COMPLEX SINGULARITIES AND DISTRIBUTION OF ZEROS IN ISING AND GAUGE MODELS

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1. Introduction

This talk will report on a study of properties of lattice gauge theories for complex values of the coupling, namely of possible singularities and distribution of zeros of their partition function[1]. It may seem to be a rather bizarre or perverse idea to look at complex temperatures (= couplings) when interesting physics only takes place along the real axis - actually mainly in the vicinity of a critical point. I would like to convince you that such a study may however uncover new interesting phenomena, and yield useful information on the physical, critical behavior. On general grounds, any information on the analyticity properties of thermodynamic quantities as functions of the (complex) temperature may be useful : the radius of convergence is controlled by the closest singularity, more detailed information might allow to write dispersion relations, etc... Let us look at the strong coupling expansions of the plaquette energy in the four-dimensional Z_2, U(1) and SU(2) lattice gauge theories. These series have been computed to eleventh order in t^2 by Wilson[2], t being the first character expansion parameter :

$$t = \tanh\beta \;,\; I_1(\beta)/I_o(\beta) \quad , \quad I_2(\beta)/I_1(\beta)$$

for Z_2, U(1) and SU(2) respectively. A glance at these series indicates that the closest singularity is located on the real *negative* axis : indeed the coefficients of the series have alternating signs. A more careful analysis, using for instance Padé approximants confirms it and also points to a second singularity, along the positive axis. The latter is interpreted either as the end of the metastability region beyond the first order transition in the case of Z_2, or as the real deconfining phase transition of U(1). In the second case of SU(2), it has been argued[3] that this real singularity should split into two complex nearby

singularities, causing the bump in the specific heat. The situation is summarized in Fig. 1.

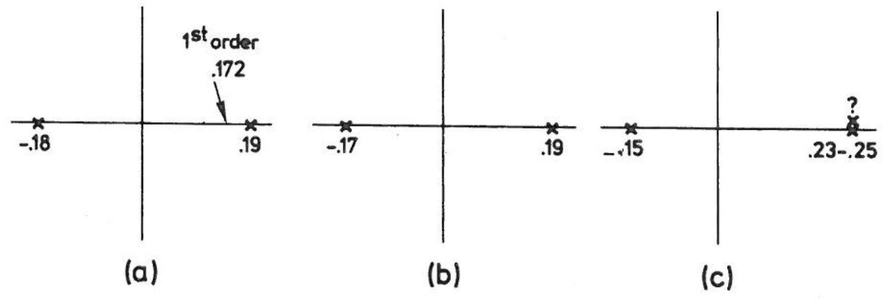


Figure 1. Singularities in the complex t^2 plane of four-dimensional gauge theories : a) : Z_2 ; b) : U(1) ; c) : SU(2).

In any event, the negative singularity is always closer to the origin and we would like to understand better the occurrence of this singularity, its properties and its possible interpretation. As a similar singularity exists in the three-dimensional model, we shall mainly dwell on the case of the dual Ising model. A particularly interesting issue at stake is the possible relevance of these nearby singularities to the physics of random surfaces.

2. Complex singularities of the three-dimensional Ising model

2.1. General features

Consider the low-temperature expansion of the 3-d Ising model, the equivalent by duality of the strong coupling expansion of the 3-d Z_2 gauge model. The expansion parameter is

$$t^2 = \tanh^2\beta = \exp - 4\beta_I \qquad (2.1)$$

(β = gauge inverse coupling, β_I = Ising inverse temperature). Rather long series have been derived on various lattices[4], and on the simple cubic lattice, it has been known for a long time[5] that the closest singularities arise at

$$t_u^2 = -.286 \qquad (2.2)$$

and $$t_c^2 = .412$$

The latter correspond to the Curie temperature, the former is the subject of this analysis.

