

Location of the Lee-Yang zeros and absence of phase transitions in some Ising spin systems

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We consider a class of Ising spin systems on a set Λ of sites. The sites are grouped into units with the property that each site belongs to either one or two units, and the total internal energy of the system is the sum of the energies of the individual units, which in turn depend only on the number of up spins in the unit. We show that under suitable conditions on these interactions none of the $|\Lambda|$ Lee-Yang zeros in the complex $z = e^{2\beta h}$ plane, where β is the inverse temperature and h the uniform magnetic field, touch the positive real axis, at least for large values of β . In some cases one obtains, in an appropriately taken $\beta \nearrow \infty$ limit, a gas of hard objects on a set Λ' ; the fugacity for the limiting system is a rescaling of z and the Lee-Yang zeros of the new partition function also avoid the positive real axis. For certain forms of the energies of the individual units the Lee-Yang zeros of both the finite- and zero-temperature systems lie on the negative real axis for all β . One zero-temperature limit of this type, for example, is a monomer-dimer system; our results thus generalize, to finite β , a well-known result of Heilmann and Lieb that the Lee-Yang zeros of monomer-dimer systems are real and negative. © 2012 American Institute of Physics. [<http://dx.doi.org/10.1063/1.4738622>]

Dedicated to Elliott Lieb on the occasion of his eightieth birthday, in friendship and admiration.

I. INTRODUCTION

We consider a system of Ising spins on a finite set Λ of sites; we often think of Λ as a subset of some lattice \mathbb{L} . Writing $\underline{\sigma} = (\sigma_i)_{i \in \Lambda}$, with $\sigma_i = \pm 1$, for a spin configuration, we let $N = N(\underline{\sigma}) = \sum_{i \in \Lambda} (1 + \sigma_i)/2$ be the total number of up spins. We will sometimes think of this system as a lattice gas in which $\eta_i = (1 + \sigma_i)/2$ is the indicator of a particle at site i ; N is then the total number of particles in the system and $N/|\Lambda|$, with $|\Lambda|$ the number of sites, the average density ρ . The average magnetization per site is $m = |\Lambda|^{-1} \sum \sigma_i = |\Lambda|^{-1} (2N - |\Lambda|) = 2\rho - 1$. The thermodynamic properties of this system are determined¹ by the partition function,

$$Z_\Lambda(z, \beta) = \sum_{\underline{\sigma}: \Lambda \rightarrow \pm 1} z^{N(\underline{\sigma})} e^{-\beta U(\underline{\sigma})}, \quad (1.1)$$

where $U(\underline{\sigma})$ is the internal energy of the configuration $\underline{\sigma}$, β is the inverse temperature, and z is the magnetic fugacity, that is, $z = e^{2\beta h}$ with h the magnetic field. Z_Λ is a polynomial in z of order $|\Lambda|$, with positive coefficients.

The zeros in the complex fugacity plane of $Z_\Lambda(z, \beta)$, usually called Lee-Yang zeros, have been of interest since the original studies of Yang and Lee² and Lee and Yang.³ For finite systems none of the $|\Lambda|$ zeros can lie on the physically relevant positive real axis. But when Λ is a subset of some periodic lattice \mathbb{L} and $U(\underline{\sigma})$ is the restriction to Λ of a translation invariant energy (with some boundary conditions), so that we may speak of the thermodynamic limit $\Lambda \nearrow \mathbb{L}$, the zeros can in this limit approach the real axis, signaling (typically) the existence of a phase transition in the model.² The nature of the phase transition depends on the manner in which the zeros approach the positive z

axis as β or other parameters in U are changed. Speaking loosely, there will be a discontinuity in the magnetization per site, that is, a first order transition, at a value H of the magnetic field if the density of zeros on the real axis at $z = e^{2\beta H}$ is nonzero, and a higher order transition if there is a nonzero density arbitrarily close to this point.²

In their second paper,³ Lee and Yang proved that for the Ising model with ferromagnetic pair interactions, that is, for

$$U(\sigma) = - \sum_{\{i,j\} \in \Lambda, i \neq j} J_{ij} \sigma_i \sigma_j, \quad (1.2)$$

with all $J_{ij} \geq 0$, all the zeros of Z_Λ lie on the unit circle $|z| = 1$. Consequently, the only possible thermodynamic phase transition in this system takes place at $z = 1$ or $h = 0$. The Lee-Yang theorem has been extended in many ways to a variety of classical and quantum systems; see Refs. 4 and 5 for reviews. One can also prove in many cases that there is indeed a first order phase transition at sufficiently large β , so that the zeros must have a nonzero density at $z = 1$ in the thermodynamic limit.

Much less is known rigorously for general spin systems in which the zeros do not lie on the unit circle. This has led to numerical studies of these zeros for Λ a subset of a lattice \mathbb{L} ; in particular, the cases in which \mathbb{L} is either \mathbb{Z}^2 or the planar triangular lattice, and in which the internal energy is given by (1.2) with uniformly antiferromagnetic nearest-neighbor interactions, that is, with $J_{ij} = J\delta_{|i-j|,1}$, $J < 0$, have been investigated extensively.⁶⁻⁸ These systems can be proven to undergo phase transitions in the thermodynamic limit $\Lambda \nearrow \mathbb{L}$, for large values of β , at nonzero values of h .⁹⁻¹¹ This implies that the zeros of their partition functions must converge to the real axis at some point $z(\beta) \neq 1$. More recently, there have also been results for systems in which the zeros lie on the unit circle for large β but not for small β .¹² In some cases they touch the real axis, either for finite β or in the limit $\beta \nearrow \infty$.

