-W(-b\sqrt{N})]\left[1+O\left(\dfrac{1}{N}\right)\right], & \mathrm{Re}(b)<0\end{cases} \tag{5.6}$$

where $W(z)=\sqrt{\pi}\, z e^{z^2}\operatorname{erfc}(z)$. This is an asymptotic expansion which is uniformly valid in the coupling (away from the Stokes curve). To proceed further analytically (in particular with regard to the calculation of asymptotic expressions for the Lee–Yang zeros in the next section), we define

$$\tau=b\sqrt{N} \tag{5.7}$$

and *also* take $\tau\to\infty$. $\tau=O(1)$ corresponds to $a-1=O(1/N^{1/2})$. As will become clearer in the Section 7, this is the scaling region (see also Fig. 2). The resulting double asymptotic expansion should thus be a good approximation for $N$ large and for the complex coupling constant outside the scaling region. In the thermodynamic limit the scaling region shrinks. In order to have a uniform approximation to the partition function, one must not neglect this region.

To obtain the double asymptotic expansion, we rewrite (5.5) as

$$\frac{a^2 f_N(a)}{2b}=\frac{\Theta(\mathrm{Re}(b))}{(1-b^2)^N}+\frac{1}{\tau^3}I(N,\tau^2) \tag{5.8}$$

where

$$I(N, \tau^2) = \frac{\tau^2}{2\pi} \int_0^\infty dx \left(1 + \frac{x}{N}\right)^{-N} \frac{\sqrt{x}}{x + \tau^2} \tag{5.9}$$

We approach the double asymptotic expansion of (5.8) by first evaluating the asymptotic expansion in $\tau^2$ with $N$ fixed. This is easily done by expanding $1/(x + \tau^2)$ using the geometric series and then doing the $x$ integrals using 6.2.1 of ref. 17 to obtain

$$I(N, \tau^2) = \frac{\alpha(N)}{4\sqrt{\pi}} \left[1 + \sum_{n=1}^{\infty} \left(\frac{-1}{\tau^2}\right)^n \frac{\Gamma(n + 3/2)}{\Gamma(3/2)} \beta(N, n)\right] \tag{5.10}$$

where

$$\begin{aligned} \alpha(N, n) &= N^{n+3/2} \frac{\Gamma(N - n - 3/2)}{\Gamma(N)} \\ \beta(N, n) &= \frac{\alpha(N, n)}{\alpha(N, 0)} \end{aligned} \tag{5.11}$$

To obtain the double asymptotic expansion, we then substitute the asymptotic expansions in $N$ for $\alpha(N)$ and $\beta(N, n)$,

$$\begin{aligned} \alpha(N) &= 1 + \frac{15}{8N} + \frac{385}{128N^2} + O\left(\frac{1}{N^3}\right) \\ \beta(N, n) &= 1 + \frac{n(4 + n)}{2N} + \frac{n(47 + 72n + 28n^2 + 3n^3)}{24N^2} + O\left(\frac{1}{N^3}\right) \end{aligned} \tag{5.12}$$

Before using the above to describe the phase transition from the Stokes phenomenon viewpoint, let us first make contact with the Lee–Yang viewpoint. From (5.8) and (5.10) the free energy is readily calculated to be

$$-\beta f = \lim_{N \to \infty} \frac{1}{N} \ln Z_N^c = \begin{cases} \ln 2, & |1/(1 - b^2)| < 1 \\ \ln 2 - \ln(1 - b^2)' & |1/(1 - b^2)| > 1 \end{cases} \tag{5.13}$$

The curve $|1/(1 - b^2)| = 1$ is the anti-Stokes curve (see Fig. 2). Again we shall explain the terminology below. Thus, the free energy has two analytic forms inside and outside the anti-Stokes curve. It is plausible from the $N \lesssim 100$ calculations of the Lee–Yang zeros in Section 4 that what we have called the anti-Stokes curve is the curve on which the Lee–Yang zeros condense in the thermodynamic limit. One can also see that in regions free of zeros the free energy is analytic. This is in line with standard theorems in Lee–Yang theory.[1]

