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Zeros of Partition Functions via Correlation Inequalities

François Dunlop[1]

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We show analyticity of the pressure for some classical ferromagnetic systems in the region $\{|\mathrm{Im}\,\mu| < \mathrm{Re}\,\mu\}$ of the external field. The proof, via correlation inequalities, is simpler than existing proofs for the Lee and Yang region $\{\mathrm{Re}\,\mu \neq 0\}$ and applies, without any approximation procedure, to more general continuous spin variables, e.g., distributed as $\exp(-\kappa S^{6n} - \lambda S^{4n} + \sum_{p=1}^{n} \sigma_{2p} S^{2p})$, where σ_{2n} is an arbitrary real number and the other parameters are positive. It also applies directly to plane rotators in the region $\{|\mathrm{Im}\,\boldsymbol{\mu}| \leqslant |\mathrm{Re}\,\boldsymbol{\mu}|\}$ (Euclidean norms), but the proof will be given in a subsequent article, together with new inequalities between truncated correlation functions.

KEY WORDS: Lee–Yang zeros; correlation inequalities; ferromagnetic.

1. INTRODUCTION

Let $Z((\mu_j)_{j=1,\dots,N})$ be the partition function for a classical ferromagnetic system, with two-body interactions, in a complex external field $\mu_j = x_j + iy_j$ (at site j). We show that $|Z|^2$ has a positive expansion in the couplings J_{ij} and the combinations $x_j \pm y_j$ of the external field. In particular the partition function does not vanish when

$$|y_j| \leqslant x_j, \qquad \forall j$$

The positive coefficients in the expansion are integrals of products of

$$(S_j + S_j') \pm i(S_j - S_j'), \qquad j = 1,\dots, N \tag{1}$$

where S_j is the "spin" at site j and S_j' is an independent copy. The expressions (1) define characters on the circle group, by means of polar coordinates.

[1] Institut des Hautes Etudes Scientifiques, 91440 Bures-sur-Yvette, France.

The method will therefore apply when the duplicated individual distributions are positive definite in terms of these variables (there is some freedom in the choice of the radial variable).

Besides the Ising model, this includes the density

$$\exp\left(-\kappa S^{6n} - \lambda S^{4n} + \sum_{p=1}^{n} \sigma_{2p} S^{2p} \right) \tag{2}$$

where σ_{2n} is free (real) and the other parameters are positive (or zero, but the measure should be finite).

The sign requirements give us a familiar potential with one or two minima. More general situations should be allowed (e.g., two symmetric wide and deep wells, absolute minima, and anything between them), but we have only an implicit result: We allow the density

$$\exp(-\kappa S^6 + \lambda S^4 - \sigma S^2) \text{ with } \sigma \leqslant 3 \frac{\int_0^\infty \rho^5 \exp(-\kappa\rho^6 + \lambda\rho^4 - \sigma\rho^2)\, d\rho}{\int_0^\infty \rho^7 \exp(-\kappa\rho^6 + \lambda\rho^4 - \sigma\rho^2)\, d\rho} \tag{3}$$

Note that even if (3) contains Wick-ordered $:S^6:$, it cannot be used for a $:\varphi^6:$ field theory, because the diagonal part of the free measure gives a very large σ.

The other requirements in (2) also deserve some comments: Our method is adapted to potentials that contain an arbitrary "mass term" $\sigma_{2n} S^{2n}$ and for which the region of analyticity contains

$$\{(\mu_j)_j | -\tfrac{1}{4}\pi < \operatorname{Arg} \mu_j < \tfrac{1}{4}\pi, \quad \forall_j\}$$

The result (2) should then be compared with Newman's theorem[1]: For arbitrary σ_2 and analyticity in

$$\{(\mu_j)_j | -\tfrac{1}{2}\pi < \operatorname{Arg} \mu_j < \tfrac{1}{2}\pi, \quad \forall j\}$$

the only allowed polynomials are

$$\lambda S^4 - \sigma_2 S_2$$

We therefore make two conjectures:

1. When $\kappa = 0$ in (2), our region of analyticity can be enlarged, possibly to the whole Lee and Yang region.

2. Higher degree negative terms in (2) would reduce the region where the pressure has a uniform lower bound.

Of course the size and shape of the region are only relevant in so far as they help us to prove analyticity in a fixed neighborhood of the positive real axis. The uniform lower bound that we obtain is also a stronger result than what we need. For example,

$$\left|(2\pi)^{-1/2}\int_{-\infty}^{+\infty}\exp[-\tfrac{1}{2}S^2+(x+iy)S]\,dS\right|^2 = \exp(x^2-y^2)\neq 0, \qquad \forall x, y$$
$$\geqslant 1 \qquad \text{only if} \quad x \geqslant y$$

We view our work as being in the line of Newman's[2]: There the Lee–Yang property was also related to inequalities (for derivatives of the pressure). The improvement here is that all induction procedures have been eliminated, so that we can deal directly with general continuous spins.