There have also been many studies of the Lee-Yang zeros of the grand canonical partition function for general interacting particle systems on lattices or in the continuum. Of particular interest to us is the case of “hard” interactions, in which for every particle configuration η either $U(\eta) = 0$ or $U(\eta) = \infty$; put another way, some configurations are forbidden, while all others have no internal energy. Systems with such interactions can often be obtained as a suitable $\beta \rightarrow \infty$ limit of (1.2). In many interesting cases one may then think of the model as a system of particles (which may or may not correspond to the original particles) with fixed shapes, like dimers, diamonds, or hexagons, which cover more than one lattice site and which cannot overlap. For such systems temperature plays no role, so that the partition function does not depend on β ; we will write y for the fugacity of the new particles and $Q_\Lambda(y)$ for the corresponding partition function. It has been shown, in particular, for the case of dimers (on an arbitrary graph) that the zeros of $Q_\Lambda(y)$ all lie on the negative real y axis;¹³ any system with this property will of course not have any phase transitions in the thermodynamic limit. On the other hand, hard diamonds on \mathbb{Z}^2 and hard hexagons on the triangular lattice do have a phase transition in the thermodynamic limit.^{9,14,15}

In this note we will first describe a new class of Ising systems for which no zeros touch the positive real axis, at least for large β (low temperature). In some of these systems all the zeros lie on the negative real axis, either for all values of β or for large β ; in others, the zeros are excluded from some wedge $-\phi < \arg z < \phi$, where $0 < \phi < \pi$. We will then investigate the “hard” systems obtained from some of these, after suitable rescaling, in the limit $\beta \rightarrow \infty$; these systems will similarly have no zeros of $Q(y)$ encroaching on the real y axis and hence no phase transition. The models obtained in this way include the monomer-dimer model¹³ and the graph-counting models of Refs. 16 and 17; our results thus generalize these latter results to a wider class of “hard” systems and to related low-temperature models.

II. A CLASS OF SYSTEMS WITH LEE-YANG ZEROS BOUNDED AWAY FROM THE POSITIVE REAL AXIS

We consider Ising spin systems decomposable into subsystems, called *units*, with the property that each site belongs to either one or two units. Examples include the (three-dimensional) pyrochlore

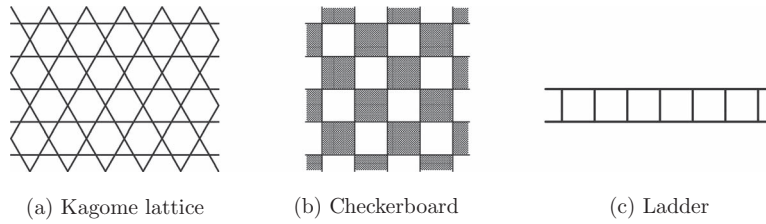


FIG. 1. Lattices decomposable into units with each site in two units.

lattice,^{18,19} in which the units are tetrahedra, the (two-dimensional) kagome lattice (Figure 1(a)), in which the units may be taken to be either the triangles or the hexagons, the *checkerboard*,^{12,20} in which the units are the alternate squares of the two dimensional square lattice (Figure 1(b)), and the *ladder*, in which every square is a unit (Figure 1(c)). We use the notation of Sec. I and write Λ_α for the set of sites of the α th unit, with $|\Lambda_\alpha| = n_\alpha$, and $\underline{\sigma}_\alpha$ for the spin configuration and $N_\alpha = N_\alpha(\underline{\sigma}_\alpha) = N_\alpha(\underline{\sigma})$ for the total number of up spins in the α th unit. Note that, in general, $N(\underline{\sigma}) \leq \sum_\alpha N_\alpha(\underline{\sigma}) \leq 2N(\underline{\sigma})$, since a site i with $\sigma_i = 1$ may belong to either one or two units.

The internal energy $U(\underline{\sigma})$ of the system is assumed to be the sum of the internal energies of the units,

$$U(\underline{\sigma}) = \sum_\alpha U_\alpha(\underline{\sigma}_\alpha), \quad (2.1)$$

and these are assumed to be symmetric in the spins of the unit, so that

$$U_\alpha(\underline{\sigma}) = F_\alpha(N_\alpha(\underline{\sigma})), \quad (2.2)$$

with F_α a polynomial of degree at most n_α . We can think of (2.2) as a mean field interaction among the spins in Λ_α . The partition functions (1.1) for a single unit and for the entire system thus become

$$Z_{\Lambda_\alpha}(z, \beta) = \sum_{\sigma_i = \pm 1, i \in \Lambda_\alpha} z^{N_\alpha(\underline{\sigma}_\alpha)} e^{-\beta F_\alpha(N_\alpha(\underline{\sigma}_\alpha))} = \sum_{l=0}^{n_\alpha} \binom{n_\alpha}{l} z^l e^{-\beta F_\alpha(l)}, \quad (2.3)$$

$$Z_\Lambda(z, \beta) = \sum_{\sigma_i = \pm 1} z^{N(\underline{\sigma})} e^{-\beta \sum_\alpha F_\alpha(N_\alpha(\underline{\sigma}))}. \quad (2.4)$$

We will prove in Sec. III that under certain conditions on the function F_α the Lee-Yang zeros of $Z_\Lambda(z, \beta)$ are bounded away from the positive real z axis at low temperature or, under stronger conditions, must lie on the negative real axis. The next result shows that such bounds on the zeros of $Z_\Lambda(z, \beta)$ follow from similar bounds on the zeros of $Z_{\Lambda_\alpha}(z, \beta)$.

Theorem 2.1: *Suppose that the angle ϕ satisfies $0 \leq \phi < \pi/2$. If each zero ζ of $Z_{\Lambda_\alpha}(z, \beta)$ satisfies*

$$\zeta \neq 0, \quad \pi - \phi \leq \arg \zeta \leq \pi + \phi, \quad (2.5)$$

then each zero ζ' of $Z_\Lambda(z, \beta)$ satisfies

$$\zeta' \neq 0, \quad \pi - 2\phi \leq \arg \zeta' \leq \pi + 2\phi. \quad (2.6)$$

In particular, if each ζ is real and negative, so is each ζ' .

Before proceeding to the proof of the theorem we give a simple example.

Example 2.2: If unit α has antiferromagnetic pair interactions of equal strength between every pair of sites then its internal energy may be written, after adding a constant, as

$$F_\alpha(N_\alpha(\underline{\sigma}_\alpha)) = -J \sum_{\{i,j\} \subset \Lambda_\alpha, i \neq j} (\sigma_i \sigma_j - 1) = -2|J| N_\alpha(n_\alpha - N_\alpha), \quad J < 0. \quad (2.7)$$

We consider several cases in which each unit has energy of the form (2.7).