As everytime we face such a singular behavior, we would like to have a classical, mean-field-like approach to study it. The simplest such approach is provided by an approximation studied by Drouffe, Parisi and Sourlas (D.P.S.) in a different context[6]. Returning to the language of gauge models at strong coupling, we imagine that the large closed surfaces of strong coupling diagrams are generated by successive decorations of each plaquette by a cube built in one of the 2d-5 (=1 for d=3) directions orthogonal to the plaquette, and not yet swept in its previous history (see Fig. 2). This is accounted for by the equation

$$p = t + (2d-5)\, p^5 \tag{2.3}$$

for the decorated plaquette p in terms of which various quantities of interest such as the internal energy, etc..., may be expressed. Singularities arise in the parametrization $p = p(t)$, at $t^2 = \pm .2862$, for d=3. The D.P.S. approximation gives two equally distant singularities on each side of the real axis. We can correct and improve this approximation if we realize that

i) in the spin picture, DPS generates configurations of overturned spins which are trees, and indeed such configurations are expected to have the largest entropy, hence to drive the closest singularity.

ii) some excluded volume effects are not properly taken into account by DPS : a correct counting of these tree-configurations amounts to solving the Ising model on an infinite tree, of coordination number q (q=6 for the cubic lattice at hand). We have in mind the so-called Bethe approximation[7,5] which discards difficult problems in the proper definition of the thermodynamic limit in such a lattice[8]. That this approximation gives a good representation of the complex singularities has been known since the work of Domb and Guttmann[5].

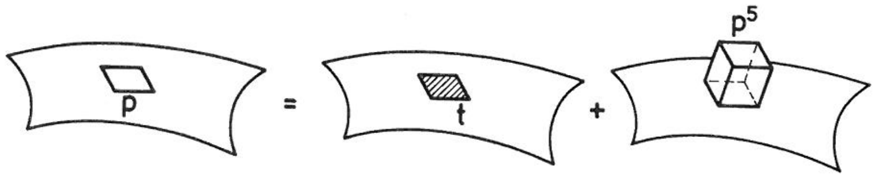


Figure 2. Possible deformations of the surface represented by the DPS equation (2.3).

2.2. The Bethe approximation

The Bethe approximation is derived from the local properties of the lattice. Consider a spin, submitted to a magnetic field h, and its q neighbors. The partition function z for this small system is computed, assuming that the q neighboring spins feel an effective field h_1, to be determined self-consistently. Defining $y = \exp -2h$, $\rho = \exp -2h_1$, we find :

$$z = \exp(q\beta + h + q\, h_1)\, [(1 + t\rho)^q + y(t + \rho)^q]$$

and ρ is obtained by equating the magnetizations of the central spin and of its neighbors :

$$M = \frac{\partial}{\partial h} \ln z = \frac{1}{q} \frac{\partial}{\partial h_1} \ln z$$

This yields

$$y = \rho \left(\frac{1+t\rho}{t+\rho}\right)^{q-1} \tag{2.4}$$

and after integration of $M = \frac{\partial F}{\partial h}$, the free energy is found to be

$$F = \frac{q}{2}\beta + h + (q-1)\ln(1 + \rho t) + (1 - \frac{q}{2}) \ln(1 + 2\rho t + \rho^2) \tag{2.5}$$

Eq. (2.4) takes a more suggestive form if we set

$$p \equiv \frac{1+\rho}{1+\rho t} \tag{2.6}$$

Then
$$p = t + y\, p^{q-1}\, (1 - pt) \tag{2.7}$$

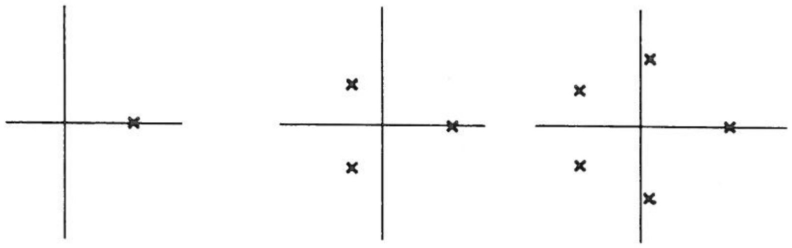
which for y = 1 (h = 0) and q = 6, should be compared to the DPS equation equation (2.3) for d = 3.

This Bethe approximation, which sums up exactly the tree configurations of overturned spins, exhibits interesting and suggestive properties :

1) on the cubic lattice, the unphysical singularity is now closer to the origin, as it should :

$$t_c^2 = (\tfrac{2}{3})^2 = .44 \quad , \quad t_u^2 = -\tfrac{1}{4} = -.25 \text{ (compare (2.2))}$$

2) more generally, the Bethe approximation reproduces correctly the number $\frac{q-2}{2}$ and approximately the location of singular points for the other standard lattices[5] : diamond (q=4), body-centered-cubic (q=8), face-centered-cubic (q=12) (see Fig.3).