Section 2 deals with the Ising model, Section 3 with continuous real spins, and Section 4 contains a heuristic discussion of the results and conjectures.

Note. Newman[3] has remarked that the inequality $U_4(i, j, k, l) \leqslant 0$ is easy in our framework. Both (2) and (3) give new examples where it holds. This result can be extended to bound higher order *truncated* functions in terms of two-point functions. We shall give the proof in a separate article about plane rotators, for which such inequalities are new.

2. ISING SPINS

Theorem 1. Given positive numbers $\{J_{ij} \geqslant 0: i = 1,..., N; j = 1,..., N\}$, let

$$Z((\mu_j)_{j=1,...,N}) = 2^{-N}\sum_{\substack{\sigma_j=\pm 1\\ j=1,...,N}}\exp\left(\sum_{\substack{i,j=1\\ i>j}}^{N} J_{ij}\sigma_i\sigma_j + \sum_{j=1}^{N}\mu_j\sigma_j\right)$$

$$(\mu_j)_{j=1,...,N} \in \mathbb{C}^N$$

$$\langle\sigma_{k_1}\cdots\sigma_{k_l}\rangle = Z((\mu_j)_j)^{-1}2^{-N}\sum_{\substack{\sigma_j=\pm 1\\ j=1,...,N}}\sigma_{k_1}\cdots\sigma_{k_l}\exp\left(\sum_{\substack{i,j=1\\ i>j}}^{N} J_{ij}\sigma_i\sigma_j + \sum_{j=1}^{N}\mu_j\sigma_j\right)$$

$$(\mu_j)_j \in \mathbb{C}^N\backslash\{(\mu_j)_j|Z((\mu_j)_j)| = 0\}; \quad k_1,..., k_l \in \{1,..., N\}$$

Then in the region

$$|\sin(\operatorname{Im}\mu_j)| \leqslant \operatorname{Sh}(\operatorname{Re}\mu_j), \qquad j = 1,..., N$$

the following inequalities hold:

$$|Z((\mu_j))_j| \geqslant Z(0) \tag{4}$$

$$\operatorname{Re}(\langle\sigma_{k_1}\cdots\sigma_{k_l}\sigma_{k_{l+1}}\rangle/\langle\sigma_{k_1}\cdots\sigma_{k_l}\rangle) \geqslant 0 \tag{5}$$

$$\operatorname{Re}(\langle\sigma_{k_1}\cdots\sigma_{k_l}\sigma_{k_{l+1}}\sigma_{k_{l+2}}\rangle/\langle\sigma_{k_1}\cdots\sigma_{k_l}\rangle) \geqslant 0 \tag{6}$$

In particular,

$$\operatorname{Re}\langle\sigma_j\rangle \geqslant 0, \qquad \forall j \tag{7}$$

$$\operatorname{Re}\langle\sigma_i\sigma_j\rangle \geqslant 0, \qquad \forall i,j \tag{8}$$

Remark. The *uniform* lower bound (4) and the inequalities (6) and (8) are new (to the author). The inequalities (5) and (7) have been proven by Newman[2] in the whole Lee–Yang region.

Proof. We introduce an independent copy, denote it by primes, and give a group structure to the new configuration space:

$$\tfrac{1}{2}(\sigma_j + \sigma_j') = \cos\tfrac{1}{2}n_j\pi, \qquad \tfrac{1}{2}(\sigma_j - \sigma_j') = \sin\tfrac{1}{2}n_j\pi, \qquad n_j = 0, 1, 2, 3 \tag{9}$$

$n_j = 0, 1, 2, 3$ have equal weights (invariant measure on Z_4) if $\sigma_j = \pm 1$ and $\sigma_j' = \pm 1$ had equal weights (invariant measures on Z_2).

We shall express duplicated expectations in terms of integrals of positive-definite functions on $(Z_4)^N$. The following formulas will be useful:

$$\begin{aligned}
\sigma_i\sigma_j + \sigma_i'\sigma_j' &= 2\cos[(n_i - n_j)\pi/2] \\
\sigma_i\sigma_j' + \sigma_i'\sigma_j &= 2\cos[(n_i + n_j)\pi/2] \\
\sigma_j\sigma_j' &= \cos(n_j\pi) \\
\mu_j\sigma_j + \bar{\mu}_j\sigma_j' &= 2x_j\cos\tfrac{1}{2}n_j\pi + 2iy_j\sin\tfrac{1}{2}n_j\pi \\
&= (x_j + y_j)e^{in_j\pi/2} + (x_j - y_j)e^{-in_j\pi/2}
\end{aligned}$$

where $\mu_j = x_j + iy_j$ and $\bar{\mu}_j = x_j - iy_j$. Then

$$Z((\mu_j)_j)Z((\bar{\mu}_j)_j) = 4^{-N}\sum_{\substack{n_j=0,1,2,3\\ j=1,\ldots,N}} \exp\Big\{2\sum J_{ij}\cos[(n_i - n_j)\pi/2] + \sum(x_j + y_j)e^{in_j\pi/2} + \sum(x_j - y_j)e^{-in_j\pi/2}\Big\} \tag{10}$$

Note that we have applied complex conjugation to the independent "copy." This can be compared with the (independent) work of Lebowitz,[4] where the two (real) "copies" differ by boundary condition terms.

