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Positivity constraints for the Ising ferromagnetic model

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Abstract. The consequences of the Lee and Yang representation for a ferromagnetic Ising model are reviewed. Bounds for the Lee and Yang angle are given and the critical magnetic behaviour is analysed. A main result is that we deduce identities for the Mayer–Yvon coefficients, which lead to introduce the expansion of the magnetization with respect to the variable $(1-\tanh^2 \beta H)$. This expansion appears to exhibit remarkable positivity properties and the corresponding coefficients are tabulated. A central role is played by the Bethe lattice which is completely analysed, since its coefficients seem to give upper bounds for the more realistic regular lattices.

1. Introduction

In 1952, Lee and Yang found the location, in the complex activity plane, of the zeros of the grand partition function of a lattice gas model, equivalent to a ferromagnetic Ising model (Lee and Yang 1952a, b). From this result they derived an integral representation satisfied by the intensity of magnetization.

This representation involves a positive measure interpreted as the density of zeros in the corresponding activity variable of the partition function.

Except for the one-dimensional case, little is known about the precise structure of this measure, although most work has been devoted to extracting, from the representation considered, information about the physical behaviour of the system. In particular inequalities for the critical indices have been deduced by Baker (1968), Gaunt and Baker (1970) (see also Griffiths 1974). The behaviour of the measure near the critical point has been analysed by Abe (1967, pp 72, 322) and Suzuki (1967, pp 1225, 1243) although the question concerning the analyticity properties near the critical point, the so called Griffiths (1967) analyticity remains to be embedded in the measure.

Our first line of research was to look for a reconstruction method of the measure from knowledge of the trigonometrical coefficients, i.e. the Mayer–Yvon coefficients appearing when expanding in the activity variable. The singular character of the measure suggests that we consider first the dominant singular part which characterizes the critical behaviour and then add less singular contributions, all terms being suitably parametrized.

The idea is then to fix the different parameters occurring in the measure from our knowledge of the low-order coefficients. We think that such a programme should be workable because it has been possible by standard methods ('ratio' method or Padé approximants) to compute the critical behaviour with high accuracy from the set of coefficients now available (see Gaunt and Guttmann 1974).

This programme is in progress, but it appears to be very difficult to set up. We have also tried first to explore more systematically a certain number of topics related to the existence of the Lee–Yang representation, concerning in particular the Lee–Yang angle and the coefficients of the Mayer–Yvon expansion.

In § 2 we give a summary of our notation and we recall previous results. In § 3, sets of monotonically decreasing upper bounds for the Lee-Yang angle are recovered from the Mayer–Yvon coefficients and a useful lower bound is recalled. In § 4 we discuss a simple sufficiency condition which must be fulfilled by the measure in order to recover the linear law for the critical magnetic indices.

Section 5 is devoted to identities satisfied by the Mayer–Yvon coefficients. These identities are induced by the positivity of the measure as well as by its support properties, some linear combinations of the Mayer–Yvon coefficients are introduced and related to the expansion in the variable $1-\tanh^2\beta H$.

In § 6, we analyse completely, from the viewpoint of its analytic structure in the activity complex plane, the Bethe lattice, for which we show that our previous identities entirely fix the solution in this simple case. Explicit expressions for the Mayer–Yvon coefficients are given in terms of classical polynomials.

Finally, in § 7 we have performed a numerical investigation, using formal languages, of the most usual lattices. This investigation is based on a linear transformation done on the Mayer–Yvon coefficients as indicated in § 5. New positivity conjectures are very strongly suggested by the inspection of the new coefficients computed to the highest available orders.

2. Definitions and notations

We shall consider a ferromagnetic Ising model on a lattice in dimension d, with c nearest neighbours, for which the Lee–Yang representation is valid (Lee and Yang 1952a, b). Since most of our results are based on this representation, these results clearly extend to systems for which this representation is true; but for clarity we shall stick to this one case.

The Hamiltonian reads:

$$\mathcal{H} = -J\sum \sigma_i\sigma_j - H\sum \sigma_i \qquad J>0, \tag{2.1}$$

the first sum being performed on nearest-neighbours pairs and the second one on all sites of the lattice. We introduce the notation:

$$\begin{aligned} x &= \mathrm{e}^{-2\beta J} \qquad 0\leq x\leq 1 \\ z &= \mathrm{e}^{-2\beta H} \end{aligned} \tag{2.2}$$

where H is the magnetic field. The thermodynamical functions satisfy the following representations. The free energy per site is given by:

$$\beta F = -\beta H - \tfrac{1}{2}c\beta J - \int_{\theta_0(x)}^{\pi} \ln(z^2 - 2z\cos\theta + 1) g(\theta, x)\,\mathrm{d}\theta. \tag{2.3a}$$

The intensity of magnetization is given by:

$$I = -\frac{\partial F}{\partial H} = 2(1-z^2)\int_{\theta_0(x)}^{\pi} \frac{g(\theta, x)}{1-2z\cos\theta + z^2}\,\mathrm{d}\theta, \tag{2.3b}$$

$\theta_0(x)$ is the Lee–Yang angle, $g(\theta, x)$ is a positive measure since it is the density of zeros (on the unit circle in the complex plane of the variable z) of the grand partition function in the thermodynamic limit. The measure g is normalized as:

$$\int_{\theta_0(x)}^{\pi} g(\theta, x)\,\mathrm{d}\theta = \tfrac{1}{2}, \tag{2.3c}$$

$I(z, x)$ satisfies the symmetry property:

$$I(z, x) = -I(1/z, x), \tag{2.4}$$

which shows the symmetry of the system on reversing the magnetic field.

Using the Poisson formula (see Szégö 1939, chap. 10), we see that the spontaneous magnetization is given by:

$$M(x) = \lim_{H\to 0^+} I(z, x) = 2\pi g(0, x) \tag{2.5}$$

and that the susceptibility $\chi(x)$ is:

$$\chi(x) = \frac{\partial I(z, x)}{\partial H}\bigg|_{H=0^+} = \beta \int_{\theta_0(x)}^{\pi} \frac{g(\theta, x) - g(0, x)}{\sin^2\frac{1}{2}\theta}\,\mathrm{d}\theta. \tag{2.6}$$

The critical temperature is given by $\theta_0(x_c) = 0$. At $x > x_c$, $g(0, x) = 0$ which implies $M(x) = 0$, there is no spontaneous magnetization and:

$$\chi(x) = 2\beta \int_{\theta_0(x)}^{\pi} \frac{g(\theta, x)}{\sin^2\frac{1}{2}\theta}\,\mathrm{d}\theta \qquad x > x_c. \tag{2.7}$$

Let us consider for $x > x_c$ the higher-order derivatives

$$\chi_k(x) = \frac{\partial^{2k+1}}{\partial H^{2k+1}} I(z, x)\bigg|_{H=0^+}. \tag{2.8}$$

Derivatives with respect to H of even order are identically zero. By re-expressing $I(z, x)$ in terms of the magnetic field H, we can write:

$$I(H, x) = \mathrm{i} \int_{\theta_0}^{\pi} g(\theta, x)\,\mathrm{d}\theta\,[\cot(\tfrac{1}{2}\theta + \mathrm{i}\beta H) + \cot(-\tfrac{1}{2}\theta + \mathrm{i}\beta H)] \tag{2.9}$$

and owing to the fact that the successive derivatives of $\cot y$ are polynomials in the variable $1/\sin^2 y$, we see that:

$$\chi_k(x) = 2\beta^{2k+1}(-1)^{k+1} \int_{\theta_0(x)}^{\pi} \frac{g(\theta, x)}{\sin^2\frac{1}{2}\theta} Q_k\left(\frac{1}{\sin^2\frac{1}{2}\theta}\right)\mathrm{d}\theta \tag{2.10}$$

where $Q_k(x)$ is a polynomial of degree k in y defined by:

$$\frac{\mathrm{d}^{2k+1}}{\mathrm{d}y^{2k+1}} \cot y = (1 + \cot^2 y) Q_k\left(\frac{1}{\sin^2 y}\right). \tag{2.11}$$

