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The Yang–Lee Edge Singularity in Spherical Models

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The density of Yang–Lee zeros in the thermodynamic limit is discussed for ferromagnetic spherical models of general dimensionalities and arbitrary range of interaction. In all cases the zeros lie on the imaginary axis in the complex magnetic field plane $H = H' + iH''$ with a density $\mathscr{G}(H'')$ that exhibits a square root singularity $\mathscr{G}(H'') \sim (H'' - H_0)^\sigma$, with $\sigma = \frac{1}{2}$, as the edge of the gap at $H'' = H_0(T)$ is approached for $T > T_c$. When $T \to T_c$ one has $H_0(T) \sim (T - T_c)^\Delta$ with critical exponent $\Delta = \beta + \gamma$.

KEY WORDS: Yang–Lee zeros; spherical models; complex magnetic field; ferromagnets; critical point singularities; critical exponents.

1. INTRODUCTION

In 1952 Yang and Lee[(1)] drew attention to the significance of the zeros of the partition function in the complex plane of an appropriate field (or activity) variable and showed how the behavior of the zeros in the thermodynamic limit was intimately related to the occurrence of phase transitions.[(2)] The concept of the distribution of zeros has proved very useful in establishing the *absence* of phase transitions in a range of models. However, application to the study of the nature of phase transitions and the behavior of thermodynamic quantities has been limited by the difficulty of obtaining concrete information about the distribution of zeros. In particular, it is important to understand the nature of any singularities in the density of the zeros, especially those lying closest to the real field (or activity) axis, since these singularities will dominate observable behavior.

In this paper we address this problem for spherical models of arbitrary dimensionality d and with general interactions. We will consider only the

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asymptotic distribution of the zeros which is attained in the thermodynamic limit of an infinitely large system. For this purpose the electrostatic analogy originally introduced by Lee and Yang,[2] and since utilized by others,[3-5] is most appropriate. In this approach an isolated zero in the complex plane is regarded as a real, positive charge; lines of charge induce discontinuities in the electric field, which, in turn, corresponds to a first derivative of the thermodynamic free energy. Thus, the locus of zeros can be found by analytically continuing the equation of state from the real axis into the complex plane and discovering those special branch cuts across which the first derivative of the free energy parallel to the cut is continuous. These cuts may then be identified with the locus of zeros and, furthermore, the discontinuity in the normal derivative across the cut will be proportional to the limiting density of zeros. In the case of a magnetic model, where the zeros in the complex magnetic field plane $(H', H'') = (\mathrm{Re}\{H\}, \mathrm{Im}\{H\})$ are usually of principal interest, the appropriate first derivative is simply the magnetization M and loci of zeros represent cuts that make the analytic function $M(H)$ single-valued.

This method is open to the technical objection that it may be misleading, since certain distributions of zeros that are everywhere analytic may be missed. In many cases this objection has no force, because the zeros are known to be restricted to certain loci and such problems cannot arise. Thus the original Lee–Yang circle theorem for spin-$\frac{1}{2}$ Ising ferromagnets shows that the zeros are confined to the pure imaginary magnetic field axis; unfortunately, the analogous theorem is not available for spherical models. However, rather than enter into these questions here, we will take the attitude that the nature of the singularities in the complex plane *of the analytically continued free energy* is, in any case, the topic of prime interest.

For the wide range of spherical models studied, we find that the zero distribution is concentrated on the imaginary magnetic field axis $H' = \mathrm{Re}\{H\} \equiv 0$ above (or below) a "gap" with "edges" at $\mathrm{Im}\{H\} = H'' = \pm H_0(T)$. The size of this gap vanishes as the temperature T approaches the critical point. Its detailed variation depends on the dimensionality of space and on the form of the interactions; however, in the critical region it exhibits the universal scaling law behavior

$$H_0(T) \sim (T - T_c)^{\Delta} \tag{1}$$

where $\Delta = \beta + \gamma$ is the thermodynamic gap exponent[6] for the appropriate class of spherical models. Explicit expressions for the value of Δ are given below: note that Δ depends on the dimensionality d and on the exponent λ of the decay law of the interactions, if these are of long range, with $J(\mathbf{R}) \sim 1/R^{d+\lambda}$ (as $R \to \infty$); but Δ is independent of other details of the lattice structure and interactions.

On the edges of the gap we find that the density $\mathscr{G}(H'')$ of the zeros exhibits a singularity of *universal type*. Explicitly, if we define $\mathscr{G}(H'')$ so that the number of zeros on the imaginary axis between iH'' and $i(H'' + dH'')$ approaches $N\mathscr{G}(H'')\, dH''$ as N, the number of spins in the system, approaches infinity, we obtain

$$\mathscr{G}(H'') \approx G[H'' - H_0(T)]^{\sigma} \qquad \text{for} \quad H'' \to H_0(T)+ \tag{2}$$

where $\sigma = \frac{1}{2}$ and G is a constant. This square root singularity is independent of the dimensionality of space and all details of the lattice structure, and of the nature of the interactions, whether of long or short range. We may remark that the singularity is of the *same* type as that found for mean field models[7] but differs strikingly from what is essentially the only other exactly known result, namely $\sigma = -\frac{1}{2}$ for the standard one-dimensional Ising model[2,7] (but see also Ref. 5).