Similarly,

$$\begin{aligned}
2\operatorname{Re}\frac{\langle\sigma_{k_1}\cdots\sigma_{k_l}\sigma_{k_{l+1}}\rangle}{\langle\sigma_{k_1}\cdots\sigma_{k_l}\rangle}
&= \frac{\langle\sigma_{k_1}\cdots\sigma_{k_l}\sigma_{k_{l+1}}\sigma'_{k_1}\cdots\sigma'_{k_l}\rangle + \langle\sigma'_{k_1}\cdots\sigma'_{k_l}\sigma'_{k_{l+1}}\sigma_{k_1}\cdots\sigma_{k_l}\rangle}{|\langle\sigma_{k_1}\cdots\sigma_{k_l}\rangle|^2} \\
&\approx \sum_{\substack{n_j=0,1,2,3\\ j=1,\ldots,N}} \cos(n_{k_1}\pi)\cdots\cos(n_{k_l}\pi)\cos(n_{k_{l+1}}\pi/2) \\
&\quad\times\exp\Big\{2\sum J_{ij}\cos[(n_i - n_j)\pi/2] \\
&\quad + \sum(x_j + y_j)e^{in_j\pi/2} + \sum(x_j - y_j)e^{-in_j\pi/2}\Big\}
\end{aligned}$$

Also

$$\operatorname{Re} \frac{\langle \sigma_{k_1} \cdots \sigma_{k_l} \sigma_{k_{l+1}} \sigma_{k_{l+2}} \rangle}{\langle \sigma_{k_1} \cdots \sigma_{k_l} \rangle}$$

$$\approx \sum_{\substack{n_j = 0,1,2,3 \\ j = 1,\ldots,N}} \cos(n_{k_1}\pi) \cdots \cos(n_{k_l}\pi) \cos[(n_{k_{l+1}} - n_{k_{l+2}})\pi/2]$$

$$\times \exp\Big\{ 2 \sum J_{ij} \cos[(n_i - n_j)\pi/2]$$

$$+ \sum (x_j + y_j) e^{in_j\pi/2} + (x_j - y_j) e^{-in_j\pi/2} \Big\}$$

where $\approx$ means proportional with a positive coefficient.

The functions to integrate are clearly positive definite on $(Z_4)^N$ when $|y_j| \leqslant x_j$ for all j. The integrals are therefore positive, and the improved lower bound (4) is obtained by expanding the exponential of the linear term and keeping only the first term.

To obtain the larger domain in the theorem, we compute

$$2^{-1} \sum_{n_j = 0,1,2,3} \exp(ipn_j\pi/2) \exp(2x_j \cos \tfrac{1}{2}n_j\pi + 2iy_j \sin \tfrac{1}{2}n_j\pi)$$

$$= \begin{cases} \operatorname{Ch} x_j + \cos y_j, & p = 0 \\ \operatorname{Sh} x_j - \sin y_j, & p = 1 \\ \operatorname{Ch} x_j - \sin y_j, & p = 2 \\ \operatorname{Sh} x_j + \sin y_j, & p = 3 \end{cases}$$

3. ONE-COMPONENT CONTINUOUS SPIN VARIABLES

Theorem 2. Given positive numbers $\{J_{ij} \geqslant 0 : i = 1,\ldots, N; j = 1,\ldots, N\}$, let $\{f_j \geqslant 0 : j = 1,\ldots, N\}$ be positive measurable functions on $\mathbb{R}$ such that

(i) $$Z((\mu_j)_{j=1,\ldots,N}) = \int \exp\Big(\sum_{i,j=1 ! i>j}^{N} J_{ij} S_i S_j + \sum_{j=1}^{N} \mu_j S_j \Big) \times \prod_{j=1}^{N} f_j(S_j)\, dS_j < \infty, \qquad \forall (\mu_j)_j \in \mathbb{R}^N$$

(ii) $$\int_0^\infty f_j(\rho \cos(\alpha - \tfrac{1}{4}\pi)) f_j(\rho \cos(\alpha + \tfrac{1}{4}\pi)) \rho^q \, d\rho$$

$j = 1,\ldots, N$; $q \geqslant q_0$, integer, are positive-definite functions of α on the circle. Here $q_0 = 2$ in general and $=5$ for even functions f_j.