Now onto the Stokes phenomenon interpretation. Looking at the form of the free energy, Eq. (5.13), one can say that the phase transition occurs due to the birth of the $-\ln(1-b^2)$ term as one crosses the anti-Stokes line. Our calculation shows that the "birth" of this term is a little more complicated. It comes from the Stokes phenomenon in the asymptotic evaluation of the partition function. We found that the asymptotic form of the partition function had a different form inside and outside the Stokes curve. In particular, simplifying our result for the purposes of exposition, we found, outside the scaling region, the behavior

$$\frac{a^2 f_N(a)}{2b} = \frac{\Theta(\mathrm{Re}(b))}{(1-b^2)^N} + \frac{1}{4\sqrt{\pi}}\frac{1}{b^3 N^{3/2}}\left[1 + O\left(\frac{1}{N}\right) + O\left(\frac{1}{\tau^2}\right)\right] \tag{5.14}$$

where we have a pole contribution and an asymptotic series. In examining the $N \to \infty$ behavior of (5.14) there are, as is typical in functions displaying the Stokes phenomenon, two important curves: the Stokes curve $[\mathrm{Re}(b) = 0]$ and the anti-Stokes curve $[|1/(1-b^2)| = 1]$. The significance of the Stokes curve is that it is where the pole term first "appears." The important thing to note here is that at this point the pole term is subdominant, i.e., exponentially small with respect to all the terms in the dominant asymptotic series. As such one can essentially neglect it. (In the recent work of Berry and others[9] the Stokes phenomenon has been studied in certain classes of function and it has been shown that the subdominant term grows smoothly out of the error term of the asymptotic expansion of the dominant series over a region about the Stokes line. A similar behavior is expected in our function.) The pole term remains subdominant until one reaches the anti-Stokes curve. At this point the pole term is of similar order as the series. Beyond the anti-Stokes curve the pole term is dominant and the series can essentially be neglected. This change in asymptotic behavior ($N \to \infty$) of a function as one changes a control parameter ($b$) is typical of the Stokes phenomenon and occurs in many special functions (where one looks at the $|z| \to \infty$ behavior as one changes arg $z$[8]). Thus, the origin of the form (5.13) in a Stokes phenomenon for the contour integral should be clear. The only thing that remains is to explain why the Lee–Yang zeros, in the limit $N \to \infty$ fall on the anti-Stokes curve. From the previous discussion we have that

$$\frac{a^2 f_N(a)}{2b} \underset{N \to \infty}{\widetilde{\quad}} \begin{cases} \dfrac{1}{(1-b^2)^N}, & \left|\dfrac{1}{1-b^2}\right| > 1 \\[2ex] \dfrac{1}{4\sqrt{\pi}}\dfrac{1}{N^{3/2} b^3}, & \left|\dfrac{1}{1-b^2}\right| < 1 \end{cases} \tag{5.15}$$

Both functional forms do not have zeros. However, near the anti-Stokes curve (and on it in the $N \to \infty$ limit) the two terms of the asymptotic expansion are of the same order and thus can balance, generating zeros of the partition function.

## 6. LEE-YANG ZEROS FOR LARGE $N$

We now calculate asymptotic expressions for the Lee–Yang zeros from the double series (5.10). This series allows us to find those zeros for which $\tau^2$ is large as $N \to \infty$.

In order to evaluate the zeros, rewrite (5.8) as a sum of two exponentials $e^f + e^g = 2e^{(f+g)/2} \cos[(f-g)/2i]$. (We assume, here and henceforth, that $N$ is even. The $N$-odd case can be treated similarly.) Then perform (another) conformal transformation of the coupling plane,

$$-e^{i\theta} = \frac{1}{1-b^2}, \qquad -\pi < \mathrm{Re}(\theta) \leqslant \pi, \qquad -\infty < \mathrm{Im}(\theta) < \infty \tag{6.1}$$

so that the zeros are given by the implicit equation

$$\theta - \theta_0 = \frac{i}{N} \log \frac{\tau^3}{I(N, \tau^2)} \tag{6.2}$$

where $\theta_0(n) = 2(n + 1/2)\pi/N$, $n = 0, \pm 1, \pm 2, \ldots$. The restrictions in (6.1) ensure that the transformation is 1–1. Looking at (6.2), one might be tempted to take $\theta_0$ as a first approximation. The conditions on the real and imaginary parts of $\theta$ in (6.1) constrain us to only take a finite number of solutions. Applying this condition to $\theta_0$ gives $N$ zeros. However, the polynomial representation tells us that there are in fact only $N-2$ zeros. At this point reference to the qualitative information from the polynomial representation helps us to avoid a trap we might otherwise have fallen into. Why are there extra zeros? Well, we only expect that the asymptotic expansion will yield a good approximation outside the scaling region. We thus only expect some of the zeros it generates to be reliable.

