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On the density of partition function temperature zeros†

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Abstract. The density of partition function 'temperature' zeros for the two-dimensional spatially anisotropic Ising model in the absence of a magnetic field satisfies a linear homogeneous partial differential equation. A generalised form of this equation, for a non-zero specific heat exponent, can be derived by applying non-linear scaling to the expression for the specific heat as an integral over the density of zeros.

1. Introduction

All the mathematical features of a partition function arise from the location and distribution of its zeros in the complex planes of appropriate variables, usually the Boltzmann factors, which combine the temperature with the mechanical parameters determining the energy of a system. In the case of magnetic systems described by Heisenberg- or Ising-type Hamiltonians, the mechanical parameters are the external magnetic field and the exchange interaction strengths. A complete description of a phase transition then involves a study of zeros in two complex variables, separately involving the magnetic field and the interaction strength. Within the scaling-law context in the vicinity of a critical point, such descriptions have been proposed by Abe (1967) and Suzuki (1967). In particular, when the magnetic field is absent, Abe (1967) has shown how to obtain linear homogeneous differential equations, which are satisfied by the density of zeros per lattice site. These differential equations can be derived by applying scaling criteria directly to the general expressions for thermodynamic functions in terms of integrals over the densities of zeros. The corresponding densities of zeros then also acquire functional forms which are characteristic of scaling theory. These theories have been used to show how certain types of zero distributions give rise to particular forms of singular behaviour at a critical point. The functional forms for the densities of zeros are often constructed by analogy with known expressions obtained from soluble models. This approach has worked well in those cases where the zeros lie on lines in the complex plane of the Boltzmann factor associated with the interaction variable. However, when the distribution of zeros is two dimensional, comparison with the forms obtained from soluble models has been less extensive and the density functions adopted have mainly been constructed by analogy with those one-dimensional densities which yield the same type of critical behaviour. It therefore becomes especially important to place the recently derived expressions for the densities of the 'temperature' zeros (Stephenson and Couzens 1984, Stephenson 1986) of the two-dimensional Ising model in the absence of a magnetic field into the theoretical scheme of scaling-law forms and differential equations referred to above.

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2. Density of zeros for the Ising model

The 'exact' expressions for the density of zeros for the two-dimensional Ising model on spatially anisotropic quadratic and triangular lattices assume the general form, for $y>0$,

$$g(x, y)=\frac{y}{4\pi^2[\det B(X-\lambda_2 y^2)(\lambda_1 y^2-X)]^{1/2}} \tag{1}$$

which represents a two-dimensional distribution in the neighbourhood of the relevent (ferromagnetic) critical point at w_c in a complex variable $w=w_c+x+iy=w_c-X+iy$. Here $x=-X=\mathrm{Re}\,(w-w_c)$ is negative for the Ising model near a ferromagnetic critical point, so X is positive. Some minor changes are needed for an antiferromagnetic critical point. Details of the derivation and the physical significance of the variables have been presented by Stephenson and Couzens (1984) and Stephenson (1986). The features we need to note here are

(i) the existence of a cusp-like region containing the zeros, with parabolic boundaries intersecting at the critical point on the real axis,

(ii) the singular nature of the density of the zeros at these boundaries,

(iii) the factor of $y=\mathrm{Im}\, w$ in the numerator,

(iv) the functional dependence on x and y.

The above expression for the density of zeros indeed has a scaling-law form, as may be seen if we rearrange it as

$$g(x, y)=\frac{y^{-1}}{4\pi^2\{\det B[(X/y^2-\lambda_2)(\lambda_1-X/y^2)]\}^{1/2}} \tag{2}$$

$$=y^{-1}f(X/y^2) \qquad \text{say.} \tag{3}$$

Furthermore it satisfies a linear partial differential equation of homogeneous form

$$g+2x\frac{\partial g}{\partial x}+y\frac{\partial g}{\partial y}=0. \tag{4}$$

However, this equation differs from the one previously obtained by Abe, who applied the usual 'linear' scaling criteria to the integral expression for the specific heat in terms of a double integral over a two-dimensional density of zeros. As we will show below, 'quadratic' scaling is needed for the Ising model, and the real and imaginary parts of the complex variable w must be scaled differently.