Equation (2.9) can also be written as:

$$I(H, x) = \sinh 2\beta H \int_{\theta_0(x)}^{\pi} \frac{g(\theta, x)}{\sin^2\frac{1}{2}\theta + \sinh^2\beta H}\,\mathrm{d}\theta. \tag{2.11a}$$

Let us consider now the Mayer–Yvon expansion which can be obtained by expanding $I(z, x)$ around $z=0$:

$$\begin{aligned} I(z, x) &= 1-2 \sum_{l\geq 1} l\mathcal{M}_l(x) z^l \\ \beta F &= \tfrac{1}{2}\ln z - \tfrac{1}{2}c\beta J - \sum_{l\geq 1} \mathcal{M}_l(x) z^l \end{aligned} \tag{2.12}$$

with

$$\mathcal{M}_l(x) = -\frac{2}{l}\int_{\theta_0}^{\pi} g(\theta, x)\cos l\theta \, d\theta. \tag{2.13}$$

Equation (2.13) defines a trigonometrical moment problem. The trigonometrical moments have the following properties (Domb 1974):

(i) $\mathcal{M}_1(x) = x^c$, c is the number of nearest neighbours.

(ii) $\mathcal{M}_l(x)$ is a polynomial of degree lc in x, the parity of which is the parity of its highest-degree term.

(iii) The term of minimal degree in $\mathcal{M}_l(x)$ is of degree:

$$N(l) = l(c-2)+2-L, \tag{2.14}$$

where the integer L can be defined in the following way. Given l points in the lattice, join all nearest neighbours taken among those and count the number of independent loops of the diagram obtained. L is the supremum of this number for all possible choices of the l points (clearly this supremum is achieved for a connected diagram).

(iv) The trigonometrical moment of order zero is:

$$\mathcal{M}_0 = \tfrac{1}{2} = \int_{\theta_0(x)}^{\pi} g(\theta, x)\, d\theta. \tag{2.15}$$

3. Bounds for the Lee–Yang angle

3.1. Upper bounds for the Lee–Yang angle

To obtain upper bounds for the Lee–Yang angle $\theta_0(x)$, we first transform the trigonometrical moment problem:

$$\int_{\theta_0(x)}^{\pi} g(\theta, x)\cos l\theta\, d\theta = \begin{cases} -\tfrac{1}{2}l\mathcal{M}_l(x) & \text{for } l\geq 1 \\ \tfrac{1}{2} = \mathcal{M}_0(x) & \text{for } l = 0 \end{cases} \tag{3.1}$$

into a proper moment problem defined by:

$$\mu_l(x) = \int_{\theta_0(x)}^{\pi} g(\theta, x)(\cos^2 \tfrac{1}{2}\theta)^l \, d\theta, \tag{3.2}$$

we have the relations for $l \geq 1$:

$$4^l \mu_l(x) = \binom{2l}{l}\mathcal{M}_0 - \sum_{p=1}^{l} \binom{2l}{l-p} p\mathcal{M}_p(x) \tag{3.3}$$

$$\mathcal{M}_l(x) = (-1)^{l+1}\frac{2}{l}\mu_0 + \sum_{p=1}^{l} (-1)^{l-p+1}\binom{l+p-1}{l-p}\frac{4^p\mu_p(x)}{p} \tag{3.4}$$

and for $l=0$:

$$\mu_0=\mathcal{M}_0=\tfrac{1}{2}. \tag{3.5}$$

In particular:

$$4\mu_1=2\mathcal{M}_0-\mathcal{M}_1=1-x^c, \tag{3.6}$$

setting $t=\cos^2\frac{1}{2}\theta$ in (3.2), we consider the Hausdorf moment problem on the finite interval $(0, \cos^2\frac{1}{2}\theta_0)$

$$\int_0^{\cos^2\theta_0/2} \mathrm{d}t\, t^l \bar{g}(t,x)=\mu_l(x), \tag{3.7}$$

where

$$\bar{g}(t,x)=[t(1-t)]^{-1/2}g(2\cos^{-1}\sqrt{t},x)>0. \tag{3.8}$$

From the knowledge of only the first $2l$ moments $\mu_0(x), \mu_1(x)\ldots\mu_{2l-1}(x)$, we can construct the set of orthogonal polynomials $\Pi_l^{(x)}(t)$ with respect to the measure $\bar{g}(t,x)$; these are the denominators of the Padé approximations built up on the moments μ_l (Baker 1975, chap. 7):

$$\Pi_l^{(x)}(t)=\begin{vmatrix} \mu_0(x) & \mu_1(x)\ldots & \mu_l(x) \\ \mu_1(x) & \mu_2(x)\ldots & \mu_{l+1}(x) \\ \vdots & \vdots & \vdots \\ \mu_{l-1}(x) & \mu_l(x)\ldots & \mu_{2l-1}(x) \\ 1 & t\quad\ldots & t^l \end{vmatrix}. \tag{3.9}$$

All the zeros of these polynomials $\Pi_l^{(x)}(t)$ belong to the support of the measure $\bar{g}(t,x)$ (see Szégö 1939, chap. 3), that is to the interval $(0, \cos^2\frac{1}{2}\theta_0)$. Therefore the largest zero of $\Pi_l^{(x)}(t)$ is a lower bound to $\cos^2\frac{1}{2}\theta_0$. Furthermore, the zeros of $\Pi_l^{(x)}(t)$ and $\Pi_{l+1}^{(x)}(t)$ interlace, and therefore the sequence of largest zeros forms a monotonically increasing set of converging lower bounds to $\cos^2\frac{1}{2}\theta_0$. For instance

$$\Pi_1^{(x)}(t)=\begin{vmatrix} \frac{1}{2} & \frac{1}{4}(1-x^c) \\ 1 & t \end{vmatrix}=\tfrac{1}{2}[t-\tfrac{1}{2}(1-x^c)] \tag{3.10}$$

from which we deduce

$$-x^c<\cos\theta_0. \tag{3.11}$$

To compute $\Pi_2^{(x)}(t)$, it is necessary to know $\mu_3(x)$, but $\mu_3(x)$ depends explicitly on the lattice, and therefore each lattice gives rise to a specific bound.

Those bounds for the angle θ_0, although monotonically converging in l are poor at low temperature (for temperature zero they only decrease like π/l). However they become close to saturation when the temperature is sufficiently high.

3.2. Lower bound for the Lee–Yang angle

We shall see, in the following, that we need a lower bound for the Lee–Yang angle. To obtain it we use the results of Ruelle (1971, 1973).