2. GENERAL SPHERICAL MODELS

We consider spherical models on a regular lattice in d-dimensional space with lattice spacing a and cell volume v_0. At the lattice sites $\{\mathbf{R}\}$ are located continuous, classical scalar spins $\{s(\mathbf{R})\}$ which interact via the Hamiltonian

$$\mathscr{H} = -\tfrac{1}{2} \sum_{\mathbf{R} \neq \mathbf{R}'} J(\mathbf{R} - \mathbf{R}')s(\mathbf{R})s(\mathbf{R}') - \mu H \sum_{\mathbf{R}} s(\mathbf{R}) + g \sum_{\mathbf{R}} [s(\mathbf{R})]^2 \tag{3}$$

Here $J(\mathbf{R}) \equiv J(-\mathbf{R})$ represents the exchange coupling, while H is the applied magnetic field and μ is the magnetic moment per unit spin length. The spins are restricted to unit mean length by the spherical condition

$$\mathscr{S}^2 = \left\langle N^{-1} \sum_{\mathbf{R}} [s(\mathbf{R})]^2 \right\rangle = 1 \tag{4}$$

where N is the number of spins, while the angular brackets denote the standard thermal expectation. The condition is to be met by adjusting the spherical field g. This formulation is essentially that of Lewis and Wannier,[8] which is thermodynamically equivalent[9] to the original formulation of Berlin and Kac.[10] Since we are interested only in the thermodynamic limit, the differences that arise for finite N are of no consequence for us.

The partition function at temperature T may be calculated exactly in the standard way[11] by introducing Fourier-transformed spin variables which diagonalize the quadratic form representing the Hamiltonian. The resulting Gaussian integrals are readily performed. The spherical condition (4) becomes the constraint equation

$$\frac{\partial F}{\partial g}(T, H; g) = 1 \tag{5}$$

where $F(T, H; g)$ is the free energy per spin. By virtue of the nature of this constraint, any thermodynamic function involving only first derivatives of F is the same whether taken at fixed g or at fixed $\mathscr{S}^2$. Specifically, we may differentiate $F(T, H; g)$ to find the reduced magnetization $m = M/\mu$, then eliminate g in favor of m in the constraint equation to obtain, finally, the equation of state in the form

$$k_B T I_d(k_B T h/m) = 1 - m^2 \tag{6}$$

where the reduced magnetic field is

$$h = \mu H/k_B T = h' + ih'' \tag{7}$$

while the basic integral is defined by

$$I_d(\zeta) = v_0 \int_{\mathbf{q}} [\zeta + \hat{J}(\mathbf{0}) - \hat{J}(\mathbf{q})]^{-1} \tag{8}$$

$$\hat{J}(\mathbf{q}) = \sum_{\mathbf{R}} [\exp(i\mathbf{q}\cdot\mathbf{R})] J(\mathbf{R}) \tag{9}$$

where $\int_{\mathbf{q}} \equiv (2\pi)^{-d} \int d^d q$, the integral running over the first Brillouin zone of the appropriate reciprocal lattice.

Now note that the Fourier transform $\hat{J}(\mathbf{q})$ is real for real $\mathbf{q}$ since $J(\mathbf{R}) = J(-\mathbf{R})$. Furthermore, we will *assume* that

$$\hat{J}(\mathbf{0}) > \hat{J}(\mathbf{q}) \qquad \text{for} \quad \mathbf{q} \neq 0 \tag{10}$$

for all $\mathbf{q}$ in the first Brillouin zone. Physically, this restriction means that the only possible phase transition in low field is of ferromagnetic character. Mathematically the restriction is satisfied trivially if we assume that the interactions are of *strictly ferromagnetic character*, that is,

$$J(\mathbf{R}) \geqslant 0 \qquad \text{all} \quad \mathbf{R} \tag{11}$$

However, (10) is actually more general than this.

From (10) it follows that the basic integral $I_d(\zeta)$ is real and strictly monotonic decreasing for real, positive ζ. Furthermore, $I_d(\zeta)$ is an analytic function in the complex ζ plane except for a cut running along the negative real axis from a branch point at $\zeta = 0$. The character of this branch point depends on the behavior of the coupling $J(\mathbf{R})$ for large $|\mathbf{R}|$ as will now be shown. If the interactions are of finite range, in the sense that $\sum_{\mathbf{R}} |R|^2 J(\mathbf{R})$ converges, the inequality (10) extends to

$$\hat{J}(\mathbf{q}) \approx \hat{J}(\mathbf{0}) - j_2(qa)^2 + \cdots \tag{12}$$

for small qa (where a is the lattice spacing). In the case of nearest neighbor coupling of strength J on the d-dimensional hypercubic lattice one has $j_2 = J$.

