

The Yang–Lee Edge Singularity in One-Dimensional Ising and N -Vector Models

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Received July 22, 1982

The distribution of zeros of the partition function in the complex magnetic field plane is studied for linear chains of n -vector spins and finite-width strips of Ising spins with nearest-neighbor interactions. By means of transfer matrix/operator techniques, the exponent σ characterizing the behavior of the density of zeros near the Yang–Lee edge is shown to have the exact value $\sigma = -1/2$ (i) analytically for n -vector chains in the high-temperature limit and for Ising strips in the low-temperature limit, and (ii) numerically for intermediate temperatures. The crossover of σ from its n -vector value to its spherical model value, $\sigma = 1/2$, as $n \rightarrow \infty$, as well as from $d = 1$ to $d = 2$ Ising as the width of the strips increases, seems to proceed by an accumulation of branch points in the spectrum of the transfer operator; for the n -vector models the position of the gap edge and the free energy at the edge approach their spherical model values with corrections of order $1/n^\zeta$ with $\zeta \approx 3/4$.

KEY WORDS: Yang–Lee zeros; complex magnetic field; one-dimensional models; transfer operators.

1. INTRODUCTION

A number of exactly solvable statistical mechanical models are provided by one-dimensional systems. Unfortunately, a one-dimensional system with short-range interactions will not, in general, display a phase transition,⁽¹⁾ so that these models are of limited interest in the study of ordinary critical behavior. On the other hand, Yang–Lee edge singularities generally do occur in these models; in fact, the nature of the edge singularity is known exactly for the ferromagnetic Ising⁽²⁾ and spherical model⁽³⁾ chains. In

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these models the zeros of the partition function concentrate, in the thermodynamic limit of an infinitely large system, along the imaginary axis of the reduced magnetic field plane,

$$h = H/k_B T = h' + ih'' \quad (1)$$

where H is the applied magnetic field in energy units, k_B is Boltzmann's constant, and T is the absolute temperature. In the limit, a density of zeros, $g(h'')$, may be defined, so that as N , the number of spins in the system, becomes infinite, the number of zeros lying in the infinitesimal interval between ih'' and $i(h'' + dh'')$ becomes asymptotically equal to $Ng(h'')dh''$. For any temperature $T > 0$, there is a gap on the imaginary axis, with edges at $\pm ih_0(T)$, within which the density of zeros vanishes; near the edges of the gap $g(h'')$ displays a power law variation,⁽⁴⁾

$$\begin{aligned} g(h'') &\sim [|h''| - h_0(T)]^\sigma & \text{for } |h''| \rightarrow h_0(T) + \\ &= 0 & \text{for } |h''| < h_0(T) \end{aligned} \quad (2)$$

where the exponent σ has the value $-1/2$ in the Ising chain⁽²⁾ and $+1/2$ for the spherical model.⁽³⁾

Indeed it is shown in Ref. 5 that the result $\sigma = -1/2$ follows for a general one-dimensional system from a simple hypothesis concerning the spectrum of the system's transfer matrix. It is known⁽⁶⁾ that zeros of the partition function may only occur in the thermodynamic limit in regions in which no single eigenvalue of the transfer matrix has largest modulus, i.e., where two or more eigenvalues share this modulus. Moreover, for a general class of Ising systems this is known to occur^(7,8) only along a set of analytic arcs in the appropriate complex field plane, even if the zeros are not confined to the imaginary axis; this criterion has been employed by several authors^(9,10) to locate the zero density for a number of models. The conclusion $\sigma = -1/2$ follows⁽⁵⁾ specifically from the further assumption that in an imaginary reduced magnetic field, $h = ih''$ (in the models we will consider, the zeros are to be found here), the transfer matrix or operator has a *single* eigenvalue of largest modulus for $|h''| < h_0(T)$, while for $|h''| \gtrsim h_0(T)$ the *two* largest eigenvalues have equal moduli and all others are smaller in magnitude, so that $h = \pm ih_0(T)$ are branch points in the spectrum at which the two dominant eigenvalues—and no others—merge. The purpose of the present work is to check the validity of this assumption for two interesting classes of systems.

Since the spherical model represents the infinite-component limit of an isotropically coupled n -vector spin model,⁽¹¹⁻¹³⁾ it is of interest to investigate the dependence of the exponent σ on n .⁽¹⁴⁾ However, renormalization group arguments⁽¹⁴⁾ indicate that σ will be *independent* of n for finite n ; this

is also known to be true for lattice models with nearest-neighbor interactions in the asymptotic high-temperature limit.⁽¹⁵⁾ In order to investigate this, we have examined ferromagnetic n -vector chains, consisting of L n -dimensional unit vector spin variables $\mathbf{s}_i = (s_i^{(1)}, s_i^{(2)}, \dots, s_i^{(n)})$, interacting through the Hamiltonian

$$\mathcal{H} = -nJ \sum_{i=1}^L \mathbf{s}_i \cdot \mathbf{s}_{i+1} - nH \sum_{i=1}^L s_i^{(1)} \quad (3)$$

where the exchange coupling J is positive and we identify $\mathbf{s}_{L+1} \equiv \mathbf{s}_1$. The factors of n are inserted to ensure that the thermodynamic free energy per spin component continues to exist in the spherical model limit $n \rightarrow \infty$. On setting $n = 1$, one recovers the spin-1/2 Ising chain. By numerically calculating the free energy per spin component in the thermodynamic limit $L \rightarrow \infty$, we find that $\sigma = -1/2$ describes the Yang–Lee edge singularity for *all* values of n and T examined. In addition, we find that the position of the Yang–Lee edge and the value of the free energy per spin component at the edge approach their spherical model values as $n \rightarrow \infty$ with corrections⁽⁵⁾ of order approximately $1/n^\zeta$ with $\zeta \cong 3/4$.

Numerical studies of the Yang–Lee edge singularity in the two-dimensional Ising model^(4,14–18) at temperatures above critical indicate that the value of σ in this model is not $-1/2$, but is appreciably higher. High-temperature series expansions give estimates⁽¹⁵⁾ near -0.163 , in good agreement with ϵ -expansion⁽¹⁶⁾ and phenomenological renormalization group⁽¹⁷⁾ estimates, (although real-space renormalization studies⁽¹⁸⁾ give estimates near -0.22 to -0.27). However, the two-dimensional model can be viewed as the infinite-width limit of Ising models on essentially one-dimensional lattices having finite width and infinite length. Since strong analogies exist between the Yang–Lee edge and an ordinary critical point,^(4,14) one would expect that the edge singularity for these finite-width models should always be given by the one-dimensional exponent $\sigma = -1/2$. We have investigated this point by examining Ising ferromagnets with nearest-neighbor interactions on $m \times \infty$ strips with periodic boundary conditions. That is, we consider an Ising lattice which may be viewed as a stack of L layers, where each layer is a ring of m spins, in the limit $L \rightarrow \infty$. The Hamiltonian is given by