In fact, we find, somewhat miraculously (although this is in fact a common miracle; cf. zeros of Bessel functions, etc.) that upon calculating higher-order terms the asymptotic expansion generated provides a good approximation for all of the zeros. How can this be the case? Well, for large $N$ the asymptotic series (5.10) is typical in that it is a sum of terms $a_n \approx \Gamma(n)/\tau^{2n}$. By forming $a_{n+1}/a_n$, one can easily see that the terms in the asymptotic expansion decrease until $n = \tau^2$ and then increase. Stopping at the minimum terms yields an error which is exponentially small.[8,9] Thus one expects that the asymptotic representation will be good down to, say, $\tau^2 = 5$ provided one takes sufficient terms. In Fig. 3 we plot the Lee–Yang zeros as a function of $\tau$(in this diagram the $N \to \infty$ limit is the scaling limit; these zeros are calculated in the next section). It is reasonably clear from this plot that the smallest zero has a value of $\tau^2$, which is large enough ($\approx 7$) for the asymptotic series to still be useful. Furthermore, for the extra zero the higher-order corrections to the asymptotic expansion have the effect of shifting $\mathrm{Re}(\theta)$ in the positive sense by a term $O(1/N)$. In fact the zero is shifted outside the range $-\pi < \mathrm{Re}(\theta) \leqslant \pi$ and thus violates the single-valuedness condition on the conformal transformation. Let us now see all this in detail.

Iterating (6.2) is quite tedious, as is trying to get the $O(1/N)$ correction out of the right hand side, grouping it with $\theta_0$, and then iterating. After a number of attempts, we settled on the following strategy to solve (6.2) asymptotically in $N$ and $\tau^2$. There are aspects of this stategy which we still find unsatisfactory. However, we are in the fortunate position of having some exact results (from the solution of the Lee–Yang polynomial) with which to compare. As a result we are able to develop reasonable confidence in our strategy, its primary virtue being the ability to systematically generate higher-order terms in the double asymptotic expansion. This procedure has been automated using *Mathematica*. Define $\delta$ by

$$\theta - \theta_0 = \frac{i}{N}\delta \tag{6.3}$$

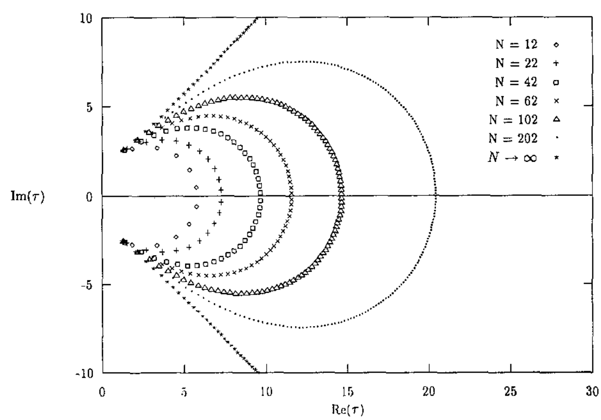


Fig. 3. The exact zeros and the scaled partition function zeros in the complex $\tau$ (scaled coupling) plane. $N \to \infty$ is the scaling limit. $\tau = b\sqrt{N}$, $b = 1 - 1/a$.

Then (6.2) can be written as $\delta = f(\tau^2, N)$. We now Taylor expand $f$ about $\theta_0$. As $\theta - \theta_0$ is small as $N \to \infty$, we expect that this expansion will converge quickly. Defining

$$\begin{aligned} c_1 &= -\frac{i}{N}\frac{d}{d\theta} f(\tau^2, N)\bigg|_{\theta=\theta_0} + 1 \\ c_n &= \frac{i}{Nn}\frac{d}{d\theta} c_{n-1}(\tau^2, N)\bigg|_{\theta=\theta_0}, \qquad n \geqslant 2 \end{aligned} \tag{6.4}$$

where $\tau_0 = \tau(\theta_0)$ and $d_n = c_n/c_1$, one obtains

$$\frac{f(\tau_0^2, N)}{c_1} = \delta + d_2\delta^2 + d_3\delta^3 + \cdots \tag{6.5}$$