Let Z be extended to a function on $\mathbb{C}^N$ and let

$$\langle S_{k_1}\cdots S_{k_l}\rangle = Z((\mu_j)_j)^{-1}\int S_{k_1}\cdots S_{k_l}\exp\left\{\sum_{i,j=1;\,i>j}^{N} J_{ij}S_iS_j + \sum_{j=1}^{N}\mu_jS_j\right\} \times \prod_{j=1}^{N} J_j(S_j)dS_j$$

$$k_1,\dots,k_l \in \{1,\dots,N\};\quad (\mu_j)_j \in \mathbb{C}^N\backslash\{(\mu_j)_j|Z((\mu_j)_j)| = 0\}$$

Then in the region

$$|\mathrm{Im}\,\mu_j| \leqslant \mathrm{Re}\,\mu_j,\qquad j = 1,\dots,N$$

the following inequalities hold:

$$|Z((\mu_j)_j)| \geqslant Z(0) \tag{11}$$

$$\mathrm{Re}\,\frac{\langle S_{k_1}\cdots S_{k_l}S_{k_{l+1}}\rangle}{\langle S_{k_1}\cdots S_{k_l}\rangle} \geqslant 0,\qquad k_1,\dots,k_{l+1}\in\{1,\dots,N\} \tag{12}$$

$$\mathrm{Re}\,\frac{\langle S_{k_1}\cdots S_{k_l}S_{k_{l+1}}S_{k_{l+2}}\rangle}{\langle S_{k_1}\cdots S_{k_l}\rangle} \geqslant 0,\qquad k_1,\dots,k_{l+2}\in\{1,\dots,N\} \tag{13}$$

Proof. We introduce an independent copy, denoted by primes, and define the polar coordinates for the sums and differences (usual variables in correlation inequalities):

$$2^{-1/2}(S_j + S_j') = \rho_j\cos\alpha_j,\quad 2^{-1/2}(S_j - S_j') = \rho_j\sin\alpha_j,$$
$$dS_j\,dS_j' \to \rho_j\,d\rho_j\,d\alpha_j,\qquad j = 1,\dots,N \tag{14}$$

The strategy will be to use positive-definite functions of $(\alpha_j)_j$ on the N-fold product of the circle group:

$$\begin{aligned} j_{ij}(S_iS_j + S_i'S_j') &= J_{ij}\rho_i\rho_j\cos(\alpha_i - \alpha_j),\qquad (J_{ij}\geqslant 0)\\ &= \tfrac{1}{2}J_{ij}\rho_i\rho_j(e^{i\alpha_i}e^{-i\alpha_j} + e^{-i\alpha_i}e^{i\alpha_j}) \end{aligned} \tag{15}$$

$$\begin{aligned} S_j^2 + S_j'^2 &= \rho_j^2\\ S_iS_j' + S_i'S_j &= \rho_i\rho_j\cos(\alpha_i + \alpha_j)\\ 2S_jS_j' &= \rho_j^2\cos 2\alpha_j\\ \mu_jS_j + \bar{\mu}_jS_j' &= 2^{1/2}x_j\rho_j\cos\alpha_j + i2^{1/2}y_j\rho_j\sin\alpha_j\\ &= \rho_j2^{-1/2}[(x_j + y_j)e^{i\alpha_i} + (x_j - y_j)e^{-i\alpha_j}],\quad (x_j \pm y_j \geqslant 0) \end{aligned}$$

where $\mu_j = x_j + iy_j$ and $\bar{\mu}_j = x_j - iy_j$.

Also, but not positive definite as they stand,

$$S_j = \rho_j\cos(\alpha_j - \tfrac{1}{4}\pi),\qquad S_j' = \rho_j\cos(\alpha_j + \tfrac{1}{4}\pi)$$

We then have

$$\begin{aligned} &Z((\mu_j)_j)Z((\bar{\mu}_j)_j)\\ &\quad= \int\exp\Big[\sum J_{ij}\rho_i\rho_j\cos(\alpha_i - \alpha_j)\\ &\qquad + \sum \rho_j2^{-1/2}(x_j + y_j)\exp(i\alpha_j) + \rho_j2^{-1/2}(x_j - y_j)\exp(-i\alpha_j)\Big]\\ &\qquad \times\prod f_j(\rho_j\cos(\alpha_j - \tfrac{1}{4}\pi))f_j(\rho_j\cos(\alpha_j + \tfrac{1}{4}\pi))\rho_j\,d\rho_j\,d\alpha_j \end{aligned} \tag{16}$$

We expand the exponential in order to factorize the radial integrals. The result is a power series in terms of the J_{ij} and $(x_j \pm y_j)_j$, where any coefficient is the integral over the group of explicit positive definite functions times a product of radial integrals of the form (ii).