$$\mathcal{H} = -J_{\parallel} \sum_{l=1}^L \sum_{j=1}^m s_{lj} s_{l+1,j} - J_{\perp} \sum_{l=1}^L \sum_{j=1}^m s_{lj} s_{l,j+1} - H \sum_{l=1}^L \sum_{j=1}^m s_{lj} \quad (4)$$

where we identify the spin variables $s_{l,m+1} \equiv s_{l,1}$ for each layer l and also $s_{L+1,j} \equiv s_{1,j}$. The couplings along the layering direction, J_{\parallel} , and normal to it, J_{\perp} , are positive. As will be seen below, the choice of periodic boundary

conditions within a layer, i.e., taking the layers to be closed rings, leads to a symmetry which affords a considerable simplification in the numerical calculation of the thermodynamic free energy. We find that the Yang–Lee edge singularity in these models for $m \leq 10$ is given by $\sigma = -1/2$ for temperatures ranging from 0.125 to 5 times the critical temperature of the two-dimensional Ising model with the same coupling strengths. We also show analytically that $\sigma = -1/2$ is the correct exponent for arbitrary finite widths m in the asymptotic low-temperature limit. From numerical analysis of the dependence of the position of the Yang–Lee edge and the free energy at the edge on m ,⁽⁵⁾ we conclude that these quantities approach their values in the two-dimensional Ising model with corrections of order $1/m^2$; such behavior has often been observed^(19,20) in models with periodic layer connections.

The next two sections contain our numerical methods and results for n -vector chains and Ising strips, respectively, together with arguments which go part way toward establishing in general, for these models, the assumption leading to $\sigma = -1/2$. In Section 4 we present further analytical results which show that the assumption is valid in certain limits. The results are recapitulated and discussed in Section 5.

2. NUMERICAL RESULTS FOR n -VECTOR MODELS

In order to investigate the nature of the Yang–Lee edge singularity in one-dimensional ferromagnetic n -vector chains with the Hamiltonian (3), we have numerically diagonalized the transfer operators for these models with an imaginary magnetic field of strength $nH = ink_B Th$. Although the zeros of the partition functions for these models are known to be confined to the imaginary field axis only for $n \leq 3$,⁽²¹⁾ we feel safe in assuming that this will be true for higher n as well. This assumption is borne out by the results of our calculations.

The linear operator which, for these systems, corresponds to the transfer matrix has the kernel

$$A(\mathbf{s}_l, \mathbf{s}_{l+1}) = c_n^{-1} \exp(K\mathbf{s}_l \cdot \mathbf{s}_{l+1} + h s_l^{(1)}) \quad (5)$$

where K is given by

$$K = J/k_B T \quad (6)$$

and

$$c_n = 2\pi^{n/2} / \Gamma(\frac{1}{2}n) \quad (7)$$

is the surface area of the n -dimensional unit sphere, which is the region of

integration. In zero field, this kernel has full n -dimensional spherical symmetry, and so the transfer operator can be diagonalized exactly⁽²²⁾ by means of the Funk-Hecke theorem.⁽²³⁾ The zero-field eigenfunctions are the n -dimensional spherical harmonics⁽²⁴⁾ $Y(l, m_1, \dots, m_{n-2}; \mathbf{s})$, which have $l \geq m_1 \geq \dots \geq m_{n-3} \geq |m_{n-2}|$; the corresponding eigenvalues depend only on l and are given by

$$\mu_l = (2/nK)^{n/2-1} \Gamma(\frac{1}{2}n) I_{n/2+l-1}(nK) \tag{8}$$

where $I_\nu(x)$ is the standard modified Bessel function.⁽²⁵⁾ The μ_l decrease with increasing l , and each has a degeneracy of

$$g_l^{(n)} = \frac{n+2l-2}{n+l-2} \binom{n+l-2}{l} \tag{9}$$

with $g_0^{(2)} = 1$; note that $g_l^{(n)}$ is just the number of spherical harmonics in n dimensions having the given value of l .

For the numerical work we expanded the field part of the integral kernel in spherical harmonics, thus converting the integral operator into an infinite matrix; the functions on which the operator acts are then represented by an infinite-dimensional vector whose elements are the coefficients in the spherical harmonic expansion of the function. (A similar technique has been developed for the case $n = 2$ by Patkos and Rujan.⁽²⁶⁾) The matrix elements $A_{l', m'_1, \dots, m'_{n-2}; l, m_1, \dots, m_{n-2}}$ vanish unless $m'_i = m_i$ for $i = 1, 2, \dots, n-2$, reflecting the fact that the kernel is still invariant under rotations of the axes of spin space which leave the direction of the magnetic field unchanged. In this case they are given by

$$A_{l', m_1; l, m_1} = \mu_{l'} \sum_{k=0}^{\infty} \langle l' m_1 | l m_1; k0 \rangle (2/nh'')^{n/2-1} \times \Gamma(\frac{1}{2}n-1) (\frac{1}{2}n+k-1) i^k J_{n/2+k-1}(nh'') \tag{10}$$

where $J_\nu(x)$ is the standard Bessel function⁽²⁵⁾ and the coefficients $\langle l' m_1 | l m_1; k0 \rangle$ arise from expanding the product of two Gegenbauer polynomials⁽²⁷⁾ in a series of Gegenbauer polynomials, namely,

$$C_{l_1-m_1}^{n/2+m_1-1}(x) C_{l_2-m_2}^{n/2+m_2-1}(x) = \sum_{l_3=m_3}^{l_1+l_2-m_1-m_2+m_3} \langle l_3 m_3 | l_2 m_2; l_1 m_1 \rangle C_{l_3-m_3}^{n/2+m_3-1}(x) \tag{11}$$

Using standard recursion relations for Gegenbauer polynomials⁽²⁷⁾ we find

that these coefficients are given in certain special cases by

$$\begin{aligned}
 \langle jm | km; l0 \rangle &= \delta_{jk} \quad \text{for } l = 0 \\
 &= \left[\frac{(n-2)}{(n+2k-2)} \right] \\
 &\quad \times \left[(k-m+1)\delta_{j,k+1} + (n+k+m-3)\delta_{j,k-1} \right] \quad \text{for } l = 1 \\
 &= (-1)^{(l+m-j)/2} \frac{\Gamma(\frac{1}{2}n+m-1)}{\Gamma(\frac{1}{2}n-1)} \\
 &\quad \times \frac{m!}{\left[\frac{1}{2}(l+m-j) \right]! \left[\frac{1}{2}(j+m-l) \right]!} \\
 &\quad \times \left(\frac{1}{2}n+j-1 \right) \frac{\Gamma\left[\frac{1}{2}(n+j+l-m)-1 \right]}{\Gamma\left[\frac{1}{2}(n+j+l+m) \right]} \quad \text{for } k = m
 \end{aligned} \tag{12}$$

where the arguments of the factorials must be nonnegative integers. The coefficients appearing in (10) are most conveniently calculated from these starting values, using the recursion relation