- (a) *The one-dimensional nearest neighbor antiferromagnetic Ising model, defined on $\Lambda = \{1, \dots, n\}$, may be regarded as a model of this type in which the units are the pairs $\alpha_i = \{i, i + 1\}$, all with the same coupling J . From (2.7) we then have $Z_{\Lambda_{\alpha_i}}(z, \beta) = z^2 + 2az + 1$ with $a = e^{2\beta|J|} > 1$; this polynomial has two negative real zeros and hence, by Theorem 2.1, the zeros $Z(z, \beta)$ are negative real.*
- (b) *When the only interactions considered for the checkerboard of Figure 1(b) are pair interactions then one may term the system the pyrochlore checkerboard,²⁰ since if each pair of vertices in a square are connected with edges one obtains a planar representation of a tetrahedron. To be concrete we choose, for example, a $2L \times 2L$ lattice with doubly periodic boundary conditions. It is then possible to check that with the unit energy (2.7), with of course $n_\alpha = 4$, all four zeros of $Z_{\Lambda_\alpha}(z, \beta)$ are on the negative real axis (this is in fact verified for arbitrary values of n_α in Theorem 3.1 below). Theorem 2.1 then states that the zeros of Z_Λ will all lie on the negative real axis; since this remains true as $\Lambda \nearrow \mathbb{Z}^2$, the system will not have a phase transition at any finite temperature. In fact, the pressure and all correlations will be analytic functions of h for all $h \in \mathbb{R}$.*
- (c) *The ladder (Figure 1(c)) illustrates the fact that two units may share several vertices and thus an edge. Note, however, that the form (2.2) of the total energy implies, with (2.7), that the coupling constant for these shared edges (vertical in Figure 1(c)) is twice that for the unshared (horizontal) edges.*

A. Proof of Theorem 2.1

The proof of Theorem 2.1 depends on two standard results, which we quote for completeness; see the Appendix of Ref. 21 for more details. We let \mathcal{A}_n denote the space of complex polynomials in z_1, \dots, z_n which are separately affine in each variable, and observe that if P is a complex polynomial of degree at most n then there is a unique symmetric $\hat{P} \in \mathcal{A}_n$ such that $\hat{P}(z, \dots, z) = P(z)$. A closed circular region is a closed subset K of \mathbb{C} bounded by a circle or a straight line.

Theorem 2.3 (Grace’s theorem): *Let P be a complex polynomial in one variable of degree at most n . If the n roots of P are contained in a closed circular region K and $z_1 \notin K, \dots, z_n \notin K$, then $\hat{P}(z_1, \dots, z_n) \neq 0$.*

If P is in fact of degree k with $k < n$ then we say that $n - k$ roots of P lie at ∞ and take K noncompact. For a proof of the result see Polya and Szegő²² Sec. V, exercise 145.

Lemma 2.4 (Asano-Ruelle) (Refs. 23 and 24): *Let K_1, K_2 be closed subsets of \mathbb{C} , with $K_1, K_2 \not\cong 0$. If Φ is separately affine in z_1 and z_2 , and if*

$$\Phi(z_1, z_2) \equiv A + Bz_1 + Cz_2 + Dz_1z_2 \neq 0,$$

whenever $z_1 \notin K_1$ and $z_2 \notin K_2$, then

$$\tilde{\Phi}(z) \equiv A + Dz \neq 0,$$

whenever $z \notin -K_1 \cdot K_2$. [We have written $-K_1 \cdot K_2 = \{-uv : u \in K_1, v \in K_2\}$].

The map $\Phi \mapsto \tilde{\Phi}$ is called *Asano contraction*; we denote it by $(z_1, z_2) \rightarrow z$. To state the next result we define, for $\epsilon > 0$ and $-\pi/2 < \theta < \pi/2$, $K_\theta(\epsilon) = \{z: \text{Re}[e^{i\theta}(z + \epsilon)] \leq 0\}$.

Lemma 2.5: If ϕ is as in Theorem 2.1 and P is a complex polynomial each of whose zeros ζ satisfies (2.5), then for any θ with $|\theta| < \pi/2 - \phi$ there is an $\epsilon > 0$ such that $\hat{P}(z_1, \dots, z_n) \neq 0$ when $z_1, \dots, z_n \notin K_\theta(\epsilon)$.

Proof: Clearly there is an $\epsilon > 0$ such that $P(z) \neq 0$ when $z \notin K_\theta(\epsilon)$, and the result follows from Grace's theorem. \square

Lemma 2.6: Suppose that ϕ is as in Theorem 2.1 and that $P_i(z), i = 1, \dots, I$, is a polynomial of degree n_i each of whose zeros ζ satisfies (2.5). Suppose further that the polynomial $\hat{Q}(z_1, \dots, z_n)$ is obtained from the product

$$\prod_{i=1}^I \hat{P}_i(z_{i,1}, \dots, z_{i,n_i}),$$

by a sequence of Asano contractions $(z_{i,j}, z_{k,l}) \rightarrow z_m$ or relabelings $z_{i,j} \rightarrow z_m$. Then each zero ζ' of $Q(z)$ satisfies (2.6).

Proof: For each θ with $|\theta| < \pi/2 - \phi$ we obtain from Lemma 2.5 and the Asano-Ruelle lemma that for some $\epsilon > 0$, $\hat{Q}(z_1, \dots, z_n) \neq 0$ when each of z_1, \dots, z_n lies in the complement of the set $-K_\theta(\epsilon) \cdot K_\theta(\epsilon)$. Thus $Q(z) \neq 0$ when z is in the complement of $-K_\theta(\epsilon) \cdot K_\theta(\epsilon)$. This complement is the interior of a parabola with focus at 0 and, in particular, contains the ray making an angle 2θ with the positive real axis. As θ varies in $\theta \in (-\pi/2 + \phi, \pi/2 - \phi)$ this ray sweeps out the complement of the region defined by (2.6). \square

We can now give the proof of the main result.