This series can be readily inverted to obtain

$$\delta = g\left(\frac{3\log[(16\pi)^{1/3}\tau_0^2]}{2a_1} - d_0\right) \tag{6.6}$$

where $g(x) = x - d_2x^2 - (2d_2^2 - d_3)\,x^3 + \cdots$ and we have separated out the log term. After some tedious, but straightforward algebra one can obtain

$$\begin{aligned} \delta = {} & \frac{-15}{8N} + \frac{3}{2\tau_0^2} + \frac{15}{4N\tau_0^2} - \frac{45e^{-i\theta_0}}{16N\tau_0^2} + \frac{3\log[(16\pi)^{1/3}\tau_0^2]}{2} \\ & + \frac{9e^{-i\theta_0}\log[(16\pi)^{1/3}\tau_0^2]}{4\tau_0^2} + O\left(\frac{(\log\tau_0^2)^2}{\tau_0^4}\right) + O\left(\frac{1}{N^2}\right) \end{aligned} \tag{6.7}$$

**Table I. A Sample of the $N = 102$ Zeros and the Asymptotic Approximation to Them, to Various Orders**

| $n$ | $\theta_{0,0}$ | $\theta_{1,1}$ | $\theta_{2,2}$ | Exact |
|---|---|---|---|---|
| 0 | 0.030799 | $0.031026 + 0.097408i$ | $0.031038 + 0.098017i$ | $0.031038 + 0.098034i$ |
| 1 | 0.092399 | $0.093079 + 0.097394i$ | $0.093114 + 0.098003i$ | $0.093114 + 0.098020i$ |
| 2 | 0.154000 | $0.155132 + 0.097367i$ | $0.155190 + 0.097974i$ | $0.155191 + 0.097991i$ |
| 3 | 0.215599 | $0.217185 + 0.097325i$ | $0.217266 + 0.097931i$ | $0.217267 + 0.097949i$ |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |
| 45 | 2.802793 | $2.823402 + 0.071229i$ | $2.826176 + 0.070759i$ | $2.826358 + 0.070881i$ |
| 46 | 2.864393 | $2.885455 + 0.068301i$ | $2.888671 + 0.067586i$ | $2.888919 + 0.067740i$ |
| 47 | 2.925993 | $2.947508 + 0.064624i$ | $2.951362 + 0.063530i$ | $2.951730 + 0.063736i$ |
| 48 | 2.987593 | $3.009561 + 0.059690i$ | $3.014436 + 0.057928i$ | $3.015069 + 0.058212i$ |
| 49 | 3.049193 | $3.071613 + 0.052187i$ | $3.078452 + 0.048897i$ | $3.079947 + 0.049251i$ |
| 50 | 3.110793 | $3.133666 + 0.036036i$ | $3.146158 + 0.025273i$ | $3.079947 + 0.049252i$ |

**Table II. A Sample of the $N=202$ Zeros and the Asymptotic Approximation to Them, to Various Orders**

| $n$ | $\theta_{0,0}$ | $\theta_{1,1}$ | $\theta_{2,2}$ | Exact |
|---|---|---|---|---|
| 0 | 0.015552 | $0.015610+0.054261i$ | $0.015611+0.054435i$ | $0.015611+0.054438i$ |
| 1 | 0.046657 | $0.046831+0.054259i$ | $0.046835+0.054433i$ | $0.046835+0.054436i$ |
| 2 | 0.077762 | $0.078051+0.054256i$ | $0.078059+0.054430i$ | $0.078059+0.054432i$ |
| 3 | 0.108867 | $0.109271+0.054250i$ | $0.109283+0.054424i$ | $0.109283+0.054427i$ |
| ⋮ | ⋮ | ⋮ | ⋮ | ⋮ |
| 95 | 2.970516 | $2.981545+0.035993i$ | $2.982925+0.035622i$ | $2.983006+0.035682i$ |
| 96 | 3.001621 | $3.012765+0.034506i$ | $3.014366+0.034017i$ | $3.014479+0.034094i$ |
| 97 | 3.032726 | $3.043986+0.032643i$ | $3.045907+0.031969i$ | $3.046077+0.032073i$ |
| 98 | 3.063832 | $3.075205+0.030146i$ | $3.077643+0.029144i$ | $3.077941+0.029290i$ |
| 99 | 3.094935 | $3.106426+0.026354i$ | $3.109858+0.024595i$ | $3.110580+0.024779i$ |
| 100 | 3.126040 | $3.137647+0.018196i$ | $3.143963+0.012695i$ | $3.110580+0.024779i$ |