More generally, in the case of long-range interactions that, for $|\mathbf{R}| \to \infty$, decay as

$$J(\mathbf{R}) \sim 1/|\mathbf{R}|^{d+\lambda} \qquad \text{with} \quad 0 < \lambda < 2 \tag{13}$$

one has, for small qa,

$$\hat{J}(\mathbf{q}) \approx \hat{J}(\mathbf{0}) - j_\lambda (qa)^\lambda + \cdots \tag{14}$$

If we formally set $\lambda = 2$ in this relation, and all others below, we obtain (12) and thereby include a description of the short-range case. [Note, however, that the excluded borderline case $\lambda = 2$ in (13) leads to logarithmic factors in the Fourier transform, which are not allowed for in our analysis.]

If the expressions (14) and (12) are substituted into the definition (8) for $I_d(\zeta)$, the integral may be evaluated asymptotically for small ζ in a straightforward manner for general d (including nonintegral d). Specifically, for $d < \lambda$ one may put $d^d q = c_d q^{d-1} dq$ with $c_d = 2\pi^{d/2}/\Gamma(\frac{1}{2}d)$ and extend the range of integration to $|\mathbf{q}| = \infty$; for $d > \lambda$ the same method suffices after differentiation once to obtain $I_d'(\zeta) = (dI_d/d\zeta)$ or, for $d > 2\lambda$, twice, etc. In this way one finds

$$\begin{aligned} I_d(\zeta) &\approx A_{d,\lambda}\zeta^{-1+(d/\lambda)} && \text{for} \quad 0 < d < \lambda \\ &\approx A_{\lambda,\lambda} \ln(j_\lambda/\zeta) && \text{for} \quad d = \lambda \\ &\approx I_d(0) - A_{d,\lambda}\zeta^{(d/\lambda)-1} && \text{for} \quad \lambda < d < 2\lambda \\ &\approx I_{2\lambda}(0) - A_{2\lambda,\lambda}\zeta \ln(j_\lambda/\zeta) && \text{for} \quad d = 2\lambda \\ &\approx I_d(0) - |I_d'(0)|\zeta && \text{for} \quad d > 2\lambda \end{aligned} \tag{15}$$

as $\zeta \to 0$. The amplitudes $A_{d,\lambda}$ are all positive; otherwise their actual values will play no crucial role. Since they are universal, however, we record them here:

$$\begin{aligned} A_{d,\lambda} &= (2\pi)^{-d} c_d \pi v_0 / a^d \lambda j_\lambda^{d/\lambda} |\sin(d\pi/\lambda)| && \text{for } 0 < d < 2\lambda \text{ but } d \neq \lambda \\ &= (2\pi)^{-d} c_d v_0 / a^d \lambda j_\lambda^{d/\lambda} && \text{for } d = \lambda \text{ or } d = 2\lambda \end{aligned} \tag{16}$$

Likewise, the integrals $I_d(0)$ are positive, although their values depend on the detailed lattice structure, etc.

3. BEHAVIOR IN THE CRITICAL REGION

The behavior of the density of zeros is of most interest for temperatures close to the critical point. In addition, the analysis happens to be easiest in this region. Accordingly, we examine it first.

The ferromagnetic critical point is conveniently defined by the simultaneous vanishing of the magnetization m and the inverse susceptibility. This yields

$$k_B T_c = 1/I_d(0) \tag{17}$$

provided $I_d(0)$ is finite, as it is for $d > \lambda$; otherwise there is no phase transition for $T > 0$ and one may take $T_c = 0$. Near the critical point the inverse susceptibility is small and, hence, so is the ratio $\zeta = k_B T h/m$. Consequently the asymptotic equation of state may be found by substituting into (6) the expressions (15) for the integral $I_d(\zeta)$.

Consider first the case $d \leqslant \lambda$ for which $T_c = 0$. The equation of state may then be written asymptotically as

$$\begin{aligned} h &\approx B_{d,\lambda} m/(1 - m^2)^{\lambda/(\lambda - d)} \qquad &\text{for} \quad 0 < d < \lambda \\ &\approx B_{\lambda,\lambda} m \exp(m^2/A_{\lambda,\lambda} k_B T) \qquad &\text{for} \quad d = \lambda \end{aligned} \tag{18}$$

where the amplitudes $B_{d,\lambda}$ are finite, real, and positive for $T > 0$.