Proof of Theorem 2.1: The main statement of the theorem is an immediate consequence of Lemma 2.6, since $\hat{Z}(z_1, \dots, z_{|\Lambda|})$ is obtained from $\prod_{\alpha} \hat{Z}_{\alpha}(z_{\alpha 1}, \dots, z_{\alpha n_{\alpha}})$ by Asano contractions and relabelings. The last statement follows by taking $\phi = 0$. \square

In Sec. III A below we will need the following corollary of Lemma 2.6.

Corollary 2.7: Suppose that $P(z)$ is a polynomial of degree n for which each zero ζ is real and negative. If \hat{Q} is obtained from \hat{P} by squaring all coefficients, then each zero ζ' of Q is real and negative.

Proof: Take $\phi = 0$, $I = 2$ and $P_1 = P_2 = P$ in Lemma 2.6 and make all contractions $(z_{1j}, z_{2j}) \rightarrow z_j$. \square

III. ZEROS OF THE PARTITION FUNCTION OF A SINGLE UNIT

In this section we consider a particular unit α with n_{α} sites, energy $F_{\alpha}(N_{\alpha})$, and partition function $Z_{\Lambda_{\alpha}}$, and address the question implicitly raised by Theorem 2.1: when are all zeros of the function $Z_{\Lambda_{\alpha}}$ confined to a sector of the form (2.5) for some ϕ ? In Sec. III A we give a criterion which guarantees that for all β these zeros satisfy (2.5) with $\phi = 0$, and in Sec. III B several criteria implying bounds of the form (2.5) for various values of ϕ .

A. A quadratic interaction energy

Theorem 3.1: Suppose that $F_{\alpha}(l)$ is quadratic with positive leading coefficient: $F_{\alpha}(l) = al^2 + bl + c$ with $a > 0$. Then for any $\beta \geq 0$ all zeros of $Z_{\Lambda_{\alpha}}(z, \beta)$ are real and negative.

Note that if $F_{\alpha}(l) = al^2 + bl + c$ then the constant c is irrelevant, the constant b represents a shift in the magnetic field, and the constant a may be absorbed into the inverse temperature; thus we may (and will) assume without loss of generality that $F_{\alpha}(l) = -l(n - l)$. In the spin language this is an energy in which every pair of spins in the unit is coupled with the same antiferromagnetic

interaction and there is a uniform magnetic field, as in example 2.2; in the lattice gas language particles on each pair of sites interact with the same positive repulsive potential and there is a uniform chemical potential.

Lemma 3.2: If $b > 0$, the polynomial

$$P_{(b)}(z) = \sum_{l=0}^n \binom{n}{l} (1 + bl(n-l))z^l$$

has only real negative zeros.

Proof: We have

$$\begin{aligned} P_{(b)}(z) &= (z+1)^n + bn(n-1) \sum_{l=1}^{n-1} \binom{n-2}{l-1} z^l \\ &= (z+1)^n + bn(n-1)z(z+1)^{n-2} \\ &= (z+1)^{n-2}[z^2 + (2 + bn(n-1))z + 1], \end{aligned}$$

which has only real negative zeros.

Proof of Theorem 3.1: Starting from $P_{(2^{-k}\beta)}$ as in Lemma 3.2, we obtain by k applications of Corollary 2.7 that the polynomial

$$\sum_{l=0}^n \binom{n}{l} (1 + \beta l(n-l)2^{-k})^k z^l \quad (3.1)$$

has only real negative zeros. Letting $k \rightarrow \infty$ we find that

$$Z_{\Lambda_\alpha}(z, \beta) = \sum_{l=0}^n \binom{n}{l} e^{\beta l(n-l)} z^l \quad (3.2)$$

has only nonpositive real zeros, and we need only observe that the constant term in (3.2) is nonzero. \square

Remark 3.3:

- (a) If we consider the system to be comprised of a single unit, i.e., take $\Lambda_\alpha = \Lambda$, then Theorem 3.1 implies that in the mean-field Ising model with antiferromagnetic interactions all Lee-Yang zeros lie on the negative real axis.
- (b) If we consider this same system but with ferromagnetic pair interactions, which is equivalent to taking $\beta < 0$ in (3.2), then the standard Lee-Yang theory implies that all zeros of Z_Λ lie on the unit circle.

B. A convex interaction energy

When F_α is as in Theorem 3.1 it is convex on the range $0 \leq l \leq n_\alpha$ in the sense that

$$2F_\alpha(l) \leq F_\alpha(l+1) + F_\alpha(l-1), \quad l = 1, \dots, n_\alpha - 1. \quad (3.3)$$

In this section we consider a unit energy $F_\alpha(l)$, not necessarily quadratic, which satisfies (3.3).

We begin by introducing some notation to describe such an F_α more precisely. Let $0 = k_0 < k_1 < \dots < k_{r-1} < k_r = n_\alpha$ be indices such that strict inequality holds in (3.3) if and only if $l = k_i$ for some i with $1 \leq i \leq r-1$. To understand the role of these indices it is helpful to introduce a geometric interpretation. Let $f_\alpha(x)$ be defined on the interval $[0, n_\alpha]$ as the linear interpolation of the nodes $(l, F_\alpha(l))$, $l = 0, 1, \dots, n_\alpha$, and let $f_\alpha^* \subset \mathbb{R}^2$ be the *epigraph* of f_α : $f_\alpha^* = \{(x, y) \mid x \in [0, n_\alpha], y \geq f_\alpha(x)\}$. Then f_α^* is a convex subset of \mathbb{R}^2 with two vertical faces and r nonvertical faces. The vertices of f_α^* are the nodes $(k_i, F_\alpha(k_i))$; all other nodes $(l, F_\alpha(l))$ are interior points of the (nonvertical) faces of f_α^* . See Figure 2. For $1 \leq i \leq r$ we define $H_{\alpha, i}$ to be the