The intensity of magnetization may have its singularities in the z plane, for fixed x, only in the domain D_x of the complex z plane defined by:

$$D_x=\{\xi;\ \text{such that}\ \xi=-(-z_1)(-z_2)\ldots(-z_c)\}, \tag{3.12}$$

where $z_i \in D$ which is defined by

$$|x+z_i|<(1-x^2)^{1/2}; \tag{3.13}$$

D_x can also be described by:

$$D_x=\left\{\xi, \text{ such that } \xi^{1/c}=x\left[-\left(-\frac{z_1}{x}\right)\left(-\frac{z_2}{x}\right)\ldots\left(-\frac{z_c}{x}\right)\right]^{1/c}\right\} \tag{3.14}$$

where $|1+(z_i/x)|<(1-x^2)^{1/2}/x$. Setting $z_i'=z_i/x$, we see that when $x>1/\sqrt{2}$, the circle $|1+z_i'|<(1-x^2)^{1/2}/x$ is of radius smaller than 1, and therefore the mean geometrical value is again inside the circle (c) of centre (-1) and radius $(1-x^2)^{1/2}/x$, that is:

$$\omega=[-(-z_1')(-z_2')\ldots(-z_c')]^{1/c}$$
$$|1+\omega|<(1-x^2)^{1/2}/x. \tag{3.15}$$

This is best seen by taking the logarithms of the various expressions and transforming the geometrical mean into an arithmetical mean, and by noticing that the image of the circle (c) considered is convex.

It then follows that D_x is the image by $\xi=z^c$ of the circle

$$|x+z|<(1-x^2)^{1/2}. \tag{3.16}$$

Setting

$$x=\sin(\psi/2) \qquad 0\leqslant\psi\leqslant\pi, \tag{3.17}$$

we get the bound (for $x>1/\sqrt{2}$):

$$\pi-\theta_0\leqslant(\pi-\psi) \qquad \psi>\pi/2. \tag{3.18}$$

It is interesting to notice that ψ has a physical interpretation as the Lee–Yang angle for the one-dimensional Ising model $c=2$. At the point $\psi=\pi$ ($x=1$ infinite temperature), the upper bound (3.11) and the lower bound (3.18) give the same value $\theta_0=\pi$. However, the slopes are different for the two bounds. In fact we obtain:

$$\frac{\sqrt{c}}{2}\leqslant\frac{\mathrm{d}\theta_0}{\mathrm{d}\psi}\bigg|_{\psi=\pi}\leqslant\frac{c}{2}. \tag{3.19}$$

These bounds will be useful in the study of the behaviour of the Mayer–Yvon coefficients $\mathcal{M}_l(x)$.

4. A sufficiency condition for the critical magnetic indices to satisfy a linear law

As observed by Lee and Yang, the critical temperature is reached when $\theta_0(x)$ goes to zero. Using x as temperature scale we have at the critical point:

$$\theta_0(x_c)=0. \tag{4.1}$$

Following Gaunt and Baker (1970) and Griffiths (1974) we introduce Δ in order to describe how the critical angle goes to zero when we approach the critical temperature from above:

$$\theta_0(x)\sim A(x-x_c)^{\Delta} \qquad x\to x_c^+, \Delta\geqslant 0. \tag{4.2}$$

The magnetic susceptibilities introduced in (2.7) and (2.8) go to infinity. They behave like (Fisher 1967)

$$\gamma_k(x) \sim B_k(x-x_c)^{-\gamma_k} \qquad \gamma_k \geqslant 0. \tag{4.3}$$

From formula (2.10) it is clear that the behaviour for $x \to x_c^+$ of $\chi_{k-1}(x)$ and of the negatives moments defined by:

$$\bar{\mu}_{-k}(x) = \int_{\theta_0(x)}^{\pi} \frac{g(\theta, x)}{(\sin^2\frac{1}{2}\theta)^k} \, d\theta, \tag{4.4}$$

are governed by the same critical indices.

It was proved by Baker (1968) and Gaunt and Baker (1970) that the critical indices γ_k satisfy the convexity relation for any $k \geqslant 0$:

$$\gamma_{k+2} - 2\gamma_{k+1} + \gamma_k \geqslant 0, \tag{4.5}$$

as well as

$$\gamma_k \leqslant \gamma_{k+1} \leqslant \gamma_k + 2\Delta. \tag{4.6}$$

These two inequalities are consequences of the positivity of the measure but they are not sufficient to impose the linear law:

$$\gamma_k = \gamma_0 + 2k\Delta, \tag{4.7}$$

which can be also considered as a consequence of scaling laws (Fisher 1967).

In fact we can remark that:

(i) if γ_0 and γ_1 satisfy the relation (4.7), i.e.

$$\gamma_1 = \gamma_0 + 2\Delta, \tag{4.8}$$

then the linear law is true for any k. This result is a straightforward consequence of the combination of inequalities (4.5) and (4.6).

(ii) If we assume that there exist positive numbers P and C fixed such that in the vicinity of the critical point: $x_c < x < x_c + \epsilon$, we have:

$$\int_{\theta_0(x)}^{P\theta_0(x)} \frac{g(\theta, x)}{\sin^2\frac{1}{2}\theta} \, d\theta \geqslant C \int_{P\theta_0}^{\pi} \frac{g(\theta, x)}{\sin^2\frac{1}{2}\theta} \, d\theta \tag{4.9}$$

(this means that the interval $(\theta_0, P\theta_0)$ which shrinks to a point as $x \to x_c$, gives a contribution at least as important as the remainder, to the critical behaviour of the susceptibility), then the positivity allows us to write:

$$\frac{1}{\sin^2\frac{1}{2}P\theta_0} \int_{\theta_0}^{P\theta_0} \frac{g \, d\theta}{\sin^2\frac{1}{2}\theta} \leqslant \int_{\theta_0}^{P\theta_0} \frac{g \, d\theta}{\sin^4\frac{1}{2}\theta} \leqslant \int_{\theta_0}^{\pi} \frac{g \, d\theta}{\sin^4\frac{1}{2}\theta} \leqslant \frac{1}{\sin^2\frac{1}{2}\theta_0} \int_{\theta_0}^{\pi} \frac{g \, d\theta}{\sin^2\frac{1}{2}\theta}. \tag{4.10}$$

Using definition (4.4) we deduce:

$$\left(\frac{C}{C+1}\right) \frac{\bar{\mu}_{(-1)}}{\sin^2\frac{1}{2}P\theta_0} \leqslant \bar{\mu}_{(-2)} \leqslant \frac{\bar{\mu}_{-1}}{\sin^2\frac{1}{2}\theta_0}$$

which gives

$$\gamma_0 + 2\Delta \leqslant \gamma_1 \leqslant \gamma_0 + 2\Delta,$$

the relation (4.8) then holds, and as a consequence so also does (4.7).

In fact it should be noticed that taking into account the normalization condition (2.3c), the integral $\int_\eta^\pi g\, d\theta/\sin^2\frac{1}{2}\theta$ remains finite for any η fixed as small as one likes. Then only the contribution from the vicinity of θ_0 is important for the singular critical behaviour; the condition (4.9) makes this statement precise. One can check that representations such as those suggested by Abe (1967, pp 72, 322) or Suzuki (1967, pp 1225, 1243) satisfy our requirement. The difficult problem of reconstructing the measure and analysing its behaviour from the knowledge of the moments requires a detailed investigation of the moments themselves. In particular the consequences for the moments of the positivity of the measure will be analyzed in the next section.

5. Identities satisfied by the Mayer–Yvon coefficient, resulting from the positivity of the Lee–Yang measure

Consider the proper moments of the measure $g(\theta, x)$:

$$\mu_l(x) = \int_{\theta_0}^{\pi} g(\theta, x)(\cos^2\tfrac{1}{2}\theta)^l \, d\theta. \tag{5.1}$$

From the transformation laws (3.3) and the property of the trigonometrical moments defined in (3.1) we see that $\mu_l(x)$ is a polynomial of order lc as is $\mathcal{M}_l(x)$. In § 2, we have seen that $\mathcal{M}_l(x)$ is exactly divisible by $x^{N(l)}$, where $N(l)$ depends on the lattice and satisfies (see (2.14))

$$N(l) = l(c-2) + 2 - L. \tag{5.2}$$

Additional information on the moments is provided by the following theorem.