Having obtained the zeros via solution of the polynomial up to $N=102$, we can now compare these (essentially exact) zeros with various orders of the asymptotic expansion. We shall denote by $\theta_{a,b}$ the asymptotic expansion obtained where one neglects terms of order $((\log \tau_0^2)/\tau_0^2)^a$ and $(1/N)^b$. The comparison for $N=102$ is made in Table I. (Note: In Fig. 2 the $n=0$ zero is the first zero in the lower half-plane near the negative real axis. $n$ increases clockwise to the scaling region.) One obtains similar agreement for $N=62, 82$. We thus expect the asymptotic formulas to provide similar agreement for $N>100$. For $N>100$ we were unable to readily generate the roots of the polynomial equation. We believe the cause of this to be cancellation error. Naturally we would still prefer to be able to calculate these zeros exactly. The contour integral representation provides an alternative. For $N>100$ one can obtain the exact zeros by evaluating (5.5) numerically and calculating the zeros using the secant method starting from $\theta_{1,1}$ and $\theta_{2,2}$ (using `FindRoot` in *Mathematica*). We verified this method by using it to reproduce the $N=102$ zeros. The comparision of the asymptotic approximations and the exact results for $N=202$ is done in Table II. In Tables I and II we can also see that the extra zeros in the lowest order approximation are artifacts (the "phantom" zeros in each case iterating to the last zero).

## 7. FINITE-SIZE SCALING LIMIT

The basic hypothesis of finite-size scaling, in the context of the model studied here, is that one can introduce a finite-sized scaling variable

$$a_s = N^q \left( \frac{a - a_c^{\text{crit}}}{a_c^{\text{crit}}} \right) \tag{7.1}$$

for some exponent $q$, such that the limit

$$Z^s(a_s) = \lim_{N \to \infty} \frac{Z_N^c(a_c^{\text{crit}}[1 + a_s N^{-q}])}{Z_N^c(a_c^{\text{crit}})} \tag{7.2}$$

exists independently of $N$. The renormalization group argument for this hypothesis suggests that this choice is unique and that if an incorrect choice is made, then the above limit will not exist or will be trivial. The finite-size scaling limit reveals universal features of critical phenonmena (see, e.g., refs. 18 and 10).

Using (4.5), we can readily determine $q$ and the scaled partition function. In order to obtain a nontrivial limit as $N \to \infty$, it is clear that one requires $z = 1 + z_s/N$, so that $z^N \to e^{z_s}$. For the rest of the integrand to have a nontrivial limit, one must choose $q = 1/2$. This leads to

$$Z^s(a_s) = \frac{1}{2\sqrt{\pi}\, i} \oint_c dz_s \frac{e^{z_s}}{\sqrt{z_s - a_s}} \tag{7.3}$$

$$= 1 + a_s \sqrt{\pi}\, w(-ia_s) \tag{7.4}$$

where $w(z) = e^{-z^2} \operatorname{erfc}(-iz)$ (see ref. 17, 7.1.3). This agrees with Eq. (3.18) of Smith. We can also make contact with the asymptotic expansion of the previous section by expressing (5.6) totally in terms of $\tau$ and taking $N \to \infty$. One obtains

$$\frac{a^2 f_N(a)}{2b} \sim \Theta(\text{Re}(\tau))\, e^{\tau^2} + \frac{1}{4\sqrt{\pi}\, \tau^3}\, \Omega(\tau) \tag{7.5}$$

where $\Omega(z)$ is defined in terms of $w(z)$ and has the asymptotic limit

$$\Omega(\tau) \sim \sum_{m=0}^{\infty} \frac{1 \cdot 3 \cdot \cdots \cdot (2m+1)}{(-2\tau^2)^m} \tag{7.6}$$

These two expressions for the scaling limit agree because $\lim_{N \to \infty} \tau = a_s$.