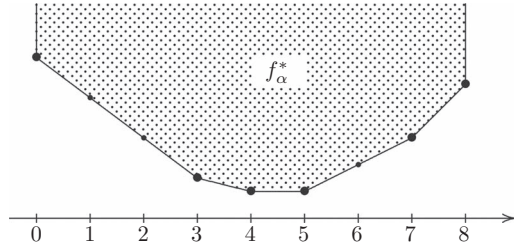


FIG. 2. Typical set f_α^* , with $n_\alpha = 8$, $r = 5$, and $(k_0, \dots, k_5) = (0, 3, 4, 5, 7, 8)$. Nodes $(l, F_\alpha(l))$ are indicated by dots, with heavier dots when $l = k_i$ for some i .

slope of the (nonvertical) face of f_α^* containing $(k_{i-1}, F_\alpha(k_{i-1}))$ and $(k_i, F_\alpha(k_i))$, and note that $H_{\alpha,i} = F_\alpha(l) - F_\alpha(l - 1)$ whenever $k_i - 1 < l \leq k_i$. Finally, for $h \in \mathbb{R}$ we define

$$E_\alpha(h) = \min_{0 \leq l \leq n} (F_\alpha(l) - hl). \tag{3.4}$$

We will be interested in Sec. IV in the set $S_\alpha(h)$ of values of l on which the minimum in (3.4) is realized; clearly if h is not equal to any of the $H_{\alpha,i}$ then $S_\alpha(h)$ contains a unique l , while for $h = H_{\alpha,i}$ it contains those l for which $(l, F_\alpha(l))$ lies in the i th nonvertical face of f_α^* .

The next result shows that at low temperature the zeros of Z_{Λ_α} fall into r groups, where the i th group is naturally associated with the i th nonvertical face of f_α^* and contains $k_i - k_{i-1}$ points, all with magnitude of order $e^{-\beta H_{\alpha,i}}$.

Lemma 3.4: For $i = 1, \dots, r$ let

$$R_i(t) = \sum_{j=k_{i-1}}^{k_i} \binom{n_\alpha}{j} t^{j-k_{i-1}}$$

and let $t_{i,1} \dots t_{i,k_i-k_{i-1}}$ be the zeros of R_i . Then one may number the zeros z_1, \dots, z_{n_α} of Z_{Λ_α} in such a way that for $k_{i-1} < j \leq k_i$,

$$\lim_{\beta \rightarrow \infty} z_j e^{\beta H_{\alpha,i}} = t_{i,j-k_{i-1}}.$$

Proof: For $l < k_{i-1}$ or $l > k_i$ the coefficient of t^l in the polynomial

$$\begin{aligned} \hat{R}_{\beta,i}(t) &= e^{\beta E_\alpha(H_{\alpha,i})} Z_{\Lambda_\alpha}(t e^{\beta H_{\alpha,i}}, \beta) \\ &= t^{k_{i-1}} R_i(t) + \sum_{l < k_{i-1} \text{ or } l > k_i} \binom{n_\alpha}{l} t^l e^{-\beta(F_\alpha(l) - H_{\alpha,i}l - E_\alpha(H_{\alpha,i}))} \end{aligned}$$

converges to zero as $\beta \nearrow \infty$. Thus, k_{i-1} of the roots converges to 0, $n_\alpha - k_i$ to infinity, and the remaining $k_i - k_{i-1}$ to the roots of R_i .²⁵ \square

To state the main result of this section we let $\delta = \max_{1 \leq i \leq r} (k_i - k_{i-1})$; $\delta + 1$ is the maximum number of nodes lying on any nonvertical face of f_α^* .

Theorem 3.5:

- (a) If $\delta = 1$, i.e. if all the inequalities in (3.3) are strict, then all roots of Z_{Λ_α} are real and negative for sufficiently large β .
- (b) If $\delta = 2$ then all roots of Z_{Λ_α} satisfy (2.5) with $\phi = \pi/3$ for sufficiently large β .
- (c) If $\delta = 3$ then there is an angle ϕ_{n_α} , which as indicated may be chosen to depend only on n_α , such that $\phi_{n_\alpha} < \pi/2$ and such that all roots of Z_{Λ_α} satisfy (2.5) with $\phi = \phi_{n_\alpha}$ for sufficiently large β .

- (d) If $k_1 \leq 4$ and $k_{r-1} \leq n_\alpha - 4$ with at least one of these an equality, and $k_i - k_{i-1} \leq 3$ for $i = 2, \dots, r - 1$ so that $\delta = 4$, then there is an angle $\phi_{n_\alpha} < \pi/2$ such that all roots of Z_{Λ_α} satisfy (2.5) with $\phi = \phi_{n_\alpha}$ for sufficiently large β .

Proof:

- (a) When $\delta = 1$ each of the polynomials $R_i(t)$ is linear, with a negative real root. From Lemma 3.4 the roots of Z_{Λ_α} for large β must be widely separated in magnitude, and since any complex roots among these occur in complex conjugate pairs, the roots must in fact be real.
- (b) It follows from Lemma 3.4 that $\arg z_j \rightarrow \arg t_{i,j-k_{i-1}}$ as $\beta \nearrow \infty$, so that it suffices to show that each root t_{ij} satisfies $|\arg t_{ij} - \pi| < \pi/3$. When $\delta = 2$ the $R_i(t)$ are either linear, with roots having argument π , or quadratic; in the latter case the quadratic formula shows that the roots t_{ij} are complex, have negative real part, and satisfy

$$\left| \frac{\operatorname{Im} t_{ij}}{\operatorname{Re} t_{ij}} \right| = \sqrt{\frac{4(k_i - 1)(n_\alpha + 1 - k_i)}{k_i(n_\alpha + 2 - k_i)} - 1} < \sqrt{3}, \quad (3.5)$$

which yields the desired bound. Improved bounds on the roots for specific values of k_i and n_α may be obtained from (3.5). For example, if $i = 1$ then $k_1 = 2$ and one obtains (2.5) with $\phi = \pi/4$ for the smallest (in magnitude, at large β) two zeros of Z_{Λ_α} , a result closely related to earlier work of Ruelle,¹⁶ as we discuss in Sec. V.