$$\begin{aligned}
 \langle jm | km; l0 \rangle &= \left[\frac{(\frac{1}{2}n+k-2)(j-m)}{(\frac{1}{2}n+j-2)(k-m)} \right] \\
 &\quad \times \langle j-1, m | k-1, m; l0 \rangle \\
 &\quad + \left[\frac{(\frac{1}{2}n+k-2)(n+j+m-2)}{(\frac{1}{2}n+j)(k-m)} \right] \\
 &\quad \times \langle j+1, m | k-1, m; l0 \rangle \\
 &\quad - \left[\frac{(n+k+m-4)}{(k-m)} \right] \langle jm | k-2, m; l0 \rangle \tag{13}
 \end{aligned}$$

which, incidentally, can be summed explicitly for $m = 0$ to give

$$\begin{aligned}
 \langle j0 | k0; l0 \rangle &= \frac{j!}{\left[\frac{1}{2}(j+k-l) \right]! \left[\frac{1}{2}(k+l-j) \right]! \left[\frac{1}{2}(l+j-k) \right]!} \\
 &\quad \times \left(\frac{1}{2}n+j-1 \right) \frac{\Gamma\left[n + \frac{1}{2}(j+k+l) - 2 \right]}{\Gamma(n+j-2)} \\
 &\quad \times \frac{\Gamma\left[\frac{1}{2}(n+j+k-l) - 1 \right] \Gamma\left[\frac{1}{2}(n+k+l-j) - 1 \right]}{\Gamma\left[\frac{1}{2}(n+l+j-k) - 1 \right]} \\
 &\quad \times \frac{1}{\left[\Gamma(\frac{1}{2}n-1) \right]^2 \Gamma\left[\frac{1}{2}(n+j+k+l) \right]} \tag{14}
 \end{aligned}$$

where the arguments of all factorials are nonnegative integers.

Note that the largest eigenvalue of the transfer matrix for *zero* field, μ_0 , corresponds to an eigenfunction having all azimuthal indices equal to zero.

Our numerical computations for $m = 0, 1$, and 2 indicate that this continues to hold for imaginary fields, at least up to the Yang-Lee edge. Accordingly, we expect that the dominant eigenfunction is always to be found among functions having full cylindrical symmetry about the magnetic field direction.

From (10) we see that every element in the l 'th row of any block of the matrix resolution of the transfer operator carries a factor μ_l . Since $I_\nu(x)$ decreases rapidly with increasing ν for fixed x , it suffices for numerical computations to retain only a rather small part of these infinite matrices. The largest eigenvalues of the $m_1 = 0$ and 1 blocks of the matrix for $n = 15$ spin components at $K = 0.5$ are plotted against h'' in Fig. 1; these eigenvalues were calculated by retaining 14 rows and columns of each block. The fractional change in the magnitudes of these eigenvalues when the number of rows and columns was doubled was at most 2%, and was as large as this only for the smallest eigenvalues displayed; the four largest eigenvalues changed by at most a part in 10^7 . The eigenvalues were also reasonably stable against small changes in the matrix elements. The value $K = 0.5$ corresponds to the mean field critical temperature T_0 of the model, defined by

$$k_B T_0 = \sum_j J_{ij} \quad (15)$$

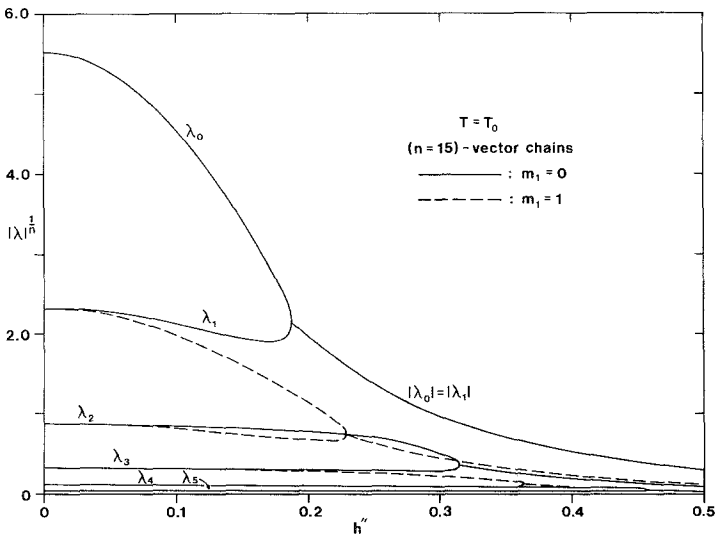


Fig. 1. Magnitudes of the largest eigenvalues λ_i of the $m_1 = 0$ and $m_1 = 1$ components of the transfer operator for the nearest-neighbor 15-vector chain at temperature $T = T_0$ in an imaginary magnetic field $nH = ink_B Th''$. The branch point at $h'' = h_0 \approx 0.187$ leads to a Yang-Lee edge singularity at $h'' = h_0$ with $\sigma = -1/2$.

where J_{ij} is the coupling strength between spins i and j . With our form of the Hamiltonian (3), this reduces to $T_0 = 2J/k_B$ for arbitrary n .

The most important feature of Fig. 1, for our purposes, is the square root branch point in the spectrum at $h'' \approx 0.187$, at which the two largest eigenvalues meet and become complex conjugates. As pointed out above, this branch point represents the Yang–Lee edge, and the merging of the two largest eigenvalues leads to an edge singularity with exponent $\sigma = -1/2$. Other eigenvalues then meet in pairs at higher values of h'' , their moduli remaining below that of the dominant eigenvalues. These features appeared in all cases for which calculations were carried out, including values of n in the range 2 to 60 and temperatures ranging from $\frac{1}{2}T_0$ to $2T_0$. Thus we see that the Yang–Lee edge singularity is given by $\sigma = -1/2$ for these models.

In fact if no eigenvalues of the transfer operator become complex *before* the largest does, then it follows that the largest eigenvalue merges only with the second largest and so $\sigma = -1/2$. To see this, let the eigenvalues of the azimuthally symmetric component of the transfer operator be $\lambda_0(h''), \lambda_1(h''), \dots$ in order of decreasing magnitude, and suppose that all of the λ_i are real for $h'' < h_0(T)$, where λ_0 (at least) becomes complex at $h_0(T)$. The eigenvalues are the zeros of the Fredholm determinant,

$$D(h'', \lambda) = \prod_{i \geq 0} [\lambda - \lambda_i(h'')] \quad (16)$$

Taking the derivative of this with respect to h'' and setting $\lambda = \lambda_0(h'')$ yields

$$\left. \frac{\partial D}{\partial h''} \right|_{\lambda=\lambda_0(h'')} = - \left(\frac{d\lambda_0}{dh''} \right) \prod_{i \geq 1} (\lambda_0 - \lambda_i) \quad (17)$$