We now calculate the zeros of the scaled partition function. As in the previous section, we can only progress analytically by solving for the zeros of the above equation as $\tau \to \infty$. Unlike the previous section, the calculation is considerably simpler because we only have one variable in which to expand. Smith performed this calculation, but his technique only allowed him to calculate to low order. We now present a technique which is able systematically to generate higher-order terms. We restrict ourselves to $\text{Re}(\tau) > 0$, as the imaginary axis is a Stokes line and the zeros lie in this half-plane. Using an argument similar to that used in the previous section, one finds that the zeros are the solutions of

$$\tau^2 = \tau_0^2(n) - 3 \log \tau + \log \Omega(\tau) \tag{7.7}$$

**Tale III. The First Few Scaling Zeros in the Upper $\tau$ Plane Together with Their Asymptotic Approximations**

| $n$ | Zeroth order | First order | Second order | Exact |
|---|---|---|---|---|
| 0 | $0.933674 + 1.692381i$ | $-0.039277 + 1.725930i$ | $-0.462563 + 1.851437i$ | $-19.50610 + 78.53459i$ |
| 1 | $1.957995 + 2.406742i$ | $1.279570 + 2.560480i$ | $1.197948 + 2.613446i$ | $1.225157 + 2.547128i$ |
| 2 | $2.633529 + 2.982303i$ | $2.049431 + 3.161082i$ | $2.013677 + 3.201256i$ | $2.025596 + 3.161939i$ |
| 3 | $3.171714 + 3.466761i$ | $2.642843 + 3.652385i$ | $2.622692 + 3.684430i$ | $2.628872 + 3.655972i$ |
| 4 | $3.632040 + 3.892348i$ | $3.141689 + 4.079199i$ | $3.128857 + 4.105702i$ | $3.132351 + 4.083384i$ |
| 5 | $4.040688 + 4.276192i$ | $3.579584 + 4.462104i$ | $3.570805 + 4.484621i$ | $3.572849 + 4.466301i$ |
| 6 | $4.411858 + 4.628515i$ | $3.974124 + 4.812570i$ | $3.967831 + 4.832095i$ | $3.969017 + 4.816595i$ |

where $\tau_0(n) = [2(n+\frac{1}{2})\,\pi i - \frac{1}{2}\log 16\pi]^{1/2}$. This equation implies that $\tau \to \tau_0$ as $\tau \to \infty$. One cannot solve this equation asymptotically by iteration because the right-hand side is not small as $\tau \to \infty$. One can overcome this problem by writing

$$\tau^2 + 3\log\tau = \left(\tau + \frac{3\log\tau}{2\tau}\right)^2 - \frac{9}{4}\left(\frac{\log\tau}{\tau}\right)^2 \tag{7.8}$$

to transform (7.7) to

$$\tau - \tau_0 = -\frac{3\log\tau}{2\tau} - \frac{3}{4\tau_0\tau^2} + \frac{9}{8\tau_0}\left(\frac{\log\tau}{\tau}\right)^2 + O\left(\frac{1}{\tau_0\tau^4}\right) \tag{7.9}$$

where the positive square root is taken, ensuring that $\mathrm{Re}(\tau) > 0$ asymptotically. This equation can now be solved asymptotically by iteration to yield

$$\tau = \tau_0 - \frac{3\log\tau_0}{2\tau_0} - \frac{9(\log\tau_0)^2}{4\tau_0^3} + \frac{9\log\tau_0}{4\tau_0^3} + O\left(\frac{1}{\tau_0^3}\right) \tag{7.10}$$

We show in Table III the first six zeros in the upper half-plane together with the predictions of the asymptotic formula to various orders of iteration. As in the previous section, the lowest order asymptotic expansion predicts an extra zero in the region of interest $[\mathrm{Re}(\tau) > 0]$, whereas higher-order terms move this zero out of the right half-plane, thus rendering it a phantom zero (Smith concluded that this was a phantom zero when he was unable to find it numerically). Again as in the previous section, the asymptotic formula is able to reproduce all zeros to a good approximation. The exact zeros are obtained as in the previous section (though here Newton's method is used). In Fig. 3 we plot the zeros in the complex scaled coupling plane $\tau$. We also plot the exact zeros for various $N$ in the same variable. One can thus see how the scaling limit is approached. Also in the above argument there is no guarantee that we have recovered all the scaling zeros (i. e., strictly speaking, we would need to check at small values of $\tau$ where the asymptotic expansion is not valid). This plot makes it reasonably clear that we have indeed recovered all the scaling zeros.