- (c) When $\delta = 3$ the polynomials R_i can be linear, quadratic, or cubic; following the analysis of (b) it suffices to show that in the cubic case all roots have negative real part. Up to a constant factor any such cubic R_i has the form

$$k(k-1)(k-2) + k(k-1)(n+3-k)t + k(n+3-k)(n+2-k)t^2 + (n+3-k)(n+2-k)(n+1-k)t^3, \quad (3.6)$$

where $n = n_\alpha$ and $k = k_i$. For $n = k = 3$ this polynomial has a triple root at $z = -1$; we may then vary n and k continuously to some desired values and ask whether roots can cross the imaginary axis during this procedure. We may assume that the intermediate values of n, k remain real and satisfy $n, k \geq 3$ and $n - k \geq 0$. Suppose (3.6) vanishes for $t = is$, s real. We cannot have $s = 0$ since $k(k+1)(k+2) \neq 0$. For $s \neq 0$ we would have both

$$(k-1)(k-2) = (n-k+2)(n-k+3)s^2$$

and

$$k(k-1) = (n-k+1)(n-k+2)s^2,$$

so that $(n-k+1)(k-2) = k(n-k+3)$, i.e., $n+1=0$, in contradiction with $n \geq 3$.

- (d) We suppose that $k_1 = 4$; the analysis when $k_{r-1} = n_\alpha - 4$ is the same. With the results (a)–(c) above it suffices to show that the roots of

$$R_1(t) = \sum_{l=0}^4 \binom{n_\alpha}{l} t^l \quad (3.7)$$

satisfy an appropriate bound of the form (2.5). The roots of $R_1(t)$ are all equal to -1 for $n_\alpha = 4$ and, treating n_α as a continuous variable, can have the form $t = is$, s real, only for n_α a root of $n^2 + 9n - 4 = 0$; as both the roots of this polynomial are less than 4 the roots of R_1 for $n_\alpha > 4$ must all lie strictly in the left half plane.

Remark 3.6:

- (a) A classical result of Newton provides a converse to Theorem 3.5(a): if all roots of Z_{Λ_α} are real for some β then either equality holds for all l in (3.3), in which case $F_\alpha(l) = A + Bl$ for some A, B , there are no interactions, and all roots of Z_{Λ_α} are equal, or strict inequality holds for all l in (3.3). For a proof see p. 104 of Ref. 26. Other related results are contained in Refs. 27–29. In particular, (a) of the theorem follows from the result of Ref. 27.

(b) By taking $k \approx n_\alpha/2$ one sees that there is no bound (2.5) on the roots of (3.6) which is uniform in n_α and k and satisfies $\phi < \pi/2$. On the other hand, one can show that such a uniform bound may be found both for the roots of (3.6) for fixed k and for the roots of (3.7).

C. An example: Quartic and quadratic interactions

As an example we consider a unit with two and four spin interactions which satisfy spin flip symmetry. In the particle language described in Sec. I the energy is

$$U_\alpha(\underline{\sigma}) = -K_2 \sum_{1 \leq i < j \leq n} (\eta_i \eta_j + \hat{\eta}_i \hat{\eta}_j) - K_4 \sum_{\substack{X \subset \{1, \dots, n\} \\ |X|=4}} (\prod_{i \in X} \eta_i + \prod_{i \in X} \hat{\eta}_i),$$

where $\hat{\eta}_i = 1 - \eta_i$, i.e.,

$$F_\alpha(l) = -K_2 \left[\binom{l}{2} + \binom{n_\alpha - l}{2} \right] - K_4 \left[\binom{l}{4} + \binom{n_\alpha - l}{4} \right].$$

We assume that K_2 and K_4 are not both zero. The convexity condition (3.3) is satisfied with strict inequality for all l , if

$$2K_2 + \frac{K_4}{2} [(l - 1)(l - 2) + (n_\alpha - l - 1)(n_\alpha - l - 2)] < 0$$

for $l = 1, \dots, n - 1$. This happens when

$$\theta_{n_\alpha} < \arg(K_2 + iK_4) < \phi_{n_\alpha}, \tag{3.8}$$

where the angles ϕ_n and θ_n are given by

$$\begin{aligned} \tan \theta_n &= -\frac{4}{(n-2)(n-3)}, & \pi/2 \leq \theta_n < \pi, \\ \tan \phi_n &= \begin{cases} -\frac{8}{(n-2)(n-4)}, & \text{if } n \text{ is even,} \\ -\frac{8}{(n-3)^2}, & \text{if } n \text{ is odd,} \end{cases} & 3\pi/2 \leq \phi_n < 2\pi. \end{aligned}$$

See Figure 3. Under condition (3.8), Theorem 3.5(a) implies that Z_{Λ_α} has its zeros on the negative real axis at low temperature, and hence by Theorem 2.1 so does Z_Λ , if all units in the system are of this type. Note that, in particular, (3.8) includes the negative K_2 -axis, where we know from Theorem 3.1 that the zeros are real and negative at all temperatures. For nonzero values of K_2 and K_4 not satisfying (3.8), Remark 3.6(a) implies that the zeros do not lie exclusively on the real z axis for any β .

If we specialize further to the case $n_\alpha = 4$, in which $\theta_n = \tan^{-1}(-2)$ and $\phi_n = 3\pi/2$, then the region in the space of interactions at which all zeros are on the negative real axis can be computed

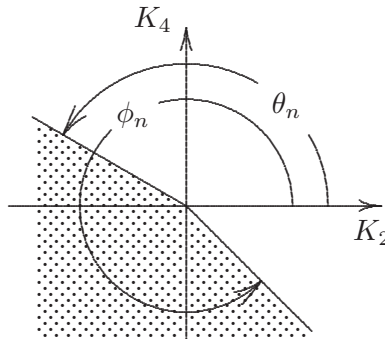


FIG. 3. In the shaded region (which extends to infinity in both the x and y directions) all zeros are real and negative at low temperature.