Since $\lambda_0(h'')$ is the largest eigenvalue, it must have a negative derivative in a domain in which it meets another real eigenvalue; since we are assuming that all eigenvalues are real for $h'' < h_0(T)$, this first branch point must lie in a region of the (h'', λ) plane in which $(\partial D / \partial h'')$ is positive. However, we also have

$$\left. \frac{\partial D}{\partial h''} \right|_{\lambda=\lambda_1(h'')} = \left(\frac{d\lambda_1}{dh''} \right) (\lambda_0 - \lambda_1) \prod_{i \geq 2} (\lambda_1 - \lambda_i) \quad (18)$$

$$\left. \frac{\partial D}{\partial h''} \right|_{\lambda=\lambda_2(h'')} = - \left(\frac{d\lambda_2}{dh''} \right) (\lambda_0 - \lambda_2) (\lambda_1 - \lambda_2) \prod_{i \geq 3} (\lambda_2 - \lambda_i) \quad (19)$$

so that the second largest eigenvalue, λ_1 , is increasing near the branch point as expected; however, the third largest eigenvalue, λ_2 , is smaller than λ_1 and must be decreasing when $(\partial D / \partial h'') > 0$. Thus only λ_1 can reach λ_0 as

h'' varies; hence the Yang-Lee edge singularity has $\sigma = -1/2$. Unfortunately, although the zero-field eigenvalues μ_l are known to be real and positive, we have not succeeded in showing that all eigenvalues are real for $h'' < h_0(T)$, so that a complete proof that $\sigma = -1/2$ is always the correct exponent for these models is still lacking. Nonetheless, the numerical evidence points to the conclusion that the Yang-Lee edge singularity for these one-dimensional n -vector models is characterized by $\sigma = -1/2$ for all finite n and at all temperatures $T > 0$.

The lack of dependence of σ on n is at first quite surprising, since the spherical model, which represents the infinite-component or $n \rightarrow \infty$ limit of the classical n -vector models,⁽¹¹⁻¹³⁾ has a different edge singularity than the finite n models, namely,⁽³⁾ $\sigma = +1/2$ rather than $\sigma = -1/2$. However, we can see how this singularity builds up as n grows by considering the positions of the branch points in the spectrum of the transfer operator in the $(h'', n^{-1} \ln \lambda)$ plane.⁽⁵⁾ These become closer to one another as n increases (as illustrated in Fig. 4 of Ref. 5), and in the spherical model limit we should expect to see infinitely many eigenvalues coalescing at the Yang-Lee edge to give the correct singularity. If $h_0^{(n)}(T)$, the position of the edge for fixed n and T , and $f_0^{(n)}(T)$, the reduced free energy at the edge,

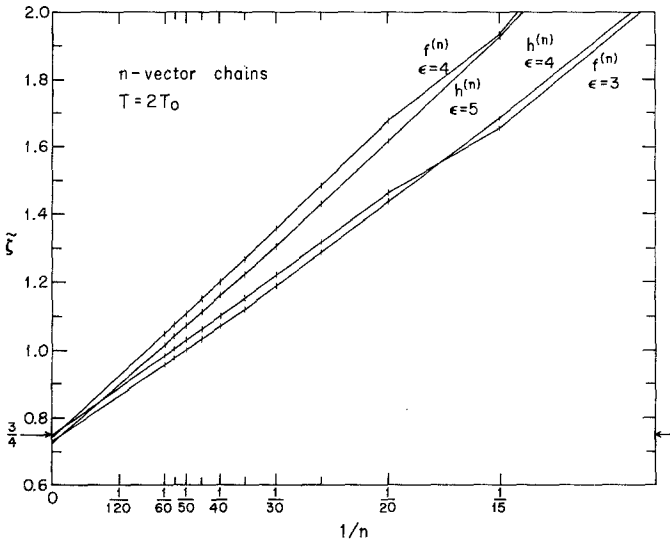


Fig. 2. Approximants $\tilde{z} = -(n + \epsilon)(a_n - a_{n-1}) / (a_n - a_\infty)$ to the exponent characterizing the approach of the Yang-Lee edge for an n -vector chain to its position in the spherical model, for $a_n = h_0^{(5n)}$ and $a_n = f_0^{(5n)}$ at a temperature $T = 2T_0$. The n -shift ϵ is varied in order to reduce the curvature of the plots.

approach their spherical model values with corrections of order $1/n^\zeta$, we may use methods similar to the ratio test⁽²⁸⁾ to estimate the exponent ζ . Thus for $K = 0.25$ we have plotted the approximants $-(n + \epsilon)(a_n - a_{n-1}) / (a_n - a_\infty)$ against $1/n$ in Fig. 2, for $a_n = h_0^{(5n)}$ and $a_n = f_0^{(5n)}$. These approximants should approach a limiting value ζ as $n \rightarrow \infty$. The n -shift, ϵ , has been varied in an attempt to reduce the curvature of the ratio plots. We conclude that

$$\zeta = 0.73 \pm 0.03 \quad (20)$$

represents the data fairly well for $K = 0.25$. Similar analyses for $K = 0.5$ ($T = T_0$) and $K = 1.0$ ($T = \frac{1}{2} T_0$) confirm this result; the values of $h_0^{(5n)}$ and $f_0^{(5n)}$ are tabulated in Ref. 29. Note that higher-order analytic corrections to the behavior of $h_0^{(n)}$ and $f_0^{(n)}$ can cause large amounts of curvature in the ratio plots. For example, $1/n$ terms in the expansion of $h_0^{(n)}$ for large n would give rise to terms of order $n^{-1+\zeta} \approx n^{-1/4}$ in the approximants; such terms decay only very slowly as n grows, and so make extrapolation difficult.

3. NUMERICAL RESULTS FOR ISING MODELS

A program of calculation similar to that for the n -vector chains has been carried out for ferromagnetic $m \times \infty$ Ising strips with the Hamiltonian (4). For these models, zeros of the partition function are known to lie only on the imaginary magnetic field axis⁽²⁾; consequently, we take $H = ik_B Th$ purely imaginary. The task of numerically diagonalizing the transfer matrices for these models is greatly simplified by the symmetry which arises from the choice of periodic boundary conditions within a layer. Specifically, if the spins in layer l are labeled $s_{l1}, s_{l2}, \dots, s_{lm}$ as in (4), then the interactions within and between layers l and $l + 1$ are unchanged if, for both layers, the spin indices are cyclically permuted, $(1, 2, \dots, m) \rightarrow (2, 3, \dots, m, 1)$, or inverted, $(1, 2, \dots, m) \rightarrow (m, m - 1, \dots, 1)$. It follows that the transfer matrix can be block diagonalized by choosing the states of a layer to be those linear combinations of the basic spin configurations (defined by specifying the value of each spin in the layer) which transform according to the irreducible representations of the corresponding symmetry group. Only the matrix elements between states belonging to the same representation can be nonzero.⁽³⁰⁾

Now note that when the magnetic field is real, the Fröbenius–Perron theorem⁽³¹⁾ tells us that a single, nondegenerate eigenvalue of the transfer matrix will have a greater modulus than any other. Furthermore, this dominant eigenvalue will be real and will correspond to an eigenvector having only positive components. The nondegeneracy of the eigenvalue

implies that its eigenvector transforms according to a one-dimensional representation of the symmetry group of the system. In such a representation, the group elements must be represented by the complex roots of unity, so that applying any symmetry operation to the dominant eigenvector yields the same vector multiplied by a root of unity. However, the operations of cyclically permuting or inverting spin labels merely exchange components of the eigenvector, thus producing a vector having only positive components. Since this new vector must be the old eigenvector multiplied by a root of unity, that root must be $+1$. In other words, the dominant eigenvalue in real fields corresponds to an eigenvector which is *invariant* under any symmetry of the Hamiltonian which only interchanges spins.