(a) (b) (c)

Figure 3. Singularity pattern of other three-dimensional Ising lattice : a) : diamond ; b) b.c.c. ; c) f.c.c. (see ref. 4).

3) all these complex singular points have the same critical behavior : the specific heat, the magnetic susceptibility and the correlation length[9,10] diverge with the classical exponents $\alpha_u = \frac{1}{2}$, $\gamma_u = \frac{1}{2}$, $\nu_u = \frac{1}{4}$ while the magnetization has a singular part of exponent $\beta_u = \frac{1}{2}$: $M \sim M_{reg} + C(t^2 - t_u^2)^{1/2}$. We recall the classical exponents at the physical singularity : $\alpha = 0$, $\beta = \frac{1}{2}$, $\gamma = 1$, $\nu = \frac{1}{2}$.

4) In the presence of a complex magnetic field, the Bethe approximation satisfies the Lee-Yang theorem[11] : thermodynamic quantities may be expressed in terms of the distribution of zeros on the unit circle in the variable $y = e^{-2h}$, the moment of which are explicitly known[12]. Moreover all the singular points, including the previous physical and complex singularities in t^2 and the Lee-Yang edge singularity on the unit circle in y lie on the same algebraic curve. The equation of the later is obtained by eliminating p between

$$\begin{cases} f(p,t,y) \equiv p - t - y(1 - pt)\, p^{q-1} = 0 \\ \dfrac{\partial f}{\partial p} = 0 \end{cases} \tag{2.8}$$

and read

$$y + \frac{1}{y} - 2 = \frac{-q^q}{(q-1)^{q-1}} \frac{1}{t^{q-2}} (t^2 - t_c^2)^3 \prod_u (t^2 - t_u^2)^2 \tag{2.9}$$

where the product runs over the $\frac{q-2}{2} - 1$ complex singularities, in zero

field, and $t_c = \frac{q-2}{q}$. For $h = 0$, $y = 1$, we recover the singularities in t^2, while for $t_c^2 < t^2 < 1$, the right hand side is negative and (2.9) has solutions at $y = e^{\pm i\theta_c}$; these edge singularities pinch the real axis ($\theta_c \to 0$) as t^2 approaches t_c^2.

Equations (2.9) also exposes the distinct behavior of t_c^2 and of t_u^2 as the real field h departs from zero. The physical singularity t_c^2 splits into three $t_c^2 \sim (\frac{q-2}{q})^2 + A \exp \frac{i\pi}{3} (1 + 2k)$, $k = 0,1,2$, the complex t_u^2 split into two.

This Bethe approximation may be improved by adding gradually larger and larger clusters of spins[4]. To any finite order in these corrections, the singularities will remain classical. As such, the Bethe approximation is not sufficient to reproduce the details of the actual critical behavior that we shall describe now.

2.3. Critical behavior at t_u^2

We have seen that the number and the location of the complex singularities depend on the lattice. However from the analysis of the series expansions, there is a fair evidence of a universal behavior at these points. Typically, a Padé analysis of the free energy series yields an exponent α_u :

$$F(t) \sim F_{reg}(t) + A(t^2 - t_u^2)^{2-\alpha_u}$$

ranging between 1.1 and 1.5, for the cubic, b.c.c and f.c.c. lattices. In particular, notice that the two pairs of singularities of the f.c.c. lattice are approximately equally distant from the origin, and have roughly the same exponent. This exponent is clearly non-classical ($\alpha = .5$) and differs from the physical one ($\alpha_c = .11$). Notice that a weak divergence of the internal energy is not ruled out by these estimates. This should not worry us, since for complex couplings the energy is no longer bounded. Finally, we observe that the expansion of the correlation length[10] also points to a singularity at t_u^2. For the cubic lattice

$$\xi \sim (t^2 - t_u^2)^{-\nu_u} \quad , \quad \nu_u \simeq \frac{1}{3}$$

so that the relation $\alpha = 2 - \nu d$ is approximately satisfied.

This suggests that there is a universal continuous theory describing this critical behavior. What is this continuous theory ? Previous considerations on the Bethe approximation have suggested a possible relationship with the Lee-Yang edge singularity, itself associated with the ϕ^3 theory with an imaginary coupling constant[13]. However comparison of the edge critical behavior, characterized by the exponent σ :

$$M - M_c \sim (h - h_c)^{\sigma} \qquad F \sim (h - h_c)^{\sigma+1}$$

with the previous estimate does not reveal a striking agreement. At d=3 Fisher gives $1 - \sigma \simeq .91$, to be compared with α_u given above.