Theorem. $\mu_l(x)$ is exactly divisible by $(1-x)^l$.

Proof. Since $g(\theta, x)$ is positive, we deduce from (5.1)

$$0 \leqslant \mu_{l+1}(x) \leqslant \mu_l(x) \cos^2\tfrac{1}{2}\theta_0 \leqslant \mu_l(x), \tag{5.3}$$

the proof will be completed by induction.

First $\mu_1(x) = \frac{1}{4}(1-x^c)$ is divisible by $(1-x)$. Then assuming $\mu_k(x)$ divisible by $(1-x)^k$ (for $k = 1, \ldots, l$), from $0 \leqslant \mu_{l+1}(x) \leqslant \mu_l(x)$ we deduce that $\mu_{l+1}(x)$ is at least divisible by $(1-x)^l$. Now we write

$$\begin{aligned} \mu_l(x) &= (1-x)^l R_l(x) \\ \mu_{l+1}(x) &= (1-x)^l R_{l+1}(x) \end{aligned} \tag{5.4}$$

where R_l and R_{l+1} are polynomials as is μ_{l+1}. But (5.3) gives us

$$0 \leqslant R_{l+1} \leqslant R_l \cos^2\tfrac{1}{2}\theta_0. \tag{5.5}$$

The bounds (3.18) on the Lee–Yang angle θ_0 show that $\theta_0(x)$ tends *continuously* towards π when $x \to 1$. Therefore R_{l+1} must vanish once at $x = 1$, and μ_{l+1} is divisible by $(1-x)^{l+1}$. The property is then true for all l; thus the theorem is proved.

This theorem clearly extends to any model for which the zeros of the partition function stay on an interval of some line of the complex activity plane, which shrinks to the point $z = -1$ when $x \to 1$.

Now we remark that if in (5.2) L were zero, $\mathcal{M}_l(x)$ which is of parity lc, would be divisible by $x^{l(c-2)+2}$ and therefore would depend only on l coefficients. But the corresponding $\mu_l(x)$ have to be divisible by $(1-x)^l$, which gives l different conditions. Therefore for such a hypothesis ($L=0$), the polynomials $\mathcal{M}_l(x)$ (or $\mu_l(x)$) are completely determined by the factorization property of $\mathcal{M}_l$ at $x=0$ and of μ_l at $x=1$. In the following we will call these polynomials tree polynomials or Bethe polynomials, since we can generate them by the Bethe approximation—or equivalently by solving an Ising model on a Bethe lattice. This will be explained in detail in the next section.

In more physical cases than the Bethe lattice (for instance any regular lattice in more than one dimension), we can draw on the lattice diagrams with loops. Then, as indicated at the end of § 2, we can factorize only a smaller power $x^{N(l)}$ in $\mathcal{M}_l(x)$. Therefore it appears that $\mathcal{M}_l$ (or μ_l) depends only on L different parameters.

In any case we shall define $\mathcal{P}_l(x)$ by:

$$4^l\mu_l(x)=(1-x)^l\mathcal{P}_l(x). \tag{5.6}$$

When c is even, the $\mu_l(x)$ are even polynomials in x. Then we can factorize $(1-x^2)^l$. For c even, we define $P_l(u)$ by:

$$4^l\mu_l(x)=(1-x^2)^lP_l(u) \qquad u=x^2. \tag{5.7}$$

In all explicit examples we have computed, we have furthermore noticed that both for $\mathcal{P}_l(x)$ in the odd c case and $P_l(u)$, in the even case, all their coefficients are integers and positive. We have no explanation for this surprising fact since it reveals positivity properties of the expansion of the free energy and not as usual of the partition function. This positivity conjecture has been checked for many lattices, up to the highest order available (see § 7).

We can connect the moment $\mu_l(x)$ to the expansion of the free energy or the intensity of magnetization in the variable (Wall 1967):

$$v=\frac{4z}{(1+z)^2}=\frac{1}{\cosh^2\beta H}=1-\tanh^2\beta H. \tag{5.8}$$

From (2.3a) and (2.3b) we deduce:

$$\beta F-\tfrac{1}{2}\ln\tfrac{1}{4}v+\tfrac{1}{2}c\beta J=-\int_{\theta_0}^{\pi}\ln(1-v\cos^2\tfrac{1}{2}\theta)g(\theta,x)\,\mathrm{d}\theta=\sum_{l\geq 1}^{\infty}\frac{v^l}{l}\mu_l(x) \tag{5.9}$$

$$I=-\frac{\partial F}{\partial H}=2(1-v)^{1/2}\int_{\theta_0}^{\pi}\frac{g(\theta,x)\,\mathrm{d}\theta}{1-v\cos^2\frac{1}{2}\theta}=2(1-v)^{1/2}\sum_{l=0}^{\infty}v^l\mu_l(x). \tag{5.10}$$

Note that $(1-v)^{1/2}=\tanh\beta H$ is the magnetization for zero coupling J. In this case the only remaining term in the last sum is $\mu_0=\frac{1}{2}$.

The factorization properties of the μ_l allow us to write:

$$I=\begin{cases}\tanh\beta H\sum\limits_{l=0}^{\infty}[v(1-x)]^l\mathcal{P}_l(x) & c\text{ odd}\\ \tanh\beta H\sum\limits_{l=0}^{\infty}[v(1-u)]^lP_l(u) & c\text{ even, }u=x^2.\end{cases} \tag{5.11}$$

Due to the fact that the Mayer–Yvon coefficients vanish strongly at the origin, it is easy to compute the lowest powers of $P_l(x)$ from the transformation law (3.3). For example the four lowest terms of $P_l(u)$ for the square lattice in two dimensions are given by (as well as for the $c=4$ Bethe lattice as shown in the next section):

$$P_l(u)=\frac{1}{2}\binom{2l}{l-1}+u\frac{l+1}{2}\binom{2l}{l-1}+u^2\frac{(l+2)(l+3)}{4}\binom{2l}{l-2}$$
$$+u^3\frac{(l+3)(l^2+9l+26)}{12}\binom{2l}{l-3}+\dots. \tag{5.12}$$

The square lattice and the Bethe $c=4$ lattice differ only at the fourth order. The diamond lattice and the Bethe ($c=4$) lattice will similarly differ only at sixth order because the first loop diagram can only appear at such an order.

6. Analysis of the Bethe lattice

6.1. Introduction

The Bethe lattice is defined as an infinite lattice without loops such that each site has c nearest neighbours. The Hamiltonian is still given by (2.1). The partition function of such a lattice system can be computed by the following trick (Domb 1960, p 149). Take one particular site and its c nearest neighbours. Consider the isolated system built with the $(c+1)$ corresponding spins. The magnetic field H is applied on the central spin and the external spins are embedded in a different effective magnetic field H_1, which can be fixed in order that the mean values of the central and the external spins are equal, assuming still that spins of neighbouring pairs contribute with the factor $-J$ to the Hamiltonian as in (2.1).