These formulas represent implicit equations for the analytic function $m(h)$ (at fixed T). To understand their significance a graphical analysis is helpful. Guided by the Yang–Lee theorem[2] for the standard Ising model, we expect the zeros of the partition function, and hence the cut needed for the function $m(h)$, to lie along the imaginary h axis. Accordingly, let us set

$$h = h' + ih'' = iy \qquad \text{and} \qquad m = m' + im'' = iw \tag{19}$$

and consider real w (i.e., pure imaginary magnetization). The equations of state (18) then yield real y (i.e., pure imaginary field). Furthermore, the general character of the (y, w) or (ih, im) relation is as illustrated in Fig. 1. Evidently y as a function of w exhibits a simple, analytic maximum at (h_0, m_0) [and a corresponding conjugate minimum at $(-h_0, -m_0)$]. Con-

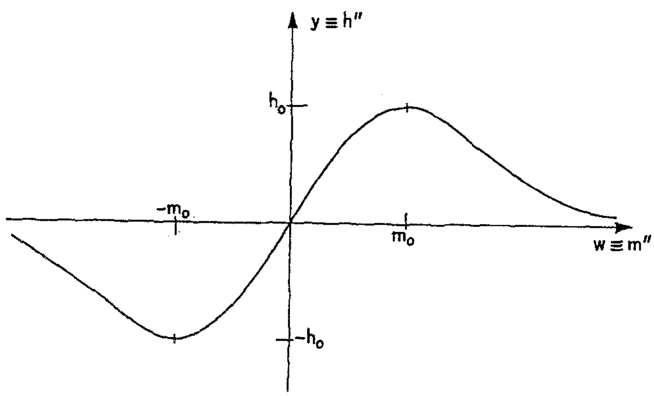

Fig. 1. Variation of $y \equiv h'' = \mathrm{Im}\{h\}$ with real $w \equiv m'' = \mathrm{Im}\{m\}$ for spherical models with $d \leq \lambda$, which implies $T_c = 0$. The maximum at $y = h_0$, $w = m_0$ corresponds to a square root branch point in the function $m(h)$.

versely, w as a function of y, or m as a function of h, must exhibit conjugate square root branch points at $y = \pm h_0$ or $h = \pm ih_0$. Note, furthermore, that the nature of this branch point is quite independent of the "critical character" of the spherical model as exemplified by the exponent $\lambda/(\lambda - d)$; this, indeed, enters only into the dependence of y on w (or h on m) for large values of w. In the inverse function $w(y)$ [or $m(h)$] this dependence is effectively concealed on the second sheet of the function.

The heuristic arguments just presented confirm, for $d \leqslant \lambda$, the conclusion (2) stated in the introduction. The arguments can be made more rigorous by noting that some sufficiently high derivative of $m(h)$ should diverge at any branch point. In fact, it suffices to solve the equation $(dh/dm) = 0$ to locate the branch point. As $T \to 0$ this yields explicitly

$$\begin{aligned} h_0(T) &\approx C_{d,\lambda}(k_B T)^{d/(\lambda - d)} && \text{for} \quad 0 < d < \lambda \\ &\approx C_{\lambda,\lambda}(k_B T)^{-1/2} \exp(-1/A_{\lambda,\lambda} k_B T) && \text{for} \quad d = \lambda \end{aligned} \tag{20}$$

where

$$C_{d,\lambda} = [(\lambda - d)/(\lambda + d)]^{1/2}[A_{d,\lambda}(d + \lambda)/2\lambda]^{\lambda/(\lambda - d)} \quad \text{for} \quad 0 < d < \lambda \tag{21}$$

$$C_{\lambda,\lambda} = j_\lambda (A_{\lambda,\lambda}/2e)^{1/2} \quad \text{for} \quad d = \lambda \tag{22}$$

In addition, the calculation shows that there are no other branch points. Since y is real for real w, the branch cuts may be placed along the imaginary h axis as anticipated. Note that when $T \to 0$ the branch points, which in fact locate the edges of the gap in the zero distribution, approach the real h axis as a power law for $d < \lambda$ but exponentially fast for $d = \lambda$.

Near the branch points we may clearly write

$$h \approx ih_0 + \tfrac{1}{2}(d^2h/dm^2)_0(m - im_0)^2 \tag{23}$$

where the second derivative is evaluated at $m = im_0$ and is found to be purely imaginary, as may be anticipated from Fig. 1. Inversion of this relation confirms the square root nature of the branch points and shows that the imaginary part of m will be continuous across the cuts *only* if they lie along the imaginary h axis. If $Ng(h'')\,dh''$ represents asymptotically the number of zeros on the imaginary h axis between ih'' and $i(h'' + dh'')$, the discontinuity of the real part of m across the cut is equal[2] to $2\pi g(h'')$. In accord with the conclusion (2), this finally yields

$$\begin{aligned} g(h'') &\approx G_{d,\lambda}(T)[|h''| - h_0(T)]^{1/2} && \text{for} \quad |h''| \to h_0+ \\ &= 0 && \text{for} \quad |h''| \leqslant h_0 \end{aligned} \tag{24}$$

where the amplitudes are given by

$$\begin{aligned} [\pi G_{d,\lambda}(T)]^2 &= 2\lambda(\lambda - d)/(\lambda + d)^2 h_0(T) && \text{for} \quad 0 < d < \lambda \\ &= A_{\lambda,\lambda} k_B T/2h_0(T) && \text{for} \quad d = \lambda \end{aligned} \tag{25}$$