If (ii) would hold for all integers q, we could say that a product of positive-definite functions is again positive definite, so that the integral over the group is positive. The improved lower bound (11) and the inequalities (12) and (13) then follow as for the Ising system. Hypothesis (i) legitimates interchanges of limits and integrals.

But we have made a weaker hypothesis and should look at what happens when some q is less than q_0. For this purpose the angle integral should be factorized, using (15), so that the complete integral at a given site in a given term reads

$$\int e^{ip_j\alpha_j}\rho_j^{q_j-1}f_j(\rho_j\cos(\alpha_j - \tfrac{1}{4}\pi))f_j(\rho_j\cos(\alpha_j + \tfrac{1}{4}\pi))\rho_j\,d\rho_j\,d\alpha_j \qquad (17)$$

If $q_j = 1$, p_j must be zero. If q_j is even, p_j must be odd. The integral vanishes for even f_j because of the symmetry

$$\alpha_j \to \alpha_j + \pi$$

If $q_j = 3$, either $p_j = 0$ and everything is positive, or $p_j = 2$ and the integral vanishes for even f_j due to the symmetry

$$\alpha_j \to \alpha_j + \pi/2$$

When $q_j \geqslant q_0$, hypothesis (ii) is equivalent to (17) being positive for all p_j, and we obtain a power series expansion with positive coefficients in terms of the J_{ij} and $(x_j \pm y_j)$.

Theorem 3. Condition (ii) in Theorem 2 is satisfied by the density

$$\exp\left(-\sum_{3n\geq k>n}\lambda_{2k}S^{2k} + \sigma_{2n}S^{2n} + \sum_{n>p\geq 1}\sigma_{2p}S^{2p}\right)$$

where

$$\sigma_{2p} \geqslant 0, \quad n > p \geqslant 1; \qquad \sigma_{2n} \in \mathbb{R}; \qquad \lambda_{2k} \geqslant 0, \quad 3n \geqslant k > n$$

If $n \geqslant 4$, $\lambda_{2k} = 0$ except for $k = 2n, 3n$.

Proof. $n = 1$:

$$S^4 + S'^4 = (S^2 + S'^2)^2 - 2S^2S'^2 = \rho^4 - \tfrac{1}{2}\rho^4\cos^2 2\alpha$$

$$S^6 + S'^6 = (S^2 + S'^2)^3 - 3S^2S'^2(S^2 + S'^2) = \rho^6 - \tfrac{3}{4}\rho^6\cos^2 2\alpha$$

but

$$S^8 + S'^8 = (S^2 + S'^2)^4 - 4S^2S'^2(S^2 + S'^2)^2 + 2S^4S'^4$$
$$= \rho^8 - \rho^8\cos^2 2\alpha + \tfrac{1}{8}\rho^8\cos^4 2\alpha$$

The duplicated density can be written as

$$\exp(-\kappa S^6 - \lambda S^4 + \sigma S^2)\exp(-\kappa'^6 - \lambda S'^4 + \sigma S'^2)$$
$$= \exp(-\kappa\rho^6 - \lambda\rho^4 + \sigma\rho^2)\exp[(\cos^2 2\alpha)(\tfrac{3}{4}\kappa\rho^6 + \tfrac{1}{2}\lambda\rho^4)]$$

which for any ρ is a positive-definite function of α, provided κ and λ are positive (σ arbitrary).

On the other hand, condition (ii) is violated in the presence of an eighth-degree term (and $n = 1$). For example,

$$\int \exp(-\lambda\rho^8 + \sigma\rho^2)\exp[\lambda\rho^8(\cos^2 2\alpha - \tfrac{1}{8}\cos^4 2\alpha)]$$
$$\times\ \rho^5\exp(8i\alpha)\,d\rho\,d\alpha < 0, \qquad \sigma < 0, \quad \lambda \text{ small}$$

Proof. $n > 1$: σ_{2n} may have the "wrong" sign, so we choose

$$S^{2n} + S'^{2n} = \tau^{2n} \tag{18}$$

as our new radial variable.

Let us express ρ in terms of τ and α:

$$S^{2n} + S'^{2n} = (S^{2(n-1)} + S'^{2(n-1)})(S^2 + S'^2) - S^2S'^2(S^{2(n-2)} + S'^{2(n-2)})$$
$$= \cdots \quad \text{(induction)}$$
$$= \sum_{r=0,\, r\,\text{even}}^{n} (-)^{r/2} A_r^{2n}(SS')^r(S^2 + S'^2)^{n-r}$$
$$= (S^2 + S'^2)^n \sum_{r=0;\,\text{even}}^{N} (-)^{r/2} A_r^{2n}\left(\frac{SS'}{S^2 + S'^2}\right)^r$$