This discussion leaves clearly several open questions.

· What is the continuum theory and the upper critical dimension associated with the complex singularities ?

· If this theory has some bearing on a theory of random surface, as suggested by the reformulation of Ising models in terms of closed surfaces[14], what forbids the occurrence of a complex singularity in the diamond lattice ?

2. The four-dimensional gauge theory

Let us now discuss briefly the case of four dimensions. The singularity pattern has been presented in the Introduction and may be again roughly reproduced by DPS or better by the Bethe approximation. The DPS approximation $p = t + 3p^5$ leads to singularities at $t^2 = \pm 0.165$. The Bethe approximation is most easily gotten by solving the model on a Cayley tree of cubes. Such a lattice may be defined recursively, by building successive generations of cubes (fig.4). On a cube of generation ℓ, will be added (2d-5) cubes of generation $\ell+1$ on each of its five free faces. On the resulting lattice, 2(d-2) cubes are incident on each face, and there is no cluster nor cycle of cubes. Accordingly, the Bethe approximation resums all strong coupling diagrams which may be considered as trees of cubes, but misses diagrams as those depicted on fig.5. On the other hand, as every link is shared by an infinite number of plaquettes, there is no weak coupling expansion. To solve the model in its strong coupling phase, we consider a cube C of the ℓ-th generation, and the plaquette p separating it from its ancestor. We call x_ℓ the sum of closed diagrams made of C and its descendants not containing p, ty_ℓ the sum of such diagrams containing p (fig.4). We leave it to

the reader to convince himself that we may write recursion formulae of the form :

$$d = 3 \qquad \begin{cases} x_\ell = (x_{\ell+1} + t\, y_{\ell+1})^5 \\ y_\ell = (t\, x_{\ell+1} + y_{\ell+1})^5 \end{cases} \qquad (3.1)$$

$$d = 4 \qquad \begin{cases} x_\ell = (x^3_{\ell+1} + 3t x^2_{\ell+1} y_{\ell+1} + 3x_{\ell+1} y^2_{\ell+1} + t y^3_{\ell+1})^5 \\ y_\ell = (t x^3_{\ell+1} + 3x^2_{\ell+1} y_{\ell+1} + 3t x_{\ell+1} y_{\ell+1} + y^3_{\ell+1})^5 \end{cases} \qquad (3.2)$$

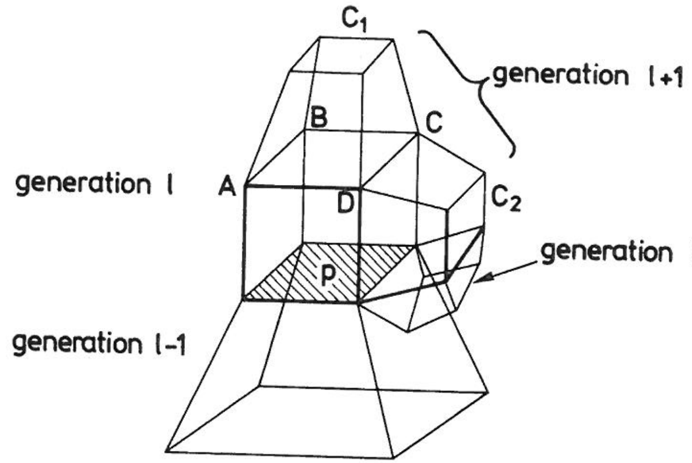


Figure 4. *Constructing a Cayley tree of cubes : each face like ABCD has 2(d-2) adjacent "cubes" (only two have been represented here); cubes built on the faces of C_1 and C_2 will never meet.*