One can also see that the dominant eigenvector in an imaginary field also belongs to the fully invariant representation of the symmetry group in both the high- and low-temperature limits, as we now show. Both the state with all spins “up” and that with all spins “down” belong to this representation; any state in any other representation must have both up and down spins. Thus in the low-temperature limit, the ratio of the largest noninvariant eigenvalue to the largest invariant one must vanish at least as quickly as $\exp(-J_{\perp}/k_B T)$.

In the high-temperature limit the $m \times \infty$ strip behaves as a collection of m independent one-dimensional chains. The eigenvalues of the transfer matrix for a single chain are given by

$$\lambda_{\pm} = \exp(K) \left\{ \cosh h \pm \left[\sinh^2 h + \exp(-4K) \right]^{1/2} \right\} \quad (21)$$

with

and so the eigenvalues for the strip are $\lambda_+^k \lambda_-^{m-k}$ for $k = 0, 1, \dots, m$, each having degeneracy $m!/k!(m-k)!$. The largest invariant eigenvalue is λ_+^m , which is nondegenerate, and so the largest noninvariant eigenvalue is $\lambda_+^{m-1} \lambda_-$, which is smaller in magnitude for $h'' < h_0(T)$. Accordingly, we will assume that this continues to hold at intermediate temperatures, and so seek the dominant eigenvector of the transfer matrix among vectors which are invariant under cyclic permutations and inversions of spin labels.

Numerically, this simplification is enormous. For an $m \times \infty$ strip, the full transfer matrix has dimension 2^m , while that part of it connecting vectors which are invariant under cyclic permutations only has a dimension given by

$$d_m = \sum_{k|m} b_k \quad (23)$$

where the sum runs over all divisors of m (including 1 and m), while b_k is the number of configurations of a layer of $k \geq 1$ spins which are *not* reproduced by cyclically permuting the spins by less than k places. The b_k can be defined and calculated from the identities

$$\sum_{l|k} lb_l = 2^k \quad \text{for each } k \geq 1 \quad (24)$$

so that

$$b_1 = 2, \quad b_2 = 1, \quad b_3 = 2, \quad b_4 = 3, \quad b_5 = 6, \quad b_6 = 9, \quad \text{etc.} \quad (25)$$

$$d_1 = 2, \quad d_2 = 3, \quad d_3 = 4, \quad d_4 = 6, \quad d_5 = 8, \quad d_6 = 14, \quad \text{etc.} \quad (26)$$

These identities follow from the fact that each configuration of a layer of k spins enters into exactly one cyclically invariant combination, which also contains contributions from the $l - 1$ distinct configurations obtained by permuting it by $1, 2, \dots, l - 1$ places if the configuration is reproduced by permuting it by l places. Such a state may be viewed as consisting of k/l copies of a configuration of an l -spin layer. Classifying the various configurations of a layer of k spins by respective values of l leads to (24).

For $m \geq 6$, the requirement of invariance under inversions further reduces the size of the matrix to be diagonalized. For example, for $m = 8$ the full transfer matrix has dimension $2^8 = 256$ and we find $d_8 = 36$, but when inversion symmetry is included the dimension of the invariant part of the matrix is only 30. Similarly, for $m = 9$ the dimension of the matrix to be diagonalized is reduced from 512 to 46, and for $m = 10$ from 1024 to 78.

Figure 3 shows the dependence of the magnitudes of the eigenvalues of the transfer matrix on the imaginary field, $h = ih''$, for the $4 \times \infty$ strip with $J_{\parallel} = J_{\perp} \equiv J$. The temperature is chosen to be $T = 2T_{c,2}$, where $T_{c,2}$ is the critical temperature of the two-dimensional Ising model with the same coupling strengths, given for this isotropic case by

$$T_{c,2} = T_0 / \left[2 \ln(\sqrt{2} + 1) \right] \cong 0.56731 T_0 \quad (27)$$

where T_0 , the mean field critical temperature defined by (15), is $T_0 = 4J/k_B$. The important features of this plot are much the same as those of Fig. 1: the two largest eigenvalues meet at a square root branch point at $h'' = 0.078\pi$, giving rise to a Yang-Lee edge singularity with $\sigma = -1/2$; the other eigenvalues merge in pairs at higher values of h'' . The ranges $0.287\pi \lesssim h'' \lesssim 0.293\pi$ and $0.495\pi \lesssim h'' \lesssim 0.505\pi$, in which the two dominant eigenvalues are again real and unequal, correspond to gaps in the zero density with square root ($\sigma = -1/2$) singularities on either side; however,

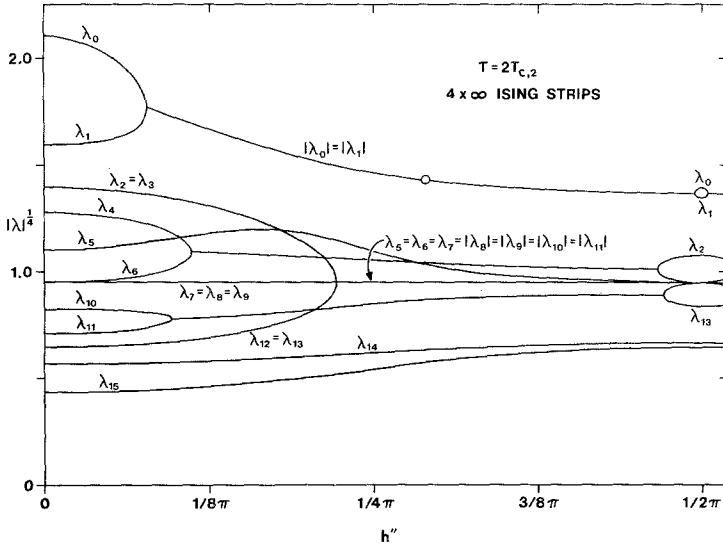


Fig. 3. Magnitudes of the eigenvalues of the transfer matrix for the $4 \times \infty$ Ising strip with periodic layer connections at a temperature $T = 2T_{c,2}$ in an imaginary magnetic field $H = ik_B Th''$. The eigenvalues which, for small h'' , are labelled $\lambda_0, \lambda_1, \lambda_5, \lambda_{10}, \lambda_{11}$, and λ_{15} belong to the invariant representation of the symmetry group.

we are more interested in the branch points closest to the real h'' axis. There are two pair of degenerate eigenvalues and one set of three degenerate eigenvalues plotted, so that all 16 eigenvalues of the transfer matrix in fact appear on the figure. These degenerate eigenvalues are among those which belong to noninvariant representations of the symmetry group; their degeneracy is due in particular to the inversion symmetry described above.