3. Derivation of the differential equation

A more general form of the above differential equation can be derived in the case when the specific heat exponent α is non-zero, provided the scaling criteria are applied separately to the real and imaginary parts of the variable w in the vicinity of the critical point. In order to take into account the cusp-like boundaries we employ 'non-linear' scaling by setting

$$x=a^n x' \qquad y=ay' \tag{5}$$

where n is an extra new exponent, which assumes the value 2 for parabolic boundaries.

Starting from the partition function

$$Z_N(w) = Z_N(0) \prod_r (1 - w/w_r) \tag{6}$$

we have for the internal energy, as shown by Abe, as $N \to \infty$, with $\beta = 1/kT_B$

$$\frac{E}{N} = \frac{1}{N}\left(\frac{\mathrm{d}w}{\mathrm{d}\beta}\right)\sum_r \frac{1}{w_r - w} \sim \left(\frac{\mathrm{d}w}{\mathrm{d}\beta}\right)\int\int \mathrm{d}x\,\mathrm{d}y \frac{g(x,y)}{(w_c + x + \mathrm{i}y - w)} \tag{7}$$

whence the specific heat is

$$\frac{C}{Nk} = -\frac{1}{N}\left(\beta\frac{\mathrm{d}w}{\mathrm{d}\beta}\right)^2 \sum_r \frac{1}{(w - w_r)^2} \sim -\left(\beta\frac{\mathrm{d}w}{\mathrm{d}\beta}\right)^2 \int\int \mathrm{d}x\,\mathrm{d}y \frac{g(x,y)}{(w_c + x + \mathrm{i}y - w)^2}. \tag{8}$$

Using the fact that zeros occur in conjugate pairs, the expression for the specific heat becomes, with $u = x + w_c - w$,

$$\frac{C}{Nk} = -2\int\int \mathrm{d}x\,\mathrm{d}y\, g(x,y)\frac{(u^2 - y^2)}{(u^2 + y^2)^2} \qquad y > 0. \tag{9}$$

Now make the non-linear scaling substitution (5), with a identified as $w - w_c$, so the specific heat divergence of the LHS is of order $a^{-\alpha}$. Then up to a constant factor, the singular parts in (9) are

$$a^{-\alpha} \sim -\int\int \mathrm{d}x'\,\mathrm{d}y'\, a^{n-1} g(a^n x', ay')\frac{[(1 + a^{n-1}x')^2 - y'^2]}{[(1 + a^{n-1}x')^2 + y'^2]^2}. \tag{10}$$

Next we require the combination

$$a^{\alpha+n-1} g(a^n x', ay')\frac{[(1 + a^{n-1}x')^2 - y'^2]}{[(1 + a^{n-1}x')^2 + y'^2]^2} \tag{11}$$

to be independent of a for small a, in the sense that the derivative of this expression is zero, as $a \to 0$. Differentiate (11) with respect to a, equate the result to 0, reintroduce x and y via (5) and rearrange to obtain

$$\begin{aligned}(\alpha + n - 1)g(x,y) + nx\frac{\partial g}{\partial x} + y\frac{\partial g}{\partial y} &\\ = g(x,y)2(n-1)x(x+a)&\frac{[(x+a)^2 - 3y^2)]}{[(x+a)^4 - y^4)]}\\ \to g(x,y)2(n-1)x^2&\frac{(x^2 - 3y^2)}{(x^4 - y^4)} \qquad \text{as } a \to 0.\end{aligned} \tag{12}$$

If $n = 1$, as in the linear case discussed by Abe, the RHS vanishes immediately. When $n \neq 1$, we examine the behaviour of the RHS along a 'scaling line' $x = cy^n$, where $x/y = cy^{n-1}$ is 'small' near a critical point on the real axis, so $x \ll y$. Now the RHS is approximately

$$g(x,y)2(n-1)3x^2/y^2$$

which is 'small' compared with all the terms on the LHS. So we we are left with a partial differential equation for the density of zeros:

$$(\alpha + n - 1)g + nx\frac{\partial g}{\partial x} + y\frac{\partial g}{\partial y} = 0. \tag{13}$$

If we set $\alpha = 0$, and $n = 2$, we regain the differential equation (4) satisfied by the Ising model density of zeros.