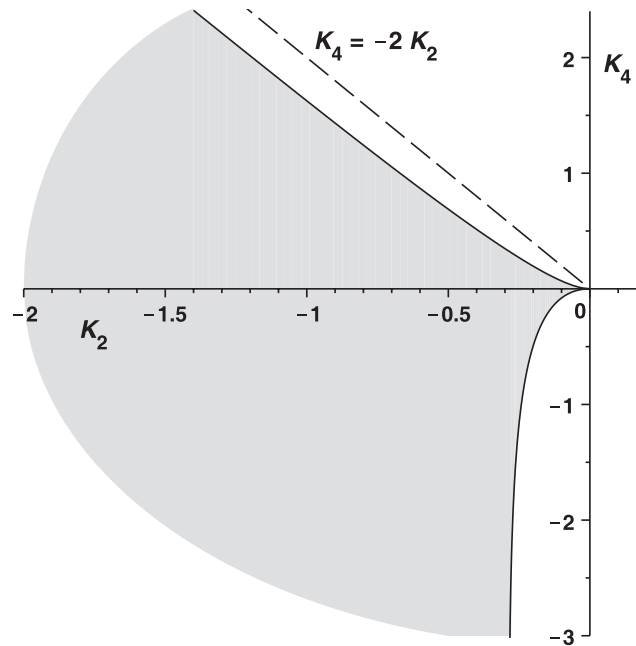


FIG. 4. The case $n_\alpha = 4$. When $\beta = 1$ all zeros are real and negative if and only if (K_2, K_4) lies in the shaded region (which extends to infinity in both the x and y directions).

exactly. Since a change of temperature is equivalent to a rescaling of (K_2, K_4) it is convenient to take $\beta = 1$; then this region is given by

$$\log \left[\frac{3 - \sqrt{9 - 8a^2}}{2a^4} \right] > K_4 > \begin{cases} \log \left[\frac{4a-3}{a^4} \right], & \text{if } K_2 > \log(3/4), \\ -\infty, & \text{otherwise,} \end{cases}$$

where $a = e^{K_2}$. See Figure 4. The computation follows that in the proof of Proposition 6 of Ref. 12, and we omit details.

IV. GROUND STATES AND ZERO TEMPERATURE LIMITS

Consider a system which is assembled from units, as described in Sec. II, such that the energy F_α for each unit is convex in the sense of (3.3). In this section we suppose further that each site belongs to exactly two units.

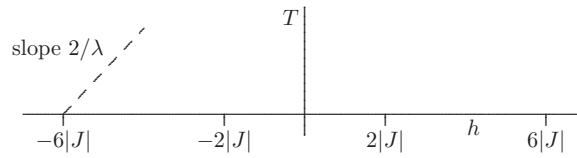
Let us fix, for the moment, a magnetic field h_0 . The total energy of the system in spin configuration $\underline{\sigma}$, including the magnetic energy, is then

$$U(\underline{\sigma}) - 2h_0N(\underline{\sigma}) = \sum_\alpha [F_\alpha(N_\alpha(\underline{\sigma})) - h_0N_\alpha(\underline{\sigma})]. \tag{4.1}$$

From (4.1) and (3.4) it follows that this energy is bounded below by $E_0 = \sum_\alpha E_\alpha(h_0)$. On the other hand, if we recall the definition of $S_\alpha(h_0)$ given below (3.4) we see that E_0 is in fact the ground state energy of the system—the minimum value of (4.1)—if and only if it is possible to find a spin configuration $\underline{\sigma}$ such that $N_\alpha(\underline{\sigma}) \in S_\alpha(h_0)$ for each α . When this is true we say that the system is *not frustrated*.

Now we assume that our system is not frustrated and consider a zero temperature limit $\beta \nearrow \infty$ with a β -dependent fugacity $z(\beta) = e^{2\beta h(\beta)}$ such that $h(\beta) \rightarrow h_0$ as $\beta \nearrow \infty$; specifically, for some $\lambda \in \mathbb{R}$ we take

$$h(\beta) = h_0 + \frac{\lambda}{2\beta}. \tag{4.2}$$

FIG. 5. The h - T plane for the pyrochlore checkerboard with pair interactions.

In the h - T phase plane (where $T = 1/\beta$ is the temperature) this corresponds to approaching $(h_0, 0)$ along a line with slope $2/\lambda$.³⁰ Then with $y = e^\lambda$ the limiting partition function is

$$\begin{aligned} Q_\Lambda(y, h_0) &= \lim_{\beta \nearrow \infty} e^{\beta E_0} Z_\Lambda(z(\beta), \beta) \\ &= \lim_{\beta \nearrow \infty} \sum_{\sigma} y^{N(\sigma)} e^{-\beta(U(\sigma) - 2h_0 N(\sigma) - E_0)} = \sum_{\sigma \in \mathcal{G}(h_0)} y^{N(\sigma)}, \end{aligned} \quad (4.3)$$

where $\mathcal{G}(h_0)$ is the set of ground-state configurations. We are of course interested in the behavior of the zeros of Z_Λ under the limiting process (4.3). If $N_{\min}(h_0) = \min_{\sigma \in \mathcal{G}(h_0)} N(\sigma)$ and $N_{\max}(h_0) = \max_{\sigma \in \mathcal{G}(h_0)} N(\sigma)$ then N_{\min} zeros will converge to 0 and $|\Lambda| - N_{\max}$ to ∞ ,²⁵ while the remaining zeros converge to the (nonzero) roots of $y^{-N_{\min}} Q_\Lambda(y, h_0)$.

When for each α one has $|S_\alpha(h_0)| = 1$, that is, when $h_0 \neq H_{\alpha,i}$ for any α, i , there is a unique ground state configuration and $Q(y, h_0)$ is rather uninteresting. When there are many ground state configurations, however, they can in some cases be identified with configurations of “hard objects” and $Q(y, H_0)$ is then the partition function for these.

In the next example we illustrate these ideas by revisiting example 2.2(b). In Sec. V we describe a family of examples involving *graph-counting polynomials*.