Our numerical calculations confirm that the same salient features—the two largest eigenvalues meeting at some value of h'' , with other pairs coming together at higher values of h'' —appear for all values of the parameters we have examined. Specifically, we have calculated the eigenvalues of the invariant block of the transfer matrix for strips of width $m \leq 10$ at temperatures in the range $0.125T_{c,2} \leq T \leq 5T_{c,2}$, with couplings J_{\parallel} and J_{\perp} not necessarily equal.

Note that the argument of Section 2, to the effect that if all eigenvalues are real for h'' less than its value $h_0(T)$ at the Yang-Lee edge, then the edge singularity is given by $\sigma = -1/2$, is still valid here, with the Fredholm determinant replaced by the secular determinant of the invariant block of the transfer matrix. Again, we have not succeeded in showing that all eigenvalues are real for $h'' < h_0(T)$ and so have not proven that $\sigma = -1/2$ is correct; however, on the basis of our numerical evidence we expect that

$\sigma = -1/2$ characterizes the edge singularity for ferromagnetic $m \times \infty$ Ising strips in general.

If we let the width m of the strip become infinite,⁽⁵⁾ the value of σ must cross over to that appropriate to the two-dimensional Ising model. As in the spherical model limit of the n -vector chains, this appears to happen by means of a coalescence of infinitely many branch points in the eigenvalue spectrum as $m \rightarrow \infty$. (This is illustrated for m up to 10 in Fig. 2 of Ref. 5 and Fig. 3.5 of Ref. 29.) The buildup of the two-dimensional singularity may be analyzed⁽⁵⁾ using finite-size scaling ideas,⁽¹⁹⁾ namely, that the position of the Yang-Lee edge, $h_0^{(m)}(T)$, and the value of the reduced free energy at the edge, $f_0^{(m)}(T) = m^{-1} \ln \lambda_0[T, h_0^{(m)}(T)]$, should differ from their infinite- m limits by amounts of order $1/m^\theta$. The value of the exponent θ should be $1/\nu_c$, where ν_c is the exponent describing the divergence of the correlation length at the Yang-Lee edge in the two dimensional Ising model,⁽¹⁴⁾ although the value $\theta = 2$ is often observed in

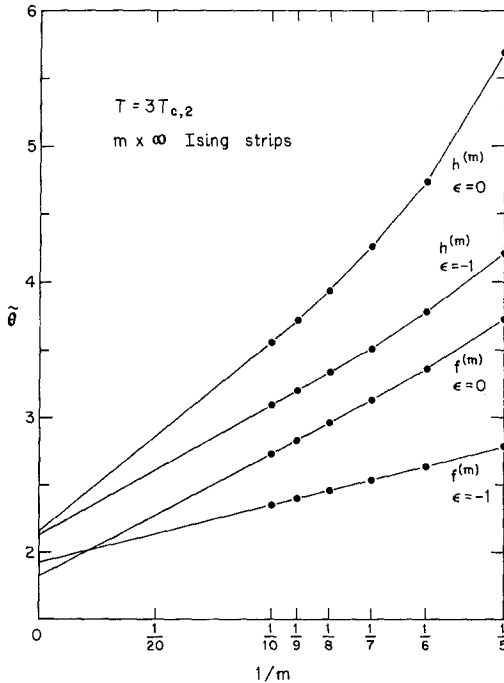


Fig. 4. Approximants $\tilde{\theta} = 1 - (m + \epsilon)(a_m - 2a_{m-1} + a_{m-2}) / (a_m - a_{m-1})$ to the exponent characterizing the dependence of the position of the Yang-Lee edge in $m \times \infty$ Ising strips on the width m for large m . We take $a_m = h_0^{(m)}$ and $a_m = f_0^{(m)}$ for a temperature $T = 3T_{c,2}$, and vary ϵ in an attempt to reduce the curvature of the plots.

systems having periodic boundary conditions.^(19,20) If an estimate of ν_c can be obtained, then a hyperscaling argument⁽¹⁴⁾ leads to an estimate of σ , namely,

$$\sigma = d\nu_c - 1 \quad (28)$$

with $d = 2$ dimensions in this case. The high-temperature series estimate⁽¹⁵⁾ $\sigma = -0.163 \pm 3$ for the two-dimensional model then yields $\nu_c = 0.419 \pm 2$ or $1/\nu_c = 2.39 \pm 1$.

We have analyzed the variation of $h_0^{(m)}(T)$ and $f_0^{(m)}(T)$ with m by methods akin to the ratio test.⁽²⁸⁾ Thus for $T = 3T_{c,2}$ we have formed the approximants $1 - (m + \epsilon)(a_m - 2a_{m-1} + a_{m-2})/(a_m - a_{m-1})$ for $a_m = h_0^{(m)}$ and $a_m = f_0^{(m)}$. These approximants, which should approach θ as $m \rightarrow \infty$, are plotted against $1/m$ in Fig. 4 with m -shifts ϵ chosen to reduce the curvature of the ratio plots. The data are consistent with

$$\theta = 2.0 \pm 0.2 \quad (29)$$

which also agrees with similar analysis for $T = 5T_{c,2}$. (See Ref. 29 for tabulated values of $h_0^{(m)}$ and $f_0^{(m)}$.) Since the expected value of $1/\nu_c$ is *greater* than 2, one might expect that any possible corrections of order $1/m^{1/\nu_c}$ could well be masked behind $1/m^2$ corrections.

4. ANALYTICAL RESULTS

Although we have not found a proof that $\sigma = -1/2$ characterizes the Yang-Lee edge singularity for all temperatures in all of the one-dimensional models considered above, we have succeeded in showing this for (i) n -vector chains in the asymptotic *high*-temperature limit, and (ii) $m \times \infty$ Ising strips in the asymptotic *low*-temperature limit. For the n -vector chains this is just an instance of a more general result, namely, that σ is independent of n in the high-temperature limit for n -vector models on a lattice with general nearest-neighbor interactions⁽¹⁵⁾; however, for the one-dimensional chains we are able to show this directly, without appealing to the solution of the one-dimensional Ising chain. As this argument is much simpler than that for the Ising strips, we present it first.