4. Distributions of zeros

The general solution of (13) is

$$g(x, y) = y^{1-\alpha-n} f(x/y^n). \tag{14}$$

Then the integrated density of zeros is

$$g(y) = \int_{x_1}^{x_2} \mathrm{d}x\, g(x, y) = \int_{x_1}^{x_2} \mathrm{d}x\, y^{1-\alpha-n} f(x/y^n). \tag{15}$$

The natural 'scaling lines' are $x = cy^n$, so we introduce a scaling variable $u = x/y^n$. The integrand can be expressed in terms of the scaling variable u, so

$$g(y) = y^{1-\alpha} \int_{u_1}^{u_2} \mathrm{d}u\, f(u) \propto y^{1-\alpha}. \tag{16}$$

The two-dimensional problem is thus reduced to an effectively equivalent one-dimensional one of the same form as discussed previously by Abe.

Some heuristic generalisations can easily be constructed. For example, for $y > 0$ with $0 < m < 1$, set

$$\begin{aligned} g(x, y) &= \frac{y}{[(x - \lambda_1 y^n)(\lambda_2 y^n - x)]^{(m+1)/2}} \\ &= y^{1-n(1+m)} f(x/y^n). \end{aligned} \tag{17}$$

The cusp boundaries are at $u_1 = x_1/y^n = \lambda_1$ and $u_2 = x_2/y^n = \lambda_2$. Again introducing the scaling variable $u = x/y^n$, the integrated density of zeros becomes

$$g(y) = \int_{x_1}^{x_2} \mathrm{d}x\, g(x, y) = y^{1-nm} \int_{u_1}^{u_2} \mathrm{d}u\, f(u). \tag{18}$$

The corresponding specific heat exponent α is now nm, so setting $n = 1$ and $m = \alpha$ yields the linear wedge case considered by Abe.

A further possible similar generalisation of the density of zeros is

$$g(x, y) = \frac{h(y)}{[(x - x_1)(x_2 - x)]^{(m+1)/2}}. \tag{19}$$

In any case where the cusp or wedge boundaries are at x_1 and x_2, integrating across the cusp gives

$$\begin{aligned} g(y) &= \int_{x_1}^{x_2} \mathrm{d}x \frac{h(y)}{[(x - x_1)(x_2 - x)]^{(m+1)/2}} \\ &= h(y)[(x_2 - x_1)/2]^{-m} B(1/2 - m/2, 1/2). \end{aligned} \tag{20}$$

If the cusp boundaries are at $x_1 = \lambda_1 y^n$ and $x_2 = \lambda_2 y^n$, then

$$g(y) \propto h(y) y^{-nm} \tag{21}$$

where one could choose $h(y) \propto y$, as before.

If in the Ising model density of zeros (1), we set $X = -x$ and $Y = y^2$, we have

$$\begin{aligned} g(x, y)\, \mathrm{d}x\, \mathrm{d}y &= \frac{y\, \mathrm{d}x\, \mathrm{d}y}{4\pi^2[\det B(X - \lambda_2 y^2)(\lambda_1 y^2 - X)]^{1/2}} \\ &= \frac{\mathrm{d}x\, \mathrm{d}Y}{8\pi^2[\det B(X - \lambda_2 Y)(\lambda_1 Y - X)]^{1/2}} \end{aligned} \tag{22}$$

which has a 'linear' cusp, or wedge, like the cases considered by Abe. X and Y are the 'natural' variables which arise in the quadratic forms associated with the density of zeros for the Ising model, as discussed by Stephenson and Couzens (1984) and Stephenson (1986). Of course the physical nature of the transition is unchanged, so it is likely this result is only a mathematical curiosity.

5. Discussion

We discuss briefly some of the ways in which non-linear scaling may be of technical importance. So far we have considered only partition function temperature zeros in the absence of a magnetic field. It is now necessary to extend the theory to incorporate magnetic field (Yang–Lee) zeros. It would also be interesting to examine the theory of zeros of correlation functions, particularly in cases where the zero distributions are two dimensional. Such developments have already been made by Abe (1967) and Suzuki (1967) for one-dimensional zero distributions.