Example 4.1: We consider again example 2.2(b): pair interactions on a $2L \times 2L$ pyrochlore checkerboard with doubly periodic boundary conditions. The unit energy of the model is given in (2.7), with $n_\alpha = 4$ for all α . Since the energy for all units has the same form $F_\alpha(l) = -2|J|l(4-l)$ we will omit the subscript α on F and similar quantities when no confusion can arise. The fields $H_l = F(l) - F(l-1)$ defined in Sec. III B are $H_1 = -6|J|$, $H_2 = -2|J|$, $H_3 = 2|J|$, and $H_4 = 6|J|$. For $H_l < h_0 < H_{l+1}$ (with $H_0 = -\infty$ and $H_5 = \infty$) the zero temperature limit along the line (4.2) is independent of λ and the ground state configurations each have exactly l up spins in each unit, that is, $N_\alpha = l$ for each α . If we take the $T \rightarrow 0$ limit of the partition function along a line (4.2) with $h_0 = H_l$ we obtain ground states in which both $N_\alpha = l$ and $N_\alpha = l-1$ are possible, with the total value of N controlled by the fugacity $y = e^\lambda$. The situation in the h - T plane is shown in Figure 5, with a typical line (4.2) for $h_0 = H_1 = -6|J|$.

We may interpret the ground state configurations in terms of hard objects by considering dimers on the new lattice Λ' obtained from Λ by shrinking each unit to a vertex and introducing an edge joining two of these points when the corresponding units share a site; Λ' is again a square lattice with certain periodic boundary conditions. An occupied site in Λ corresponds to a dimer covering the corresponding edge in Λ' , so that a ground state for $H_l < h_0 < H_{l+1}$, with $N_\alpha = l$ for each α , corresponds to a dimer configuration on Λ' in which every vertex is covered by exactly l dimers. In a ground state with $h_0 = H_l$ each site of Λ' is covered by either l or $l-1$ dimers. Thus, for example, for $h_0 = H_1 = -6|J|$ these are monomer-dimer configurations; for $h_0 = H_2 = -2|J|$ they are a restricted class of unbranched subgraphs.¹⁷ In each case, Theorem 3.5(a) implies that all zeros of the partition function lie on the negative real axis, a result originally obtained for the monomer-dimer system (in much more generality) in Ref. 13.

V. GRAPH-COUNTING POLYNOMIALS

Consider a graph G with sets V of vertices and E of edges, such that each edge connects a pair of distinct vertices. Note that such graphs may have several edges joining the same pair of vertices. We let d_0 be the maximum vertex degree in G . A *subgraph* M of G is a graph with vertex set V and edge set contained in E ; $|M|$ denotes the number of edges of M and for any vertex $v \in V$ we let $d_M(v)$ denote the vertex degree of v in M that is, number of edges of M incident on v .

A *graph-counting polynomial*¹⁶ is a polynomial

$$\tilde{Q}_C(y) = \sum_{M \in (C)} y^{|M|},$$

where (C) is the collection of subgraphs of G associated with some set C of non-negative integers via $(C) = \{M \mid d_M(v) \in C, \forall v \in V\}$. For $C = \{0, 1\}$, (C) is the class of *dimer subgraphs* of G ; in this case it was shown by Heilmann and Lieb¹³ that all the zeros of \tilde{Q}_C are real and negative. For $C = \{0, 1, 2\}$, (C) is the set of *unbranched subgraphs* of G and it is shown in Ref. 17 that the zeros of \tilde{Q}_C lie in the left half plane; results for other choices of C are given in Ref. 16. In this section we study \tilde{Q}_C for C a nonempty interval $C_{pq} = \{p, p+1, \dots, q\}$ of non-negative integers.

Given the graph G and the set C_{pq} we introduce a statistical mechanical system of the type described in Sec. II. In this system $\Lambda = E$; we may think of starting with a geometric realization of the graph and then putting a site of Λ at the center of each edge. For each $v \in V$ there is a unit α_v which contains those sites of Λ which correspond to edges of G incident on v . Since in G each edge is incident on two vertices, this system has the property, assumed in Sec. IV, that every site belongs to exactly two units. Finally, we introduce a unit energy $F(l)$, $l = 0, 1, \dots, d_0(G)$, the same for all units, which satisfies (3.3) and is such that, with k_i the indices defined in Sec. III B, (i) $p = k_{i-1}$ and $q = k_i$ for some i , and (ii) $k_j = k_{j-1} + 1$ for all $j \neq i$. In other words, the i th nonvertical face of the convex set f^* associated with F (see Figure 2) contains the nodes $(l, F(l))$ for $l = p, \dots, q$, and all other faces contain exactly two nodes.

Now consider the limit (4.3) with $h_0 = H_i = (F(q) - F(p))/(q - p)$. The ground state configurations at magnetization H_i are precisely those in which $N_{\alpha_v} \in C_{pq}$ for each v , and the assumption that the system is not frustrated is precisely the assumption that such configurations exist. Each such configuration, however, has an immediate interpretation as a subgraph of G : an edge $e \in E$ belongs to the subgraph if and only if the corresponding site in Λ is occupied (using the lattice gas language). With this identification the ground state configurations then give rise precisely to the subgraphs belonging to (C_{pq}) , and the limiting partition function $Q_\Lambda(y, H_i)$ is the same as the graph-counting polynomial $\tilde{Q}_{C_{pq}}(y)$.

The next result, which describes the behavior of the zeros of $Q_{C_{pq}}$ for certain choices of p, q , follows immediately from Theorem 3.5.

Theorem 5.1: *Suppose that p and q are such that (C_{pq}) is nonempty. Then:*

- (a) *If $q = p + 1$ then all the nonzero roots of $\tilde{Q}_{C_{pq}}(y)$ are real and negative.*
- (b) *If $q = p + 2$ then all the nonzero roots of $\tilde{Q}_{C_{pq}}(y)$ satisfy (2.6) with $\phi = \pi/3$.*
- (c) *If $q = p + 3$ then there is an angle ϕ , which may depend on p, q , and $d_0(G)$ but not on the size of the graph, such that $\phi < \pi/2$ and such that all the nonzero roots of $\tilde{Q}_{C_{pq}}(y)$ satisfy (2.6) with the angle ϕ .*
- (d) *If $p = 0$ and $q = 4$ or $p = d_0(G) - 4$ and $q = d_0(G)$ then there is an angle $\phi < \pi/2$, which depends on $d_0(G)$ but may be chosen uniformly in the size of G , such that all the nonzero roots of $\tilde{Q}_{C_{pq}}(y)$ satisfy (2.6) with the angle ϕ .*

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