In order to examine the behavior of the eigenvalues of the transfer operator for one-dimensional n -vector chains at high temperatures, we turn to the matrix resolution (10) of the integral operator. For high temperatures, the reduced coupling K defined in (6) is small, and so we evaluate the zero-field eigenvalues μ_l asymptotically, using the small-argument form of the modified Bessel function,

$$I_\nu(x) \approx (\frac{1}{2}x)^\nu / \Gamma(\nu + 1) \quad (30)$$

to obtain, from (8),

$$\mu_l \approx \left[\Gamma(\frac{1}{2}n) / \Gamma(\frac{1}{2}n + l) \right] (\frac{1}{2}nK)^l \quad (31)$$

Since every element of any row of the matrix carries a factor $\mu_l = O(K^l)$ for some l , we need only retain those rows carrying factors of μ_0 or μ_1 in order to find the eigenvalues to leading order in K . This gives us one eigenvalue of order K in the $m_1 = 1$ component of the matrix; more importantly, the azimuthally symmetric ($m_1 = 0$) component reduces to a 2×2 matrix, given explicitly by

$$[A_{ll'}] = \begin{bmatrix} C_n(\frac{1}{2}n - 1)J_{n/2-1}(nh'') & iC_n(\frac{1}{2}n)J_{n/2}(nh'') \\ iKC_n(\frac{1}{2}n)J_{n/2}(nh'') & KC_n(\frac{1}{2}n - 1)J_{n/2-1}(nh'') \end{bmatrix} \quad (32)$$

where we have set

$$C_n = (2/nh)^{n/2-1} \Gamma(\frac{1}{2}n - 1) \quad (33)$$

The eigenvalues of this matrix are

$$\begin{aligned} \lambda_{\pm} &= \frac{1}{2} C_n (\frac{1}{2}n - 1) J_{n/2-1}(nh'') \\ &\times \left\{ 1 + K \pm \left[(1 - K)^2 - 4Kn^2 J_{n/2}^2(nh'') / (n - 2)^2 J_{n/2-1}^2(nh'') \right]^{1/2} \right\} \end{aligned} \quad (34)$$

and so the Yang-Lee edge singularity is clearly given by $\sigma = -1/2$ in the high-temperature limit; in addition one can see that the edge lies at

$$h_0(T) \approx x_{n/2-1} - \left[J_{n/2}(nx_{n/2-1}) / (\frac{1}{2}n - 1) J'_{n/2-1}(nx_{n/2-1}) \right] K^{1/2} \quad (35)$$

where $x = nx_{n/2-1}$ is the smallest zero of $x^{-n/2+1} J_{n/2-1}(x)$.

We analyze the $m \times \infty$ Ising strips in the low-temperature limit by expanding in the variable

$$u = \exp(-2J_{\perp} / k_B T) \quad (36)$$

which is small for positive J_{\perp} and small T , while treating the coupling *along* the layering direction exactly. To zeroth order in u , the m spins in any layer are frozen together into the same state (+1 or -1), and so the strip effectively reduces to a single Ising chain with nearest neighbor coupling mJ_{\parallel} . The two largest eigenvalues are then given by (22) (with an overall factor of $u^{-m/2}$) with K now denoting

$$K = mJ_{\parallel} / k_B T \quad (37)$$

All other eigenvalues vanish to this order. Note that the eigenvectors corresponding to the dominant eigenvalues are linear combinations of the

states having all spins “up” and all spins “down,” and so belong to the invariant representation of the symmetry group.

In order to calculate the leading corrections to these eigenvalues, we define the transfer matrix A in such a way that the element connecting a state α having spins s_1, s_2, \dots, s_m and a state α' with spins s'_1, s'_2, \dots, s'_m is given by

$$A_{\alpha\alpha'} = \exp(-\mathcal{H}_{\alpha\alpha'}/k_B T) \quad (38)$$

where

$$\mathcal{H}_{\alpha\alpha'} = -J_{\parallel} \sum_{j=1}^m s_j s'_j - \frac{1}{2} J_{\perp} \sum_{j=1}^m (s_j s_{j+1} + s'_j s'_{j+1}) - \frac{1}{2} H \sum_{j=1}^m (s_j + s'_j) \quad (39)$$

Then the only entries in the transfer matrix which do not vanish to relative order u are those connecting two states in which a total of at most two J_{\perp} bonds are unfavorable. This occurs only if one of the states has all spins either “up” or “down” and the other has k contiguous up-spins and $m - k$ contiguous down-spins for $k = 0, 1, \dots, m$. Now since in zeroth order the dominant eigenvectors belong to the invariant representation of the symmetry group, we need only consider contributions from states which are invariant. We let $\alpha = 1$ denote the state with all spins “up,” $\alpha = 2$ the state with all spins “down,” and $\alpha = k + 2$ the state which is invariant under cyclic permutations of spin labels and is built up of spin configurations having $m - k$ contiguous up-spins and k contiguous down-spins, with $k = 1, 2, \dots, m - 1$. With this labeling of layer states, the transfer matrix takes the form

$$[A_{\alpha\alpha'}] = \begin{bmatrix} P & Q & a_1 u & \cdots & a_{m-1} u \\ R & S & b_1 u & \cdots & b_{m-1} u \\ c_1 u & d_1 u & & & \\ \vdots & \vdots & & 0 & \\ c_{m-1} u & d_{m-1} u & & & \end{bmatrix} \quad (40)$$

where we have dropped all entries of relative order u^2 and set

$$\begin{aligned} P &= \exp[\beta m(J_{\parallel} + J_{\perp} + H)] & S &= \exp[\beta m(J_{\parallel} + J_{\perp} - H)] \\ Q &= R = \exp[\beta m(-J_{\parallel} + J_{\perp})] \\ a_k &= c_k = P m^{1/2} \exp[\beta k(-J_{\parallel} - \frac{1}{2} H)] \\ b_k &= d_k = Q m^{1/2} \exp[\beta k(J_{\parallel} - \frac{1}{2} H)] \end{aligned} \quad (41)$$

One can readily show that the secular equation for the matrix (40) is given by

$$0 = \lambda^{m-2} \left\{ \lambda^3 - (P + S)\lambda^2 + \left[PS - QR - u^2 \sum_{k=1}^{m-1} (a_k c_k + b_k d_k) \right] \lambda + u^2 \sum_{k=1}^{m-1} (Pb_k d_k - Qb_k c_k - Ra_k d_k + Sa_k c_k) \right\} \quad (42)$$

Note the absence of terms of order u in this equation; this is due to the fact that any term in the expansion of the determinant $\det(A - \lambda I)$ which contains at least *one* factor of order u must in fact contain at least *two*. Similarly, entries in the matrix which are of order u^2 will contribute to the secular equation only in order u^3 . To zeroth order in u , the nonzero roots of (42) are

$$\lambda_{\pm} = \frac{1}{2}(P + S) \pm \frac{1}{2}[(P - S)^2 + 4QR]^{1/2} \quad (43)$$

The perturbation terms may be viewed as affecting the eigenvalues in two ways: (i) shifting the position of the Yang–Lee edge at which $\lambda_+ = \lambda_-$, and (ii) changing the magnitude of the eigenvalues at the edge. Accordingly, we seek the leading-order corrections to (43) by writing

$$\lambda = \frac{1}{2}(P + S) + xu^2 \pm \frac{1}{2}[(P - S)^2 + 4QR + yu^2]^{1/2} \quad (44)$$

fixing x and y by requiring that (42) be satisfied for both choices of sign. This leads to

$$x = \frac{1}{2} \left[\sum_{k=1}^{m-1} (Pb_k d_k - Qb_k c_k - Ra_k d_k + Sa_k c_k) \right] / (PS - QR) \quad (45)$$

$$y = 4 \left[\sum_{k=1}^{m-1} (a_k c_k + b_k d_k) + (P + S)x \right] \quad (46)$$

provided $PS - QR \neq 0$. For our choice of parameters (41) this is satisfied if J_{\parallel} is nonvanishing. The explicit expressions obtained for x and y are not very enlightening, but they have one important feature: both carry an overall factor of m . Thus we see that, although the perturbation preserves the value $\sigma = -1/2$ of the Yang–Lee edge singularity for *finite* widths m in the low-temperature limit, our analysis must break down, as expected, for infinite m , which represents the two-dimensional Ising model.