The analysis for the cases $d > \lambda$, for which a phase transition occurs with $T_c > 0$, proceeds in a completely analogous way. It is convenient, as usual,[6] to set

$$t = (T - T_c)/T_c \tag{26}$$

Then the asymptotic equation of state for $d > \lambda$ but $d \neq 2\lambda$ may be written

$$h \approx B_{d,\lambda} m(t + m^2)^\gamma \tag{27}$$

where the susceptibility exponent for the spherical model is given by[6,11,12]

$$\begin{aligned} \gamma &= \lambda/(d - \lambda) \qquad \text{for} \quad \lambda < d \leqslant 2\lambda \\ &= 1 \qquad\qquad\quad\;\; \text{for} \quad d \geqslant 2\lambda \end{aligned} \tag{28}$$

For the borderline case $d = 2\lambda$ the equation of state is more complicated and involves logarithms. However, this does not alter any of the analysis in a significant way. From (27) one easily sees that the exponent for the spontaneous magnetization is $\beta = \frac{1}{2}$. Furthermore, the equation of state may be cast in scaling form[6] in terms of the scaled variables m/t^β and h/t^Δ with gap exponent[6]

$$\begin{aligned} \Delta &= \beta + \gamma = (d + \lambda)/2(d - \lambda) \qquad \text{for} \quad \lambda < d \leqslant 2\lambda \\ &= 1\tfrac{1}{2} \qquad\qquad\qquad\qquad\qquad\quad\;\, \text{for} \quad d \geqslant 2\lambda \end{aligned} \tag{29}$$

On making the transformation (19) to imaginary field and magnetization, one again finds that real w (or pure imaginary m) yields real y (i.e., pure imaginary h). The general appearance of the (y, w) relation for $T > T_c$ is now as shown in Fig. 2. Although the behavior of the plot for large w (or m'') is different, the crucial analytic maximum at (h_0, m_0) remains and locates a square root branch point in the function $m(h)$. The specifically critical nature

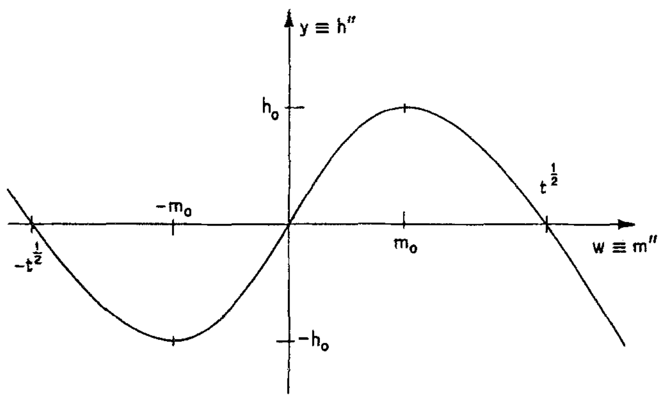

Fig. 2. Variation of $y \equiv h''$ with real $w = m''$ for spherical models with $d > \lambda$, for which $T_c > 0$. As in Fig. 1, the extrema yield square root branch points in $m(h)$.

of the equation of state, now exemplified by the exponent γ, determines the behavior of y only at large w and thus is confined to the second sheet of the function $m(h)$.

On calculating explicitly, the branch point is found to vary as $t \to 0+$ according to

$$h_0(T) \approx C_{d,\lambda} t^{\Delta} \tag{30}$$

for $d > \lambda$ but $d \neq 2\lambda$, which confirms the conclusion (1) stated in the introduction. For $d = 2\lambda$ one finds instead

$$h_0(T) \approx C_{2\lambda,\lambda} t^{3/2} / \ln t^{-1} \tag{31}$$

but this behavior in fact corresponds precisely to the expected borderline critical behavior of quantities scaling like the magnetic field[6,11,12] [and is still consistent with (1)]. The amplitudes appearing in these expressions are given explicitly by

$$\begin{aligned} C_{d,\lambda} &= \left(\frac{d-\lambda}{d+\lambda}\right)^{1/2} \left(\frac{2\lambda}{A_{d,\lambda}(d+\lambda)}\right)^{\gamma} (k_B T_c)^{-d/(d-\lambda)} \qquad \text{for} \quad \lambda < d \leqslant 2\lambda \\ &= \frac{2}{3\sqrt{3}\,|I_d'(0)|(k_B T_c)^2} \qquad \text{for} \quad d > 2\lambda \end{aligned} \tag{32}$$

Finally, on utilizing (23) as before, the density of zeros is again found to obey the square root law (24) but with amplitudes given by

$$\begin{aligned} [\pi G_{d,\lambda}(T)]^2 &= 2\lambda(d-\lambda)t/(d+\lambda)^2 h_0(T) \qquad \text{for} \quad \lambda < d \leqslant 2\lambda \\ &= 2t/9h_0(T) \qquad \text{for} \quad d \geqslant 2\lambda \end{aligned} \tag{33}$$

Note that these singularity amplitudes $G_{d,\lambda}$ diverge when $T \to T_c+$ since $h_0(T) \to 0$ more rapidly than t as the gap closes. Consequently, one should *not* expect a square-root singularity in the density of zeros *at* $T = T_c$. On the contrary, it is easy to see from the equation of state (27) that the density of zeros is characterized by an exponent $\sigma = 1/\delta$ at the critical point, where $\delta = \Delta/\beta = 1 + (\gamma/\beta)$ is the standard exponent for the critical isotherm.[6]

4. HIGH AND INTERMEDIATE TEMPERATURES

We will demonstrate now that the square root singularity in the density of zeros on the imaginary field axis, which characterizes the asymptotic critical region, in fact remains for all temperatures. Furthermore, we will show that no density of zeros appears anywhere else in the complex field plane.