In general the scaling theory of phase transitions has been carried out in the context of real physical variables, such as the temperature and the interaction strengths, magnetic field, etc, and extension to complex variables has been made by formally extending the real variables into the complex plane, making the tacit assumption that the thermodynamic functions have the same formal functional features in the complex plane as they had in the original real variable. Although such an assumption is entirely reasonable with regard to the analytical properties of the thermodynamic functions in question, our results show that the assumption fails with respect to the analytical and scaling properties of the densities of zeros, at least in the particular case of the temperature zeros of the two-dimensional Ising model. In fact the density of zeros is not an analytic function of a single complex variable, but of the real and imaginary parts separately. This is evident for the specific example of the Ising model from the critical region formula (1) and from a general expression for the Ising model density of zeros recently derived by the author (Stephenson 1987) and also for some other exactly soluble models previously analysed by Suzuki (1967). In other words, the scaling transformations, which mathematically describe the physical scaling process, are also not functions of a single complex variable, but of the real and imaginary parts separately, which can then scale differently, via what we have termed 'non-linear' scaling.

The geometrical consequences of non-linear scaling are mainly evident in the cusp-like approach of the 'scaling lines', and the associated boundaries, to the critical point(s) on the real axis. This has immediate practical consequences for the location and estimation of critical points from partition function zeros. Some authors (e.g. Abe 1967, Katsura 1967, Ono *et al* 1967, 1968, 1969, Suzuki 1967, Abe and Katsura 1970) have calculated partition function zeros numerically, typically for small finite lattice systems, and have then attempted to extrapolate these zeros geometrically in the complex plane in order to locate the critical point. Obviously such extrapolation methods could be quite misleading, and seriously in error, if the wrong geometry for the scaling lines were assumed. For example, a linear extrapolation would be most inappropriate for the two-dimensional Ising model. However, it seems that often zeros approach the real axis 'vertically', or 'at right angles', which assists the extrapolation. (For examples of a similar nature on other models, refer to Rammel and Maillard (1983) and Martin and Maillard (1986).) Nevertheless, a more systematic extrapolation procedure, involving numerical analysis of the locations of the zeros in the vicinity of the critical point, would generally involve making some assumptions about the geometrical form of the approach to the real axis. For example, one could assume a linear or a quadratic form for the scaling lines and boundaries, or a more general form described by an (unknown) exponent like our 'n', which could then be determined numerically, along with the critical point, during the extrapolation procedure.

Moreover, awareness of the possibility of non-linear scaling of zeros occurring in the vicinity of a critical point could be of considerable importance in any systematic (numerical) study of the 'movement' of zeros under finite lattice 'renormalisation' type transformations, which have been made (e.g. by Derrida and Flyvbjerg 1985, Wood 1985, Wood and Turnbull 1986) for the Ising and other lattice models.

Of course we are not yet in a position to be able to predict the nature of zero distributions in the neighbourhood of critical points for a lattice model purely on the basis of (the spin-space 'dimension' and symmetries of) its Hamiltonian or the lattice type and dimension. But for certain soluble models, and for models which are known to obey scaling and for which the critical exponents are known exactly, or have been estimated numerically by series expansion or renormalisation group techniques, we can make some plausible suggestions as to the types of distributions which can be expected to occur (refer also to Suzuki (1967)).

In the model zero distributions considered in this paper, the 'non-linear' scaling aspects of the full two-dimensional zero distributions are immediately integrated out when one calculates the thermodynamic functions (in a good approximation, the nature of which gives cause for further study elsewhere) using the integrated density of zeros. So one would not immediately expect non-linear scaling to have any direct physical consequences. Of course this may not be the situation for other models. In any case one may expect that non-linear scaling will play a role in the understanding and construction of theories and models in the context of critical phenomena in statistical physics, with subsequent possible ramifications for other branches of physics, wherever distributions of partition (and other) function zeros are of interest.

6. Summary

We have found that in order to fit the Ising model density of zeros into the scaling context, one has to use 'quadratic' scaling and to scale the real and imaginary parts of the relevant complex variable differently. For a general specific heat exponent, the two-dimensional density of zeros satisfies a linear homogeneous partial differential equation, which can be derived by applying non-linear scaling to the singular part of the specific heat.

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