The roots of the scale-invariant polynomial are obtained from

$$S^2 = e^{i\theta}, \qquad S'^2 = e^{-i\theta}, \qquad S^{2n} + S'^{2n} = 2\cos n\theta = 0$$

so that

$$S^{2n} + S'^{2n} = (S^2 + S'^2)^n \prod_{r=0;\,\text{even}}^{n-2}\left[1 - \cos^2\frac{(r+1)\pi}{2n}\left(\frac{2SS'}{S^2 + S'^2}\right)^2\right]$$
$$\tau^{2n} = \rho^{2n}\prod_{r=0;\,\text{even}}^{n-2}\left(1 - \cos^2\frac{(r+1)\pi}{2n}\cos^2 2\alpha\right) \tag{19}$$
$$\rho = \tau\prod_{r=0;\,\text{even}}^{n-2}\left(1 - \cos^2\frac{(r+1)\pi}{2n}\cos^2 2\alpha\right)^{-1/2n}$$

When τ is fixed, ρ is a positive-definite function of α, as one can see by a power series expansion. Therefore

$$\exp\sigma_2 S^2\exp\sigma_2 S'^2 = \exp\sigma_2\rho^2$$

will be allowed in the individual distribution provided σ_2 is positive. Similarly

$$S^{2p} + S'^{2p} = \rho^{2p} \prod_{s=0,\,\text{even}}^{p-2} \left(1 - \cos^2 \frac{(s+1)\pi}{2p} \cos^2 2\alpha\right)$$

$$= \tau^{2p} \prod_{s=0,\,\text{even}}^{p-2} \left(1 - \cos^2 \frac{(s+1)\pi}{2p} \cos^2 2\alpha\right) \times \prod_{r=0,\,\text{even}}^{n-2} \left(1 - \cos^2 \frac{(r+1)\pi}{2n} \cos^2 2\alpha\right)^{-p/n}$$

$$S^{2p} + S'^{2p} = \tau^{2p} \exp \sum_{m=1}^{\infty} \frac{\cos^{2m} 2\alpha}{m} \times \left\{\frac{p}{2n} \sum_{r=0,\,\text{even}}^{2(n-1)} \cos^{2m} \frac{(r+1)\pi}{2n} - \frac{1}{2} \sum_{s=0,\,\text{even}}^{2(p-1)} \cos^{2m} \frac{(s+1)\pi}{2p}\right\} \tag{20}$$

We insert

$$\cos^{2m} \frac{(r+1)\pi}{2n} = 2^{-2m}\binom{2m}{m} + 2^{-2m+1} \sum_{m'=1}^{m} \binom{2m}{m-m'} \cos \frac{m'(r+1)\pi}{n}$$

$$\sum_{r=0,\,\text{even}}^{2(n-1)} \cos \frac{m'(r+1)\pi}{n} = \begin{cases} n, & m' = 2kn \\ -n, & m' = (2k+1)n \\ 0, & \text{otherwise} \end{cases}$$

to obtain

$$S^{2p} + S'^{2p} = \tau^{2p} \exp \sum_{m=1}^{\infty} \frac{\cos^{2m} 2\alpha}{m} \times 2^{-2m} p \left\{ \sum_{\substack{m'=1 \\ \text{multiple} \\ \text{of } n}}^{m} (-)^{m'/n} \binom{2m}{m-m'} - \sum_{\substack{m''=1 \\ \text{multiple} \\ \text{of } p}}^{m} (-)^{m''/p} \binom{2m}{m-m''} \right\} \tag{21}$$

The sum inside the brackets is

$$\binom{2m}{m-p} - \binom{2m}{m-2p} + \binom{2m}{m-3p} - \cdots - \binom{2m}{m-n} + \binom{2m}{m-2n} - \binom{2m}{m-3n} + \cdots$$

where the combinatoric coefficients decrease.

The first three terms give a positive contribution:

$$\binom{2m}{m-p} - \binom{2m}{m-2p} - \binom{2m}{m-n} \geqslant 0$$

(the worst case is $n = p + 1$). The rest is a positive, alternating sum. Therefore $S^{2p} + S'^{2p}$ is also a positive definite function of α, at fixed τ.

The two higher degree terms in the density are dealt with as for $n = 1$, provided their power is a multiple of $2n$:

$$S^{4n} + S'^{4n} = (S^{2n} + S'^{2n})^2 - 2S^{2n}S'^{2n}$$

$$S^{6n} + S'^{6n} = (S^{2n} + S'^{2n})^3 - 3S^{2n}S'^{2n}(S^{2n} + S'^{2n})$$

They give a positive-definite factor:

$$\exp(-\kappa\tau^{6n} - \lambda\tau^{4n})\exp[2^{-2n}(\cos^{2n} 2\alpha)\tau^{2n}(3\kappa\tau^{2n} + 2\lambda)]$$

When $n = 2, 3$ and $k \neq 2n, 3n$, the proof relies on a calculation which we have not been able to extend to $n \geqslant 4$. We believe, however, that the last restriction in the theorem is purely artificial.