For high temperatures, it is natural to attempt an expansion in powers of the variable $K_{\perp} = J_{\perp}/k_B T$. This gives good results for an Ising chain with a ferromagnetic second-neighbor interaction, $J_2 \sum s_i s_{i+2}$, when one

expands the eigenvalues of the transfer matrix in powers of $J_2/k_B T$ in a manner similar to that described above; this procedure verifies that $\sigma = -1/2$ is the correct exponent of the edge singularity in this model at high temperatures. However, in the $m \times \infty$ strips one encounters severe difficulties in trying to apply this method. The problem stems from the fact that if one neglects K_\perp , the model reduces to a set of m independent Ising chains. Accordingly one finds that the eigenvalues of the transfer matrix in this limit are all of the form $\lambda_+^k \lambda_-^{m-k}$ for $k = 0, 1, \dots, m$, where λ_+ and λ_- , the eigenvalues for the Ising chain, are given by (21) with $K = J_\parallel/k_B T$. Thus *all* of the eigenvalues are degenerate at $h'' = \sin^{-1}[\exp(-2K)]$, and this degeneracy makes the analytical problem of finding even the leading correction to the largest eigenvalues prohibitively difficult. Some idea of this difficulty is provided by the example of the $2 \times \infty$ strip. In this case the invariant block of the transfer matrix has dimension 3, and so its secular equation is cubic. By applying the well-known prescription for obtaining the roots of a cubic polynomial, one finds that the leading correction to the position of the Yang–Lee edge is of order $K_\perp^{2/3}$. For wider strips the appropriate secular equation is of higher degree, and so the difficulties encountered will be worse.

Finally, we note that our matrix resolution of the transfer integral operator for n -vector chains does not lend itself to a large- n expansion of the eigenvalues. To see this, consider the azimuthally symmetric ($m_1 = 0$) component of the infinite matrix. From the expression (14) for the coefficients $\langle j0 | k0; l0 \rangle$ and standard asymptotic expansions of the Bessel functions, one finds that the (l', l) element of this matrix is given asymptotically for large n by

$$A_{l',l} \approx D_n n^l \left\{ 2K / \left[1 + (1 + 4K^2)^{1/2} \right] \right\}^{l'} \left\{ 2ih'' / \left[1 + (1 - 4h''^2) \right]^{1/2} \right\}^{l+l'} \quad (47)$$

where the coefficient D_n depends on n but *not* on the indices l' and l . Thus every element in the l th column carries a factor n^l in the large- n limit. The inapplicability of our matrix methods in the spherical model limit of infinite n is to be expected, since the evidence presented in Section 2 leads to the conclusion that infinitely many eigenvalues of the transfer operator become degenerate at the Yang–Lee edge in the limit $n \rightarrow \infty$. Furthermore, this evidence suggests that attempts to carry out such expansions may well encounter nonintegral powers of $1/n$. Nevertheless, it remains an interesting and, probably, tractable problem to understand in more detail the crossover from $\sigma = -1/2$ for finite n to $\sigma = +1/2$ at $n = \infty$ and so see how the exponent ζ estimated in (20) enters analytically.

5. DISCUSSION

The exponent $\sigma = -1/2$ is, as noted above, known to be correct⁽²⁾ for the one-dimensional Ising chain at all temperatures. Thus σ also takes this value for n -vector chains with nearest-neighbor interactions, for n finite and nonnegative, in the asymptotic high-temperature limit.⁽¹⁵⁾ Moreover, $\sigma = -1/2$ is also correct for ferromagnetic one-dimensional n -vector chains with *negative* n at temperatures slightly above the critical temperature⁽³²⁾ (which is positive in these models⁽³²⁾). The numerical analyses presented above indicate that this value of σ should in fact be characteristic of all one-dimensional models with short-range interactions, in accordance with the exact results. Although we have not succeeded in proving this in general, the analytical work of Sections 2 and 4 is most suggestive, and engenders the hope that complete proofs may ultimately be found.

Our work adds significantly to the somewhat limited numerical evidence presented by Kortman and Griffiths⁽⁴⁾ in support of the conclusion that for a given model, σ is independent of temperature for temperatures above critical. This is also predicted by renormalization group analysis.⁽¹⁴⁾ It is known that σ is independent of n in the asymptotic high-temperature limit⁽¹⁵⁾ for n -vector models on a lattice of any dimensionality with general interactions between nearest-neighbor spins. Thus temperature-independence of σ would, barring nonuniformity of the $T \rightarrow \infty$ limit, imply its independence of n for the models we study. All our results accord with this expectation.

Strong analogies have been pointed out^(4,14) between the Yang-Lee edge singularity and critical behavior; these have been invoked⁽¹⁴⁾ in proposing relations among various exponents characterizing the edge, such as the hyperscaling relation (28). One such analogy is provided by the transfer matrix method, which predicts that the correlation length diverges at the Yang-Lee edge. The observed independence of σ on the width m of the Ising strips is to be expected on this basis; sufficiently near the edge, the correlation length is large enough for the system to perceive its one-dimensional nature.

Our numerical results indicate that the crossover of the exponent σ from its finite- n value to its spherical model value, and that from its one-dimensional to its two-dimensional value, both proceed by a common mechanism, namely, an accumulation of branch points in the spectrum of the transfer operator or matrix. One may hope that it will prove possible in the future to analyze the density of these branch points and of their amplitudes in the infinite-component or infinite-width limit. Note that the amplitudes can be obtained from the rate of approach of the dominant eigenvalue to its value at the edge.⁽²⁹⁾ This should, in turn, show how the spherical model exponent,⁽³⁾ $\sigma = 1/2$, arises, and perhaps also lead to the value of σ for two-dimensional models.

ACKNOWLEDGMENTS

The author wishes to thank Professor Michael E. Fisher for many helpful and enlightening discussions and Professor James Langer for his support. This work was supported by the National Science Foundation, in part through the Materials Science Center at Cornell University.

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