Setting

$$z=\mathrm{e}^{-2\beta H}\qquad z_1=\mathrm{e}^{-2\beta H_1}\qquad x=\mathrm{e}^{-2\beta J}, \tag{6.1}$$

one gets after some calculation:

$$Z=\mathrm{e}^{-\beta F}=z^{-1/2}(xz_1)^{-c/2}[(1+xz_1)^c+z(x+z_1)^c] \tag{6.2}$$

where z_1 is related to z by the algebraic equation:

$$\frac{z}{z_1}=\left(\frac{1+xz_1}{x+z_1}\right)^{c-1}. \tag{6.3}$$

When $z=0$, z_1 is chosen as $z_1=0$ and for $z\neq 0$ we must select the corresponding root by continuity.

It is convenient to introduce the variable:

$$\phi=\frac{1+xz_1}{x+z_1}. \tag{6.4}$$

For $z=0$, $\phi=x^{-1}$ and is defined by continuity for $z\neq 0$. ϕ satisfies:

$$z=\phi^c\frac{\phi^{-1}-x}{\phi-x}. \tag{6.5}$$

The intensity of magnetization is then given by:

$$I=\frac{\phi^2-1}{\phi^2-2\phi x+1}=1-\frac{2z}{\phi^c+z}. \tag{6.6}$$

6.2. *The case* $c=2$

For $c=2$ we recover the solution of the Ising model in one dimension; the intensity of magnetization is given by:

$$I=\frac{1-z}{[z^2-2z(1-2x^2)+1]^{1/2}}, \tag{6.7}$$

or equivalently:

$$I=\left(\frac{1-z}{1+z}\right)\left(1-\frac{4z}{(1+z)^2}(1-x^2)\right)^{-1/2}. \tag{6.8}$$

By using the generating function of Legendre polynomials we can expand (6.7) in powers of z:

$$I=1+\sum_{n=1}^{\infty} z^n(P_n(1-2x^2)-P_{n-1}(1-2x^2)), \tag{6.9}$$

and thus by comparison with (2.12), we get for $l\geqslant 1$:

$$c=2: \qquad -2l\mathcal{M}_l(x)=P_l(1-2x^2)-P_{l-1}(1-2x^2). \tag{6.10}$$

Expanding (6.8) in powers of $v=4z/(1+z)^2$ gives:

$$I=\frac{1-z}{1+z}\sum_{p=0}^{\infty}\frac{(2p)!}{2^{2p}(p!)^2}v^p(1-x^2)^p,$$

and thus we get (see (5.10))

$$c=2: \qquad \mu_l(x)=\frac{1}{2}\frac{(2l)!}{2^{2l}(l!)^2}(1-x^2)^l. \tag{6.11}$$

6.3. *Analytic structure of the solution*

When c is greater than 2, the Ising model on a Bethe lattice exhibits a phase transition because the point $z=1$ (zero magnetic field) becomes a singular point for the function $\phi(z)$ defined by (6.5), for a value of x different from zero.

A careful but straightforward analysis of the analytic structure of $\phi(z)$ at fixed x gives the following results.

The singular points of $\phi(z)$ are $z=0$, $z=\infty$ and the two points $z(\phi_\pm)$ where $\phi_\pm$ are solution of the equation:

$$\phi^2+\phi\frac{x^2c+c-2}{x(1-c)}+1=0. \tag{6.12}$$

If this equation is satisfied, $dz/d\phi$ as derived from (6.5) vanishes. When $1-2/c\leqslant x\leqslant 1$, the solutions $\phi_\pm$ are complex conjugate numbers with modulus one.

When $0 \leqslant x \leqslant 1-2/c$, they become real positive and inverse from each other. The critical temperature is thus given by

$$x_c = 1 - \frac{2}{c}. \tag{6.13}$$

Knowing the singularities of ϕ, we must select the correct sheet by continuity from $\phi(z=0) = 1/x$. From (6.6) we get the analytic structure of the function $I(z)$. The result is:

(i) When $x > x_c$: $I(z)$ is analytic in the complex plane cut along an arc of the $|z| = 1$ circle containing the point (-1) and limited by the points $z(\phi_\pm)$ which are also complex conjugate of modulus one. The point $z = 1$ is inside the domain of analyticity and there is no spontaneous magnetization. Due to the relation

$$I(z) = -I(z^{-1}) = -I(z^*), \tag{6.14a}$$

when $|z| = 1$, we see that the discontinuity along the cut is purely real and it can be shown that it never vanishes except at the end points of the cut. The discontinuity has therefore a definite sign and $I(z)$ admits a Lee–Yang-type representation. The angle $\theta_o(x)$ is given by:

$$\theta_0(x) = \operatorname{Arg} z(\phi_+(x)), \tag{6.15}$$

from (6.12) and (6.5) we can prove that the bound (3.18) is also satisfied.

(ii) When $x < x_c$ the function $I(z)$ is split into two different functions: $I_+(z)$ defined for $|z| < 1$ and $I_-(z)$ defined for $z > 1$. For the Bethe lattice, $I_+(z)$ can be analytically continued outside $|z| = 1$ into the z plane cut along the real axis from $z(\phi_+)$ to ∞ where ϕ_+ is the greatest root of equation (6.12). The point $z(\phi_+)$ increases from one to infinity when x decreases from x_c to zero. The discontinuity of $I_+(z)$ across the cut is purely imaginary and does not change sign. As a consequence the function $\bar{I}_+(z)$ defined by:

$$I_+(z) = 1 - 2z\bar{I}_+(z), \tag{6.16}$$

is a Stieltjes function in z. The definition and properties of Stieltjes functions can be found in Baker (1975, chap. 15).

The properties of $I_-(z)$ are deduced from

$$I_-(z) = -I_+(1/z). \tag{6.14b}$$

The analytic properties of the intensity of magnetization which has four singular points $(0, \infty, z^+, z^-)$ are best visualized in figures 1 and 2.

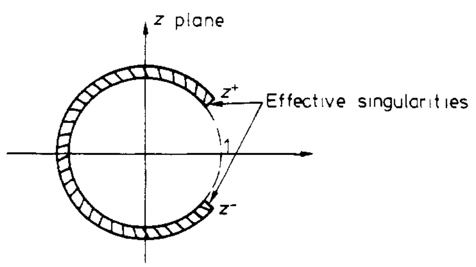

Figure 1. The analytic properties of $I(z, x)$ in the Bethe lattice for $x > x_c$.

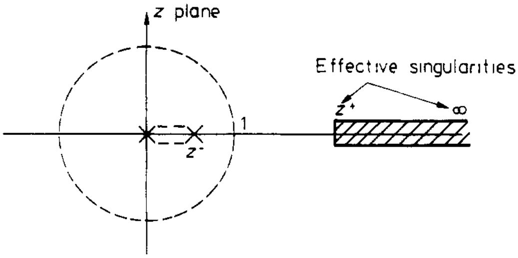

Figure 2. The analytic properties of $I(z, x)$ in the Bethe lattice for $x < x_c$.