It is instructive to consider first the high-temperature limit. This is described by large ζ, for which, from (8), we find

$$I_d(\zeta) \approx K_0/\zeta \qquad \text{with} \quad K_0 = v_0 \Omega_0 \tag{34}$$

where Ω_0 is the volume of the first Brillouin zone. The equation of state (6) then becomes a quadratic equation which is readily solved to yield

$$m(h) = h/[\tfrac{1}{2}K_0 + \tfrac{1}{2}(K_0{}^2 + 4h^2)^{1/2}] \tag{35}$$

This exhibits only the expected pair of square root branch points at $h = \pm ih_0$ where

$$h_0(T) = \mu H_0(T)/k_B T = \tfrac{1}{2}K_0 \tag{36}$$

The density of the zeros can be read off from the discontinuity, which, for the amplitude $G_{d,\lambda}$ in (24), yields

$$[\pi G_{d,\lambda}]^2 = 2/h_0(T) \qquad (\text{all } d, \lambda) \tag{37}$$

This square root branch point can be followed to lower temperatures by expanding $I_d(\zeta)$ systematically in inverse powers of ζ, which, in turn, yields an expansion of $h_0(T)$ in inverse powers of T. More generally, the fact that $I_d(\zeta)$ is real for real ζ implies that at all temperatures above critical the graph of y for real w (or pure imaginary m) has essentially the same form as shown in Figs. 1 and 2. Specifically, the plot will exhibit at least one analytic maximum which will correspond to a square root branch point in $m(h)$. If there are a number of maxima at $w = m_0 < m_1 < m_2 < \cdots$, only the one nearest the origin, namely m_0, will be relevant. In principle, two of these maxima could merge in special conditions to yield a vanishing second derivative $(d^2h/dm^2)_0$ in (23); in such a case the branch point would correspond to a fourth root, $\sigma = \frac{1}{4}$; however, we will show that this does not happen.

In more concrete terms, any branch points, real or complex, will be identified by $(dh/dm) = 0$, and hence satisfy

$$k_B Th/m = \zeta_0 = u + iv \tag{38}$$

where u and v are real, and ζ_0 is a root of

$$k_B T\zeta_0 I_d'(\zeta_0) = 2m^2 \tag{39}$$

If the equation of state (6) is used to eliminate the magnetization m, the equation for $\zeta_0(T)$ becomes

$$\zeta_0 I_d'(\zeta_0) + 2I_d(\zeta_0) = 2/k_B T \tag{40}$$

We will now show (i) that there is a unique real, positive solution of this equation which determines a branch point of $m(h)$ on the imaginary axis with exponent $\sigma = \frac{1}{2}$ and cut running along the axis; (ii) that any complex roots of (40) have negative real part, i.e., $u = \text{Re}\{\zeta_0\} < 0$; but, conversely, (iii) that throughout the physical sheet of the function $m(h)$ the ratio $\zeta_0 = k_B Th/m$ has nonnegative real part. In sum, then, the limiting zero density under all conditions is confined to the imaginary h axis and terminates in a branch point of invariant character.

It is convenient to introduce the real integration variable

$$x = \hat{J}(\mathbf{0}) - \hat{J}(\mathbf{q}) \tag{41}$$

in place of $\mathbf{q}$, and the corresponding "density of states" $\nu(x)$ in terms of which the basic integral (8) can be written

$$I_d(\zeta) = \int_0 (\zeta + x)^{-1} \qquad \text{with} \qquad \int_0 \equiv \int_0^X dx\, \nu(x) \tag{42}$$

where $X = \sup_{\mathbf{q}}\{\hat{J}(\mathbf{0}) - \hat{J}(\mathbf{q})\}$. Note that, by (10), negative values of x do not enter. Then the real and imaginary parts of (40) become

$$\int_0 \frac{uv^2 + (u + 2x)(u + x)^2}{[(u + x)^2 + v^2]^2} = \frac{2}{k_B T} \tag{43}$$

$$v\int_0 \frac{u^2 + v^2 + 4ux + 3x^2}{[(u + x)^2 + v^2]^2} = 0 \tag{44}$$

Clearly, $v = 0$ yields a solution of (44) and then (43) reduces to

$$\int_0 \left[\frac{1}{u + x} + \frac{x}{(u + x)^2}\right] = \frac{2}{k_B T} \tag{45}$$

The left-hand side is a continuous, monotonic decreasing function of $u = \mathrm{Re}\{\zeta_0\}$ approaching zero as $u \to \infty$, and $2/k_B T_c$ as $u \to 0+$. Hence there is a unique real solution of (40) for $T > T_c$. Now, as already remarked, $I_d'(\zeta_0)$ is real but negative for real, positive ζ_0. It thus follows from (39) that the real, positive solution ζ_0 determines a unique pair of complex conjugate branch points at which m and, hence, h are both pure imaginary.