Indeed, looking at (20), we see that all the coefficients in the exponential are now negative ($p > n$). If they grow fast enough in magnitude with m, the expansion of the exponential will have all negative coefficients, which is what we need. But the first term has a factor of p, so the mth term should be larger than of order p^m, which should give an upper bound on p.

We also remark that if the monomials of even degree between $2n$ and $4n$ are negative definite (modulo a function of τ alone), then the full range of even integers $(2n, 6n)$ is allowed in Theorem 3:

$$S^{4n+2q} + S'^{4n+2q} = (S^{2n} + S'^{2n})(S^{2n+2q}) - S^{2n}S'^{2n}(S^{2q} + S'^{2q}), \qquad 0 < q < n \quad (22)$$

To complete the proof of the theorem, we check this assumption for $n = 2, 3$, using (20):

$$S^6 + S'^6 = (S^4 + S'^4)^{3/2}\left(1 - 3\frac{\cos^2 2\alpha}{4}\right)\left(1 - 2\frac{\cos^2 2\alpha}{4}\right)^{-3/2}$$

$$S^8 + S'^8 = (S^6 + S'^6)^{4/3} \times \left[1 - 4\frac{\cos^2 2\alpha}{4} + 2\left(\frac{\cos^2 2\alpha}{4}\right)^2\right]\left(1 - 3\frac{\cos^2 2\alpha}{4}\right)^{-4/3}$$

$$S^{10} + S'^{10} = (S^6 + S'^6)^{5/3} \times \left[1 - 5\frac{\cos^2 2\alpha}{4} + 5\left(\frac{\cos^2 2\alpha}{4}\right)^2\right]\left(1 - 3\frac{\cos^2 2\alpha}{4}\right)^{-5/3}$$

We expand the last factor and collect the two or three terms which contribute to a given power of the cosine. Besides the desired result, we get that monomials of degree larger than $3n$ ($n = 2, 3$) are not negative definite for fixed τ.

Lemma 1. Condition (ii) in Theorem 2 is satisfied by the density

$$\exp(-\kappa S^6 + \lambda S^4 - \sigma S^2), \qquad \kappa, \lambda \geqslant 0$$

provided

$$\sigma \leqslant 3\,\frac{\int_0^\infty S^5 \exp(-\kappa S^6 + \lambda S^4 - \sigma S^2)\, ds}{\int_0^\infty S^7 \exp(-\kappa S^6 + \lambda S^4 - \sigma S^2)\, ds} \tag{23}$$

Remark. It is precisely for this application that we introduced the restriction $q \geqslant q_0$ in Theorem 2. For $q_0 = 1$, (23) would be replaced by the smaller interval

$$\sigma \leqslant \frac{\int_0^\infty S \exp(-\kappa S^6 + \lambda S^4 - \sigma S^2)\, ds}{\int_0^\infty S^3 \exp(-\kappa S^6 + \lambda S^4 - \sigma S^2)\, ds}$$

Proof. The condition refers to

$$\int \exp(-\kappa\rho^6 + \lambda\rho^4 - \sigma\rho^2) \exp[(\cos^2 2\alpha)(\tfrac{3}{4}\kappa\rho^6 - \tfrac{1}{2}\lambda\rho^4)]\rho^q\, d\rho$$
$$q \geqslant 5$$

We expand the second factor and let

$$A(p, q) = \int \rho^q(6\kappa\rho^6 - 4\lambda\rho^4)^p \exp(-\kappa\rho^6 + \lambda p^4 - \sigma\rho^2)\, d\rho$$

We should prove

$$A(p, q) \geqslant 0, \qquad \forall p, \forall q \geqslant 5$$

Only p odd is a problem. We first study the dependence on q by separating the function to integrate into its positive and negative parts: The corresponding integrals satisfy

$$A_+(p, q) \geqslant (2\lambda/3\kappa)^{1/2} A_+(p, q - 1), \qquad A_-(p, q) \leqslant (2\lambda/3\kappa)^{1/2} A_-(p, q - 1)$$

so that

$$A(p, q) = A_+(p, q) - A_-(p, q) \geqslant (2\lambda/3\kappa)^{1/2} A(p, q - 1)$$

But then

$$\begin{aligned} A(p, q) &= 36\kappa^2 A(p - 2, q + 12) - 48\lambda\kappa A(p - 2, q + 10) \\ &\quad + 16\lambda^2 A(p - 2, q + 8), \qquad p \geqslant 3 \\ &\geqslant 16\lambda^2 A(p - 2, q + 8) \end{aligned}$$