The property that $\bar{I}_+(z)$ be a Stieltjes function does not extend to the realistic lattices, because it can be shown by computing some low-order Hadamard determinants that $\bar{I}_+(z, x)$, which is a Stieltjes function for the Bethe lattice, cannot be analytically continued any further into a Stieltjes function for the realistic case of a regular lattice (square lattice in two dimension for instance). For the Bethe lattice, it is interesting to remark that the poles of $I(\phi) = (\phi^2 - 1)/(\phi^2 - 2\phi x + 1)$ do not appear in the corresponding physical Riemann sheet but can only be encountered after turning around the singularities $z(\phi_\pm)$. However, there is an exception to this statement in the case $c = 2$, where these poles coincide with the beginning of the cut. As a consequence, the behaviour of the discontinuity (i.e. the measure of Lee and Yang) near the end point of the cut is different for $x > x_c$:

$$g(\theta, x) \sim \begin{cases} \dfrac{1}{(\theta - \theta_0(x))^{1/2}} & \theta \sim \theta_0 \qquad \text{for } c = 2 \\ (\theta - \theta_0(x))^{1/2} & \theta \sim \theta_0 \qquad \text{for } c > 2. \end{cases} \tag{6.17}$$

Analysis of the critical behaviour of the intensity of magnetization shows that its critical indices are classical (i.e. given by the Landau theory). From the universality point of view, the Bethe lattice can be considered as a limiting case when the dimension of the space goes to infinity.

6.4. *Mayer–Yvon expansion for the Bethe lattice*

It is possible to compute the expansion of $I(\phi(z))$ in powers of z by means of contour integration. Writing:

$$I(z, x) = 1 - 2z\bar{I}(z, x) \qquad \bar{I}(z, x) = \sum_{n \geq 1}^{\infty} n\mathcal{M}_n z^{n-1} \tag{6.18}$$

we get:

$$n\mathcal{M}_n(x) = \frac{1}{2\pi i} \oint \frac{\bar{I}(z, x)\,dz}{z^n}, \tag{6.19}$$

where the contour is a small circle around zero.

From (6.8) we obtain:

$$\bar{I}(z, x) = \frac{1}{\phi^c + z}. \tag{6.20}$$

Taking $\xi = x\phi$ as variable of integration instead of z, we get after some algebraic computation:

$$n\mathcal{M}_n = x^{n(c-2)+2} R_n, \tag{6.21}$$

with

$$R_n = \frac{1-c}{2\pi i} \oint d\xi\, \xi^{-nc+n-1} \frac{(\xi - x^2)^{n-1}}{(1-\xi)^n} + \frac{c-2}{2\pi i} \oint d\xi \frac{(\xi - x^2)^{n-2} \xi^{-nc+n}}{(1-\xi)^n (\xi^2 - 2x^2\xi + x^2)}. \tag{6.22}$$

Expanding the first integral gives rise to Jacobi polynomials in the variable $(1-2x^2)$ while the expansion of the second integral gives products of Tchebicheff polynomials of the second kind and Jacobi polynomials (we use Bateman's 1953 conventions).

The final result is:

$$n\mathcal{M}_n = x^{n(c-2)+2}\Big((c-1)P_{n-1}^{(n(c-2)+1,0)}(1-2x^2)$$
$$-(c-2)\sum_{k=0}^{n-1} (1-x^2)^{k/2} \mathcal{U}_k((1-x^2)^{1/2}) P_{n-1-k}^{(n(c-2),k)}(1-2x^2)\Big). \tag{6.23}$$

Equation (6.23) gives the general solution of the problem mentioned in § 5: that of determining the polynomials $\mathcal{M}_n(x)$ of degree nc, having a definite parity (even or odd according to the parity of nc), in which we can factorize $x^{n(c-2)+2}$, and such that the corresponding proper moments $\mu_l(x)$ vanish like $(1-x)^l$ when x goes to 1. It is easy to verify that when $c=2$, formulae (6.23) and (6.10) are equivalent.

7. Numerical investigations for the most usual lattices, and resulting positivity conjectures

In this section we will first report the lowest-order expressions of the proper moments (defined in (5.1)) $\mu_l(x)$ for several lattices.

For the Bethe lattices, direct calculations have been performed by solving the linear system deduced from the constraints indicated in § 5: taking as unknown the n independent coefficients appearing in $n\mathcal{M}_n(x)$, we first express $\mu_n(x)$ in terms of those unknowns by performing the linear transformation (3.3), and then we require $\mu_n(x)$ to vanish as $(1-x)^n$. Using equations (5.6) and (5.7) we have tabulated the resulting polynomials $\mathcal{P}_l(x)$ for $c=3$, and $P_l(u)$ for $c=4$ and 6.

We have also computed the corresponding polynomials $\mathcal{P}_l(x)$ for the honeycomb lattice ($c=3$, dimension 2), and $P_l(u)$ for simple quadratic ($c=4$, dimension 2), diamond ($c=4$, dimension 3) triangular ($c=6$, dimension 2) and simple cubic ($c=6$, dimension 3) lattices. We have used the tables given by Sykes *et al* (1973) and performed the transformation (2.3). Here we give tables for the difference $\Delta\mathcal{P}_l(x)$ (or $\Delta P_l(u)$) for the realistic associated lattices between the polynomials of the Bethe lattice and the corresponding polynomial of the realistic lattice (tables 1–8).

All calculations involving only integers are made exactly with formal languages.

Analysis of tables 1–8 leads to the following observations.

(i) All coefficients of the polynomials considered are positive integers. This leads to the following conjecture: the partial derivatives at the origin of the function

Table 1. Coefficient $\mathscr{P}_n(x)$ for the Bethe lattice ($c=3$).

$$\mathscr{P}_1(x)=x^2+x+1$$
$$\mathscr{P}_2(x)=4x^4+8x^3+9x^2+6x+3$$
$$\mathscr{P}_3(x)=19x^6+57x^5+87x^4+85x^3+60x^2+30x+10$$
$$\mathscr{P}_4(x)=98x^8+392x^7+776x^6+992x^5+917x^4+644x^3+350x^2+140x+35$$
$$\begin{aligned}\mathscr{P}_5(x)={}&531x^{10}+2655x^9+6510x^8+10330x^7+11885x^6+10521x^5+7410x^4+4200x^3+1890x^2+630x\\&+126\end{aligned}$$
$$\begin{aligned}\mathscr{P}_6(x)={}&2974x^{12}+17844x^{11}+52347x^{10}+99530x^9+137565x^8+147024x^7+126159x^6+88902x^5\\&+51975x^4+25080x^3+9702x^2+2772x+462\end{aligned}$$
$$\begin{aligned}\mathscr{P}_7(x)={}&17060x^{14}+119420x^{13}+408464x^{12}+906892x^{11}+1467067x^{10}+1841035x^9+1863435x^8\\&+1560819x^7+1099917x^6+657657x^5+333333x^4+141141x^3+48048x^2+12012x\\&+1716\end{aligned}$$
$$\begin{aligned}\mathscr{P}_8(x)={}&99658x^{16}+797264x^{15}+3117648x^{14}+7925680x^{13}+14710640x^{12}+21234192x^{11}\\&+24798256x^{10}+24065600x^9+19772325x^8+13927720x^7+8471372x^6+4453176x^5\\&+2008006x^4+760760x^3+231660x^2+51480x+6435\end{aligned}$$
$$\begin{aligned}\mathscr{P}_9(x)={}&590563x^{18}+5315067x^{17}+23400216x^{16}+67072980x^{15}+140622678x^{14}+229768182x^{13}\\&+304474884x^{12}+336235572x^{11}+315510057x^{10}+255152065x^9+179606394x^8+\\&+110715696x^7+59870328x^6+28291536x^5+11544156x^4+3967392x^3+1093950x^2\\&+218790x+24310\end{aligned}$$

Table 2. Coefficient $P_n(u)$ for the Bethe lattice ($c=4$).