Because $I_d(\zeta)$ is regular for ζ away from the negative real axis, we may expand about ζ_0 and recapture (23) again with

$$(d^2h/dm^2)_0 = -4ih_0/k_B T\zeta_0[I_d'(\zeta_0)]^2(d\zeta_0/d\Theta) \tag{46}$$

where, with $\Theta = 1/k_B T$,

$$\left(\frac{d\zeta_0}{d\Theta}\right) = \frac{2}{3I_d'(\zeta_0) + \zeta_0 I_d''(\zeta_0)} = -\frac{2}{v_0}\left[\int_0 \frac{\zeta_0 + 3x}{(\zeta_0 + x)^3}\right]^{-1} \tag{47}$$

Evidently $(d^2h/dm^2)_0$ is *strictly* positive for real $\zeta_0 > 0$. Finally, the density of zeros near the edge $h = ih_0$ is once more determined by (24) but with amplitude given by

$$[\pi G_{d,\lambda}]^2 = \frac{-k_B T\zeta_0[I_d'(\zeta_0)]^2}{[3I_d'(\zeta_0) + \zeta_0 I_d''(\zeta_0)]h_0(T)} \tag{48}$$

Now let us return to (43) and (44) and consider the possibility of negative or complex roots $\zeta_0(T)$. First note that for $v \neq 0$ the integrand in (44) is nonnegative whenever $u \geqslant 0$, so that the integral cannot vanish unless $u < 0$. It follows that any solutions of (40) beyond the real, positive solution already discussed lie in the left half-plane. However, as we will now prove, such solutions are of no concern!

To this end, first note that the *physical sheet* of the function $m(h)$ has m real and positive for h real and positive. This follows most directly from the reality and convexity of the free energy as a function of real h; however, it also follows from the equation of state (6). Second, notice that the equation of state is symmetric under change of sign of both the real and imaginary parts of h. Explicitly, if the physical sheet of $m(h)$ is known for h in the first quadrant of the complex h plane, the relations

$$m(h^*) = [m(h)]^* \qquad \text{and} \qquad m(-h) = -m(h) \tag{49}$$

suffice to determine the whole physical sheet. Accordingly, let us write

$$h = |h|e^{i\theta}, \qquad m = |m|e^{i\varphi}, \qquad \zeta = |\zeta|e^{i\psi} \tag{50}$$

where $\theta = \varphi + \psi$ is restricted by $0 \leqslant \theta \leqslant \frac{1}{2}\pi$. The imaginary part of the equation of state (6) may then be written

$$\sin\psi\, |h|(k_B T)^2 \int_0^\infty [(u + x)^2 + v^2]^{-1} = |m|^3 \sin 2\varphi \tag{51}$$

with u and v defined in analogy to (38). The coefficients of both the sine functions are positive, so that $\sin\psi$ and $\sin 2\varphi = \sin 2(\theta - \psi)$ must have the same algebraic sign. This condition restricts the allowed regions of the (θ, ψ) plane to those shaded in Fig. 3. Now, as explained, the physical sheet of $m(h)$ must include the real axis where $\theta = \varphi = \psi = 0$; indeed, for small θ one has, from (51), $\theta \approx c\psi$ with $c > 1$. Thus region I in Fig. 3 is accessible on

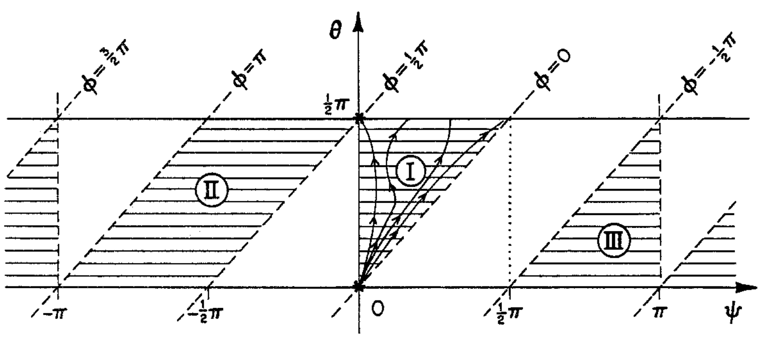

Fig. 3. Allowed regions of the $(\theta, \psi) = (\arg\{h\}, \arg\{\zeta\})$ plane following from the equation of state via (51). Region I is the only one accessible on the physical sheet of $m(h)$.

the physical sheet. (Conceivable paths of continuation from the real axis as θ increases monotonically are indicated.) However, region I communicates with other regions only at the point $\theta = \varphi = \frac{1}{2}\pi$, $\psi = 0$. Since this represents the limiting value of θ, no actual continuation to other regions is possible. Finally, notice that within region I the argument ψ of ζ is bounded by $\frac{1}{2}\pi$. Consequently, the real part of ζ is nonnegative everywhere on the physical sheet of $m(h)$. This completes the proof that the limiting density of zeros is confined to the imaginary h axis.