The result now follows by induction from

$$\begin{aligned} A(1, 5) &= \int (6\kappa\rho^5 - 4\lambda\rho^3)[\exp(-\kappa\rho^6 + \lambda\rho^4)]\rho^6 \exp(-\sigma\rho^2)\, d\rho \\ &= \int (6\rho^5 - 2\sigma\rho^7) \exp(-\kappa\rho^6 + \lambda\rho^4 - \sigma\rho^2)\, d\rho \geqslant 0 \quad \text{by hypothesis.} \end{aligned}$$

Lemma 2. Any density satisfying condition (ii) in Theorem 2 will keep this property after multiplication by a power series $\sum_{p=0}^{\infty} a_p S^p$ satisfying

(i) $a_p^2 \geqslant 2a_{p+2}a_{p-2}$

(ii) $a_{p+1}a_p \geqslant a_{p+2}a_{p-1} + a_{p+3}a_{p-2}$

Remark. It follows that powers of the power series are also allowed. One can then use Newman's approximation method[1] to recover Theorem 3 at least for $n = 1$:

$$[\exp(-n^{2/3}\kappa^{1/3}S^2](1 + n^{-1/3}\kappa^{1/3}S^2 + \tfrac{1}{2}n^{-2/3}\kappa^{2/3}S^4)^n \xrightarrow[n\to\infty]{} \exp(-\tfrac{1}{6}\kappa S^6)$$

The moral of Lemma 2 is that we should consider densities modulo entire functions of sufficiently slow growth (slower than just order zero).

Sketch of the proof:

$$\left(\sum a_p S^p\right)\left(\sum a_q S'^q\right) = \sum_{n,m=0;n-2m\geq 0}^{\infty} C_{nm}(S + S')^{\sigma(n)}(SS')^{[n-\sigma(n)]/2-m}(S^2 + S'^2)^m$$

where

$$\sigma(n) = \begin{cases} 0, & n \text{ even} \\ 1, & n \text{ odd} \end{cases}$$

$$C_{nm} = \sum_{r=0}^{[n-\sigma(n)]/2-m} (-)^{[r+\sigma(n)]/2} A_r^{2m+2r+\sigma(n)} a_{[n+\sigma(n)]/2+m+r} a_{[n-\sigma(n)]/2-m-r}$$

$$A_r^k = \begin{pmatrix} \tfrac{1}{2}[k - \sigma(k)] - \tfrac{1}{2}[r - \sigma(r)] \\ \tfrac{1}{2}[r - \sigma(r)] \end{pmatrix} \left\{\sigma(k) + [1 - \sigma(k)][1 - \sigma(r)]\frac{k}{k - r}\right\}$$

$$A_0^0 = 1$$

The hypothesis guarantees

$$C_{nm} \geqslant 0, \qquad \forall n, m$$

The result then follows from the fact that positive-definite functions form a multiplicative cone.

4. A HEURISTIC DISCUSSION

The models under consideration undergo a phase transition at strong couplings and zero external field, in suitable geometric situations, irrespective of the other parameters.[5] For the densities

$$\exp(-\lambda S^{4n} + \sigma S^2), \qquad \sigma \in \mathbb{R}$$

two pure phases are expected, corresponding to

$$\langle S \rangle_{\pm} = \pm a \approx \left(\frac{\sigma + \beta}{2n\lambda}\right)^{1/(4n-2)}$$

β is an increasing function of the J_{ij} in the interaction term

$$\exp\left(\sum J_{ij} S_i S_j\right)$$

It goes to infinity when all the J_{ij} go to infinity.

The idea of the Lee–Yang theorem is that an arbitrarily small external field is enough to pick one of the two phases, as indicated by the minimum of the potential:

$$4n\lambda S^{4n-1} - 2\sigma S - \mu = 0$$

This is clear enough when $\sigma > 0$:

$$S_{\min} = (\sigma/2n\lambda)^{1/(4n-2)} + O(\mu)$$

but not when $\sigma < 0$:

$$S_{\min} = O(\mu)$$

which is very far from $S = \langle S \rangle_+$.

As for $\sigma = 0$,

$$S_{\min} \approx (\mu)^{1/(4n-1)}$$

which is much better for small μ and large n.

Of course all the $S_{\min}$ are smaller than $\langle S \rangle_+$, but if we have gone some way ($\sigma \geqslant 0$) at the minimum of the potential, the conditions on a possible imaginary part of μ will be less stringent, and the $\exp(\sum J_{ij} S_i S_j)$ will push S for the rest of the way to its true expectation.

Needless to say, we would be very happy to replace this very tentative argument by a better one. It was an attempt at explaining why σ should be positive or zero in our Theorem 3. Because $\langle S \rangle_+$ increases with n for suitable λ, it also suggests that the region for analyticity, for σ arbitrary negative and λ arbitrary positive, should shrink as n increases, as it does from degree 4 to degree 6.

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