$$P_1(u)=u+1$$
$$P_2(u)=5u^2+6u+3$$
$$P_3(u)=31u^3+45u^2+30u+10$$
$$P_4(u)=213u^4+364u^3+294u^2+140u+35$$
$$P_5(u)=1556u^5+3060u^4+2880u^3+1680u^2+630u+126$$
$$P_6(u)=11843u^6+26334u^5+28215u^4+19140u^3+8910u^2+2772u+462$$
$$P_7(u)=92842u^7+230230u^6+276276u^5+212212u^4+115115u^3+45045u^2+12012u+1716$$
$$\begin{aligned}P_8(u)={}&744277u^8+2035800u^7+2702700u^6+2311400u^5+1416870u^4+648648u^3+220220u^2\\&+51480u+6435\end{aligned}$$
$$\begin{aligned}P_9(u)={}&6072124u^9+18156204u^8+26409024u^7+24847200u^6+16900380u^5+8743644u^4+3490032u^3\\&+1050192u^2+218790u+24310\end{aligned}$$

Table 3. Coefficient $P_n(u)$ for the Bethe lattice ($c=6$).

$$P_1(u)=u^2+u+1$$
$$P_2(u)=7u^4+8u^3+9u^2+6u+3$$
$$P_3(u)=64u^6+84u^5+105u^4+85u^3+60u^2+30u+10$$
$$P_4(u)=663u^8+984u^7+1344u^6+1232u^5+1001u^4+644u^3+350u^2+140u+35$$
$$\begin{aligned}P_5(u)={}&7391u^{10}+12235u^9+18045u^8+18255u^7+16350u^6+12006u^5+7770u^4+4200u^3+1890u^2\\&+630u+126\end{aligned}$$
$$\begin{aligned}P_6(u)={}&86488u^{12}+157920u^{11}+249348u^{10}+274340u^9+265815u^8+214632u^7+154737u^6+96822u^5\\&+53460u^4+25080u^3+9702u^2+2772u+462\end{aligned}$$
$$\begin{aligned}P_7(u)={}&1047628u^{14}+2090872u^{13}+3511417u^{12}+4159883u^{11}+4313036u^{10}+3761576u^9+2941939u^8\\&+2030743u^7+1263262u^6+696696u^5+339339u^4+141141u^3+48048u^2+12012u\\&+1716\end{aligned}$$
$$\begin{aligned}P_8(u)={}&13022615u^{16}+28196560u^{15}+50108280u^{14}+63440720u^{13}+69865600u^{12}+65112432u^{11}\\&+54479152u^{10}+40582880u^9+27500265u^8+16831880u^7+9341332u^6+4636632u^5\\&+2032030u^4+760760u^3+231660u^2+51480u+6435\end{aligned}$$
$$\begin{aligned}P_9(u)={}&165170998u^{18}+385537734u^{17}+721988334u^{16}+971123844u^{15}+1129719564u^{14}\\&+1116835740u^{13}+991014252u^{12}+786879612u^{11}+570962646u^{10}+377818438u^9\\&+229558446u^8+127351692u^7+64287132u^6+29126916u^5+11639628u^4+3967392u^3\\&+1093950u^2+218790u+24310\end{aligned}$$

Table 4. Coefficient $\Delta\mathscr{P}_n(x)$ for the honeycomb lattice ($d=2$, $c=3$).

$\Delta\mathscr{P}_1=0$
$\Delta\mathscr{P}_2=0$
$\Delta\mathscr{P}_3=0$
$\Delta\mathscr{P}_4=0$
$\Delta\mathscr{P}_5=0$
$\Delta\mathscr{P}_6=(1+x)^6 3x^6$
$\Delta\mathscr{P}_7=(1+x)^6(63x^8+63x^7+42x^6)$
$\Delta\mathscr{P}_8=(1+x)^6(828x^{10}+1656x^9+1860x^8+1056x^7+360x^6)$
$\Delta\mathscr{P}_9=(1+x)^6(8775x^{12}+26325x^{11}+41850x^{10}+40446x^9+26271x^8+10557x^7+2448x^6)$

Table 5. Coefficient $\Delta P_n(u)$ for the diamond lattice ($d=3$, $c=4$).

$\Delta P_1=0$
$\Delta P_2=0$
$\Delta P_3=0$
$\Delta P_4=0$
$\Delta P_5=0$
$\Delta P_6=12\,u^6$
$\Delta P_7=336\,u^7+168\,u^6$
$\Delta P_8=5976\,u^8+5568\,u^7+2440\,u^6$
$\Delta P_9=86490\,u^9+114318\,u^8+55080\,u^7+9792\,u^6$

Table 6. Coefficient $\Delta P_n(u)$ for the simple quadratic lattice ($d=2$, $c=4$).

$\Delta P_1=0$
$\Delta P_2=0$
$\Delta P_3=0$
$\Delta P_4=4\,u^4$
$\Delta P_5=80\,u^5+40\,u^4$
$\Delta P_6=1104\,u^6+1020\,u^5+264\,u^4$
$\Delta P_7=13062\,u^7+17066\,u^6+8176\,u^5+1456\,u^4$
$\Delta P_8=142372\,u^8+236880\,u^7+160432\,u^6+52960\,u^5+1280\,u^4$
$\Delta P_9=1476639\,u^9+2959443\,u^8+2549547\,u^7+1189683\,u^6+303552\,u^5+34272\,u^4$

Table 7. Coefficient $\Delta P_n(u)$ for the simple cubic lattice ($d=3$, $c=6$).

$\Delta P_1=0$
$\Delta P_2=0$
$\Delta P_3=0$
$\Delta P_4=12\,u^8$
$\Delta P_5=360\,u^{10}+120\,u^9+120\,u^8$
$\Delta P_6=7584\,u^{12}+4716\,u^{11}+5256\,u^{10}+1584\,u^9+792\,u^8$
$\Delta P_7=138194\,u^{14}+122486\,u^{13}+150584\,u^{12}+77952\,u^{11}+48048\,u^{10}+13104\,u^9+4368\,u^8$
$\Delta P_8=2332292\,u^{16}+2648272\,u^{15}+3557616\,u^{14}+2455808\,u^{13}+1763704\,u^{12}+785760\,u^{11}$
$\quad+352800\,u^{10}+87360\,u^9+21840\,u^8$
$\Delta P_9=37591191\,u^{18}+51646923\,u^{17}+75192597\,u^{16}+62934957\,u^{15}+51030054\,u^{14}+29315790\,u^{13}$
$\quad+15935400\,u^{12}+6257088\,u^{11}+2276640\,u^{10}+514080\,u^9+102816\,u^8$

Table 8. Coefficient $\Delta P_n(u)$ for the triangular lattice ($d=2$, $c=6$).