5. DISCUSSION

As remarked in the introduction, the square root, $\sigma = \frac{1}{2}$, edge singularity in the density of zeros for spherical models is the same as found in mean field models.[7] Indeed, for $d > 2\lambda$ the asymptotic critical equation of state for spherical models is identical to that given by mean field theory. On the other hand, the one-dimensional, spin-$\frac{1}{2}$ Ising model with nearest neighbor interactions yields[2] $\sigma = -\frac{1}{2}$, corresponding to the branch point behavior $m - im_0 \sim (h - ih_0)^{-1/2}$. Indeed, it can be seen by the transfer matrix method that this latter result is characteristic of one-dimensional Ising models, including both those with further neighbor interactions and those consisting of two or more coupled chains (e.g., $m \times \infty$ strips).[13]

Numerical studies by Kortman and Griffiths,[7] based on high-temperature series expansions, suggest the distinct edge singularity exponents $\sigma = -0.125 \pm 0.05$ for the two-dimensional square Ising lattice and $\sigma = 0.125 \pm 0.05$ for the three-dimensional diamond Ising lattice. Values within these two ranges have recently been found for a number of two- and three-dimensional Ising models in the limit $T \to \infty$.[14] Thus, although σ is independent of d for spherical models, it appears to depend strongly on d for Ising models. However, a renormalization group analysis[15] suggests that σ becomes equal to the mean field/spherical value $\frac{1}{2}$ for Ising models in $d \geqslant 6$ dimensions.

It is known[16] that the spherical model corresponds to the $n \to \infty$ limit of ferromagnetic models with n-component vectorial spin variables $\vec{s}(\mathbf{R}) = [s^{\mu}(\mathbf{R})]_{\mu=1,2,\ldots,n}$. One might thus expect the edge singularity exponent σ to depend on n as well as on d, approaching the spherical model value $\sigma = \frac{1}{2}$ as $n \to \infty$.[2] This point is currently under investigation[13] by the transfer kernel method for nearest neighbor one-dimensional models; a tentative analysis, however, indicates that σ "sticks" at the Ising ($n = 1$) value, $\sigma = -\frac{1}{2}$, for all $n < \infty$ and jumps abruptly to $\sigma = \frac{1}{2}$ only for $n = \infty$. A similar result for general d is suggested by the renormalization group analysis.[15] Further work

[2] It might be remarked that for the cases $n = 2$ and 3, Dunlop and Newman[17] have established that the zeros are confined to the pure imaginary magnetic field axis.

will, we hope, confirm these results and fill in further our picture of the nature of the Yang–Lee zero distribution.

REFERENCES

1. C. N. Yang and T. D. Lee, *Phys. Rev.* **87**:404 (1952).
2. T. D. Lee and C. N. Yang, *Phys. Rev.* **87**:410 (1952).
3. P. C. Hemmer and E. H. Hauge, *Phys. Rev.* **133**:A1010 (1964); E. H. Hauge and P. C. Hemmer, *Physica* **29**:1338 (1963); P. C. Hemmer, E. H. Hauge, and J. O. Aasen, *J. Math. Phys.* **7**:35 (1966); E. Byckling, *Phys. Rev.* **140**:A1165 (1965).
4. S. Katsura, *Prog. Theo. Phys. (Kyoto)* **13**:571 (1955).
5. M. van den Berg and Th. Niemeijer, *Physica* **85A**:186 (1976).
6. M. E. Fisher, *Rep. Prog. Phys.* **30**:615 (1967); *Rev. Mod. Phys.* **46**:597 (1974).
7. P. J. Kortman and R. B. Griffiths, *Phys. Rev. Lett.* **27**:1439 (1971).
8. H. W. Lewis and G. H. Wannier, *Phys. Rev.* **88**:682 (1952).
9. C. C. Yan and G. H. Wannier, *J. Math. Phys.* **6**:1833 (1965).
10. T. H. Berlin and M. Kac, *Phys. Rev.* **86**:821 (1952).
11. G. S. Joyce, in *Phase Transitions and Critical Phenomena*, Vol. 2, C. Domb and M. S. Green, eds. (Academic Press, London, 1972).
12. G. S. Joyce, *Phys. Rev.* **146**:349 (1966).
13. D. A. Kurtze (to be published).
14. M. E. Fisher (to be published); see also G. A. Baker, Jr. and P. Moussa, in Proc. 23rd Conf. Magnetism and Magnetic Materials, *J. Appl. Phys.* **49**:1360 (1978).
15. M. E. Fisher, *Phys. Rev. Lett.* **40**:1610 (1978).
16. H. E. Stanley, *Phys. Rev.* **176**:718 (1968).
17. F. Dunlop and C. M. Newman, *Comm. Math. Phys.* **44**:223 (1975).