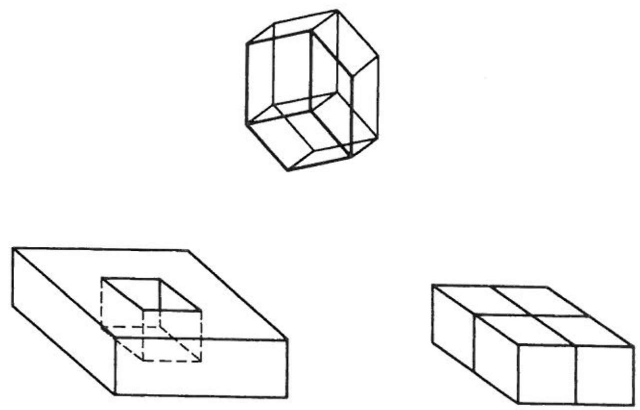


Figure 5. *Examples of diagrams omitted in the Bethe approximation.*

Assuming that $\rho_\ell = \dfrac{y_\ell}{x_\ell}$ reaches a fixed point ρ as $\ell \to \infty$ we get

$$\rho = \left(\frac{t+\rho}{1+\rho t}\right)^5 \qquad \text{for } d = 3$$

$$\rho = \left(\frac{t+3\rho+3t\rho^2+\rho^3}{1+3\rho t+3\rho^2+\rho^3 t}\right) \qquad \text{for } d = 4 \tag{3.3}$$

For arbitrary dimension, the corresponding expression is :

$$\rho = \left[\frac{(t+\rho)^{"2d-5"}}{(1+t\rho)^{"2d-5"}}\right]^5 \tag{3.4}$$

where quotation marks mean that in the binomial expansion, we set $t^{2k} \equiv 1$, $t^{2k+1} \equiv t$.

In three dimensions, all this boils down to the previous Bethe approximation of the dual Ising model, while in four dimensions, it leads to a parametric representation of the partition function in terms of a variable p

$$F - F_{triv} = 20 \ln (1 + 3\rho t + 3\rho^2 + \rho^3 t)$$

$$-14 \ln (1 + 4\rho t + 6\rho^2 + 4\rho^3 t + \rho^4) \tag{3.5}$$

$$\rho = p^5$$

$$p = t + (1-pt)\, p^5\, \frac{3+p^{10}}{1+3p^{10}}$$

where $F_{triv.}$ is the group-dependent strong coupling limit :
$F_{triv} = 6 \ln \cosh\beta + 4 \ln 2$ for Z_2, etc... This parametrization has two singular points at $t^2 = -.151$ and $t^2 = .190$. Moreover the transition from the strong coupling to the weak coupling phase $\rho = p \equiv 1$ is discontinuous (first order), as in the ordinary mean field picture. In the case of Z_2, comparing F given above to $F_{weak} = 6\beta + \ln 2$ leads to a first order transition at $t^2 = .178$. All this agrees roughly with the numbers given on fig. 1.

Concerning the critical behavior in the vicinity of the complex singularities, we can only rely on the rather scarce information contained in the series. A Padé analysis gives an exponent α_u ranging between

.45 and .6. We see that this exponent is now quite consistent with its mean field value 1/2. Does that mean that we have already reached the upper critical dimension ? Here the internal energy seems to be finite at t_u^2, and a divergence of the specific heat should signal a divergence of the correlation length, provided exponential fall-off of correlations holds at complex coupling. On the other hand, strong coupling series for the correlation length are still very short[15] and it is difficult to assert that ξ diverges at t_u^2. If so, we ask again : what is the corresponding continuous theory ?

4. Distribution of zeros.

Following earlier works on smaller lattices[16], B. Pearson has recently[17] computed exactly the partition function of a $4 \times 4 \times 4$ Ising lattice and plotted its zeros in the complex β_I plane. This plots presents several remarkable features (see Fig. 6 for a rough sketch, ref. 17) for more accuracy)

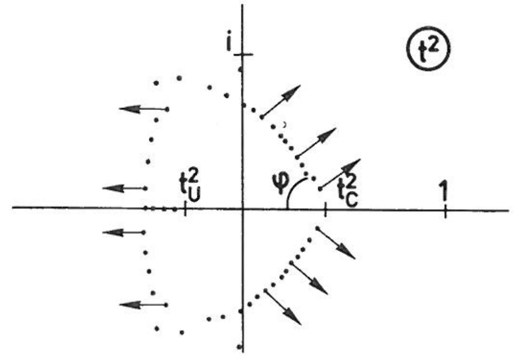


Figure 6. Sketch of the distribution of zeros on a $4 \times 4 \times 4$ Ising lattice The antiferromagnetic zeros (obtained by inversion : $t^2 \to 1/t^2$) have not been displayed. The arrows show how the zeros move under a real magnetic field.

1) The zeros lie on a rather regular, smooth curve. Contrary to the two dimensional Ising case, where it is known exactly that they lie on circles in the $t^2 = e^{-4\beta_I}$ plane[18], there is here no such guarantee.