## 8. DISCUSSION

The Lee–Yang and Stokes phenomenon viewpoints can be seen to be quite complementary. They each have their own particular utility. The Lee–Yang picture provides a good representation of the partition function for relatively small $N$ as well as giving the exact number of zeros. The contour integral representation provides a good representation for large $N$, but generates "phantom" zeros if one is not careful. In the Lee–Yang picture it is clear why a polynomial representation exists (a hard-core potential provides a cutoff in the grand partition function). In our model it is not clear why a polynomial representation arises. In fact, had we not had the Lee–Yang picture, we probably would not have found the polynomial representation.

The contour integral representation makes it very clear as to why the zeros form on curves in the coupling plane. This fact is something that the Lee–Yang picture cannot explain. Indeed they comment in the concluding remarks of their paper that they are surprised that the zeros of their polynomial should have such regular patterns. From the discussion at the end of Section 5 it is clear that the zeros lie on curves because they result from the asymptotic balance of two contributions, the bound state and the continuum. In fact with this viewpoint one can look at some of the numerical results in the literature with a different perspective. For example Pearson's[3,10] calculation of the temperature zeros for the 3D Ising model clearly suggests four different regions of the complex plane in which the partition function has a different analytic form. This is clearly a much more complicated Stokes phenomenon, strongly suggesting that in the thermodynamic limit there are four contributions to the partition function. One can imagine that a meaningful phenomenology could be attempted. We should point out that although in many cases zeros seem to form on lines in the thermodynamic limit, there are some models where they form more complicated patterns, for example, the anisotropic Ising model, where they form in areas,[20],[2] and also hierarchical models, where they form self-similar patterns.[21] It is clear that the mechanism for zero generation discussed above has no direct relevance to these examples.

The Lee–Yang and Stokes phenomenon viewpoints only provide a characterization of a phase transition. That is, they describe the function-theoretic features present in the thermodynamic functions of systems exhibiting phase transitions. They do not give sufficient and necessary conditions on the Hamiltonian, the dimensionality, and the symmetry of the system for the presence of such features. In the model we have described, however, the mechanism by which the phase transition arises is quite clear. Examining this mechanism allows us to recast the question, "Why do phase transitions occur?" As we described in Section 1, the model investigated here is essentially two dimensional ($N \times K_c$). The Green's function for the finite system is meromorphic. As one of the dimensions goes to infinity ($K_c$), the Green's function becomes double-valued, the cut arising

[2] We are grateful to a referee and J. M. Luck for pointing out this example, and to P. J. Forrester for assistance in finding the references.

from the coalescence of eigenvalues. Furthermore, there is a bound state. When the coupling lies outside the Stokes circle, the bound state is on the "physical sheet" (i.e., the sheet on which the contour lies). If it lies inside the Stokes circle, the bound state is on the second ("unphysical") sheet. It is the motion of the bound state that causes the Stokes phenomenon and thus the phase transition. It is fairly natural that the eigenvalues should form a continuum in the $K_c \to \infty$ limit. However, it is less clear as to why one state should split off from the continuum and remain discrete. It is this property which is the mechanism for the phase transition. Thus in the context of the model studied here the question, "Why is there a phase transition?," can be rephrased, "Why do bound states occur?" The usual, qualitiative, answer to both questions is that "cooperative" or "coherent" behavior occurs. In fact, within quantum scattering theory (see, e.g., ref. 19) there exist a number of bounds, calculable in terms of the potential, on the number of bound states, so that there is some understanding of how bound states occur.

We would also like to point out that we expect that the mechanism outlined above is probably quite common. In ref. 2 (pp. 141, 243) a suggestion of Kac is described in which a phase transition occurs if the largest eigenvalue is asymptotically degenerate below the critical temperature and strictly nondegenerate above the critical temperature. This viewpoint is another way of stating that the leading eigenvalue either joins the continuum or splits off as a bound state according to the value of the coupling. Also, we state above that the Green's function becomes double-valued in the $K_c \to \infty$ limit. This is not strictly true. In this limit the Green's function remains meromorphic, but varies rapidly in the vicinity of the cut. However, the double-valuedness remains if we undertake the following procedure. First consider a domain of the complex plane excluding a sufficiently large neighborhood of the eigenvalues. Then take $K_c \to \infty$ limit. Follow this with an analytic continuation. Under such a procedure the Green's function becomes double-valued. Also, the fact that there is only one bound state in our model is a consequence of the use of zero-range potentials for the sticking. The zero-range potentials manifest themselves through mixed boundary conditions (3.2).

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