$\Delta P_1 = 0$
$\Delta P_2 = 0$
$\Delta P_3 = 6\,u^6$
$\Delta P_4 = 144\,u^8 + 60\,u^7 + 48\,u^6$
$\Delta P_5 = 2535\,u^{10} + 1935\,u^9 + 1920\,u^8 + 660\,u^7 + 270\,u^6$
$\Delta P_6 = 39708\,u^{12} + 42570\,u^{11} + 49428\,u^{10} + 28584\,u^9 + 16200\,u^8 + 4752\,u^7 + 1320\,u^6$
$\Delta P_7 = 587601\,u^{14} + 796971\,u^{13} + 1048698\,u^{12} + 799078\,u^{11} + 557200\,u^{10} + 263536\,u^9 + 110838\,u^8 + 28392\,u^7 + 6006\,u^6$
$\Delta P_8 = 8428968\,u^{16} + 13676808\,u^{15} + 19979340\,u^{14} + 18318656\,u^{13} + 14865208\,u^{12} + 9031176\,u^{11} + 4822544\,u^{10} + 1950592\,u^9 + 672000\,u^8 + 152880\,u^7 + 26208\,u^6$
$\Delta P_9 = 118754268\,u^{18} + 222621804\,u^{17} + 355797360\,u^{16} + 374777028\,u^{15} + 342776394\,u^{14} + 246308040\,u^{13} + 155214207\,u^{12} + 79801335\,u^{11} + 35666541\,u^{10} + 12698235\,u^9 + 3767472\,u^8 + 771120\,u^7 + 111384\,u^6$

$I(\beta, H)/\tanh\beta H$ with respect to the variables $w=(1-x)/\cosh^2\beta H$ and x independently are positive at all orders:

$$\frac{\partial^{n+p}}{\partial w^n\,\partial x^p}\left(\frac{I(\beta,H)}{\tanh\beta H}\right)\bigg|_{w=x=0} \geqslant 0. \tag{7.1}$$

When c is even, the property holds for $w=(1-x^2)/\cosh\beta H$ as well as for $w=(1-x)/\cosh^2\beta H$. The derivatives will clearly keep their sign in the range

$$0\leqslant x\leqslant 1 \qquad 0\leqslant w\leqslant \frac{1-x}{\cos^2\frac{1}{2}\theta_0} \tag{7.2}$$

where the series (6.10) converges.

Another consequence of the positivity properties of the coefficients is that the Lee–Yang angle can be bounded from above.

Using equations (5.6) and (5.7):

$$\mu_l(x) \geqslant \begin{cases} [\frac{1}{4}(1-x)]^l \mathcal{P}_l(0) = (1-x)^l \mu_l(0) & c \text{ odd} \\ [\frac{1}{4}(1-x^2)]^l P_l(0) = (1-x^2)^l \mu_l(0) & c \text{ even.} \end{cases} \tag{7.3}$$

But $\mu_l(0)$ is easily obtained from (3.3):

$$\mu_l(0) = \frac{1}{2}\frac{1}{4^l}\binom{2l}{l}. \tag{7.4}$$

We obtain an upper bound for the radius of convergence of the series (5.10), i.e. a lower bound for $\cos^2\frac{1}{2}\theta_0$.

For c odd we have:

$$\cos^2\tfrac{1}{2}\theta_0 > \lim_{l\to\infty}\left[\frac{1}{2}\left(\frac{1-x}{4}\right)^l\binom{2l}{l}\right]^{1/l}. \tag{7.5}$$

The $l\to\infty$ limit is easily derived and gets:

$$\cos^2\tfrac{1}{2}\theta_0 > 1-x.$$

For c even we get similarly:

$$\cos^2\tfrac{1}{2}\theta_0 > 1-x^2, \tag{7.6}$$

i.e. in the c even case, θ_0 is less than the corresponding angle in the one-dimensional ($c=2$) case. Such a bound is better at low temperature that the bound given in § 3.1.

Similar considerations also lead to the following result. If the inequalities (7.1) are true, the radius of convergence of the series expansion of $I(\beta, H)/\tanh \beta H$ in powers of the variable w, will be a monotonically decreasing function of x. Thus $\cos^2(\theta_0(x)/2)/(1-x)$ is a monotonically increasing function of x.

(ii) If we compare polynomials corresponding to the same value c, and different dimension d, each coefficient appears to be an increasing function of the dimension d. The Bethe lattice enters into this scheme as the infinite-dimensional case.

If we compare polynomials corresponding to different c (having the same parity) the coefficients seem to be increasing function of c (for any dimensions considered here).

Since d and c are insufficient to characterize the lattice, some care must be taken in trying to generalize this observation. Moreover, continuation in c or d (at fixed d or c) is hard to define. However, if our assertions are true at any order in the expansion, we can deduce in the c even case that the corresponding Lee–Yang angle will be at constant c a decreasing function of the dimension and a decreasing function of c, because $1/\cos^2\frac{1}{2}\theta_0$ is the radius of convergence of the series (5.10). As an example we have for $c=4$

$$\theta_0(\text{Bethe}) < \theta_0(\text{diamond}, d=3) < \theta_0(\text{square}, d=2). \tag{7.7}$$

This gives the corresponding inequalities for the critical temperatures:

$$T_c(\text{square}) \leq T_c(\text{diamond}) \leq T_c(\text{Bethe}). \tag{7.8}$$

These following inequalities are known to be true (Domb 1974)

$$x_c(\text{square}) = \sqrt{2}-1 \simeq 0{\cdot}4142 \qquad x_c(\text{diamond}) \simeq 0{\cdot}4773 \qquad x_c(\text{Bethe}) = \tfrac{1}{2}. \tag{7.9}$$

We have not compared different lattices having same c and same d. (For example the honeycomb lattice and the so called 4–8 lattice discussed by Domb (1960, p 219) both have $c=3$, $d=2$.) Such an investigation would be interesting and in any case a counting method should be set up for the expansion in the parameter $v(1-x)$ or $v(1-x^2)$ in order to verify our observations at all orders.

Finally we want to report another numerical observation concerning the positivity of the Mayer–Yvon coefficients themselves, and the location of their zeros.

For the Bethe lattices $n(c-2)+2$ zeros of $\mathcal{M}_n(x)$ are at the origin, the other zeros form n opposite pairs (for the variable x) lying in the *real* intervals defined by $x_c^2 < x^2 < 1$, with $x_c = 1-2/c$. Furthermore these zeros interlace when l increases.

For the other lattices we observe a similar phenomenon: the first set of $n(c-2)+2$ zeros splits into $n(c-2)+2-2L$ zeros remaining at the origin, and L pairs of opposites (real or complex) slightly shifted from the origin but such that $\operatorname{Re} x^2 < 0$. The second set of l pairs of zeros remains *real*, and lies in the same interval as in the case of the Bethe lattice.

A consequence of the location of zeros is that for any lattice $\mathcal{M}_n(x)$ appears (at least up to the highest-order considered) to keep a constant positive sign in the whole interval $(0, x_c)$ where x_c is the critical temperature of the Bethe lattice having same coordination number.

The expansion (2.12) has therefore also positivity properties in the low temperature region.

8. Conclusions

The Lee–Yang representation for the Ising model is known to have important consequences for the analyticity property of the solution. We have shown that its positivity property also has a strong influence on the coefficients of the various expansions, as well as on the critical behaviour.

Therefore we believe that a constructive approximation (i.e. a set of approximations giving exact bounds) to the solution of the Ising model may be deduced from approximations on the measure itself. Such a programme would allow the greatest number of deductions to be made from the knowledge of a large (but finite!) number of coefficients of the expansion.

The situation has some similarity with elementary particle physics: the Lee–Yang representation plays the role of the dispersion relations, the measure is equivalent to the so called absorptive part of the scattering amplitudes and the spontaneous magnetization is similar to the total cross section. Consideration of the positivity properties of the absorptive part is known to have greatly increased the exact known properties of the amplitudes in particle physics (Martin 1969).

Finally we want to point out that the linear transformations we performed on the moments (which is the so called *de la Vallée Poussin* transformation) can be generalized to include more information coming from the knowledge of the type of singularity associated with the intensity of magnetization in the z variable at the ends of the arc of the Lee–Yang circle.

Such an approach with a more sophisticated (Gronwall 1932) method could be very valuable and will be investigated in the future.

More generally, it seems to us, that the impact of the renormalization group approach on the Lee–Yang measure or, vice versa, the influence of such a positive measure on the renormalization procedure, could be investigated with much profit.

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