2) The zeros accumulate in the vicinity of t_c^2 and tend to pinch the real positive axis, but also in the vicinity of t_u^2 ! This shows that the complex singularity is not an artefact of low-temperature expansions but a true feature of the model.

3) If we represent the zeros by a continuous distribution $t^2 = u(\lambda)$ with a density $g(\lambda)$, we may write

$$F = \frac{1}{N} \sum_{i=1}^{\frac{3}{2}N} \ln(t^2 - u_i) \qquad (4.1)$$

$$\simeq \int d\lambda \; g(\lambda) \ln(t^2 - u(\lambda))$$

Therefore we expect the *real part* of F to be continuous across the curve $t^2 = u(\lambda)$. In the vicinity of t_c^2, we write

$$\begin{aligned} F(t) &= F_+(t) \simeq A_+(t^2 - t_c^2)^{2-\alpha} + F_{reg}, \quad t^2 > t_c^2 \\ &= F_-(t) \simeq A_-(t_c^2 - t^2)^{2-\alpha} + F'_{reg}, \quad t^2 < t_c^2 \end{aligned} \qquad (4.2)$$

Writing that Re F_+ = Re F_- along the curve yields a relation between the angle φ (fig.6), α and A_+/A_- :

$$tg(2-\alpha)\varphi = \frac{\cos \pi\alpha - \frac{A_-}{A_+}}{\sin \pi\alpha} \qquad (4.3)$$

Pearson's plot gives $\varphi \simeq 60 \pm 5°$, while estimates of $A_+/A_- = .48 - .51$ [19], of $\alpha = .11$ leads to $\varphi = 57° \pm .7$. Notice that mean field or Bethe give a trivial high temperature phase : $A_+/A_- = 0$, $\alpha = 0$ hence $\varphi = 45°$. In two dimensions, a similar argument predicts $\varphi = \frac{\pi}{2}$, which is the exact result.

Pearson has also drawn the paths of the zeros in the presence of a (real) magnetic field : this is roughly indicated by arrows on Fig. 6. The zeros seem to fall into two families, having distinct behaviors. Zeros closer to t_c^2 move along angles of approximately $\pm$ 60°, while zeros in the left hand half-plane move parallel to the real axis. This is what was expected from t_c^2 and t_u^2 in the Bethe approximation of Sect. 2. More realistically, we expect the closest zero to the real axis $t_c(h)$ to represent the singularity in the presence of h and to obey the equation of state :

$$\frac{h}{M^\delta} = f\left(\frac{(t - t_c(0))^\beta}{M}\right) \qquad (4.4)$$

$$\text{or} \qquad h^2 \sim -(t_c(h) - t_c(0))^{2\beta\delta} \qquad \beta\delta = \beta + \gamma \qquad (4.5)$$

where the minus sign has been inserted to satisfy the Lee-Yang theorem. Hence

$$t_c(h) - t_c(0) \sim h^{1/\beta\delta} \; e^{\pm i\pi/2\beta\delta} \qquad (4.6)$$

and the angle is predicted to be $\pm 58°$. Again departure from mean field (60°) is hardly visible.

Finally, let us mention that finite size effects may be represented by the relation :

$$h^2 = -(\tau^{2\theta} + C\, N^{-2\theta/\nu})^\varepsilon \qquad (4.7)$$

where $t_c(h,N)$ is the closest zero, $\tau = t_c(h,N) - t_c(0,\infty)$, C is a positive constant, and θ and ε are two new exponents. We have the following relations between them and φ of eq. (4.3)

$$\begin{aligned} \frac{\theta}{\varepsilon} &= \beta\delta \\ \pi - \varphi &= \frac{\pi}{2\theta} \end{aligned} \qquad (4.8)$$

Eq. (4.7) says that before following the direction $\pi/2\beta$ as in Eq. (4.6) the zeros move along the angle

$$\operatorname{Arg}(\tau(h,N) - \tau(0,N)) = \left(\frac{\theta}{\beta\delta} + \frac{1}{2\theta} - 1\right)\pi \qquad (4.9)$$

This angle takes the value 35° in the mean field approximation, and about 28° at d = 3. This agrees with the observed behavior[1].

To summarize, we see that much information is contained in these distributions of zeros. An analysis of the antiferromagnetic zeros is also interesting and will be presented elsewhere.

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