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Location of zeros in the complex temperature plane: Absence of Lee–Yang theorem

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Abstract. In the Yang–Lee theory the occurrence of a phase transition at real (physical) values of the magnetic field is related to the behaviour of the density of zeros of the partition function in the complex magnetic field plane. As shown by Lee and Yang, these zeros fall on lines for a wide class of ferromagnetic models. In extensions of the Yang–Lee theory to the complex temperature plane, it has often been assumed that the zeros of the partition function would again fall on lines rather than in areas. Though this happens to be true for the isotropic Ising model, we point out that there is in general no basis for this assumption. We discuss the location of the zeros of the partition function of the anisotropic Ising model in the complex temperature plane and show that they indeed always fall in areas.

1. Introduction

An elegant characterisation of the mathematical mechanism by which certain statistical mechanical models may develop phase transitions in the thermodynamic limit was given by Yang and Lee in 1952. They pointed out that an intimate connection (discussed below) exists between the occurrence of a phase transition in a system and the distribution of zeros of the grand-canonical partition function in the complex fugacity plane. The Yang–Lee theory can alternatively be formulated in terms of the distribution of zeros of the canonical partition function in the complex magnetic field H plane. In this paper, we will use the latter formulation, and, for concreteness, only consider Ising models. While there are to our knowledge no examples where the theory has turned out to be useful in actually solving models, it has been applied profitably in rigorous statistical mechanical studies, especially in proving the *absence* of phase transitions in several systems (see for a review Kurtze 1979). The prime example of a result of this kind is the famous so-called Lee–Yang theorem (1952) that the zeros of the partition function of the ferromagnetic spin- $\frac{1}{2}$ Ising model with two-spin interactions lie on the imaginary H axis. This implies that ferromagnetic Ising models cannot have a phase transition in a finite (real) magnetic field.

The essential idea underlying the Yang–Lee characterisation of a phase transition (Yang and Lee 1952; see for introductions also Fisher 1965, Thompson 1979) may be summarised as follows. The partition function $Z_N(H, T)$ of a system of N Ising spins $s_i = \pm 1$ may be expanded in powers of $z = \exp(-2H/kT)$ as

$$Z_N(H, T) = z^{-N/2} \sum_{n=0}^N P_n z^n. \quad (1)$$

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Since Z is a polynomial in z of degree N , Z will have N roots z_r , in the complex z plane; it can therefore be written as

$$Z_N(H, T) = z^{-N/2} P_0 \prod_{r=1}^N \left(1 - \frac{z}{z_r}\right). \quad (2)$$

If in the thermodynamic limit the zeros coalesce into lines C in the complex plane, then the free energy per spin $f(H, T)$ becomes (omitting an unimportant term proportional to $\ln z$)

$$\begin{aligned} f(H, T) &= -kT \lim_{N \rightarrow \infty} N^{-1} \ln Z_N(H, T) = -kT \lim_{N \rightarrow \infty} N^{-1} \sum_{r=1}^N \ln \left(1 - \frac{z}{z_r}\right) \\ &= -kT \int_C ds g(s) \ln(1 - z/z(s)), \end{aligned} \quad (3)$$

where $Ng(s) ds$ is the number of zeros in a line element ds of C ($\int_C ds g(s) = 1$).

Since all P_n in (1) are positive, none of the roots z_r can lie on the (physical) positive real z axis, and consequently the partition function in (2) is analytic along the real z axis for any finite N . However, it is possible that in the thermodynamic limit the zeros approach the real axis at z_c . If so, this marks the occurrence of a phase transition, because f is then non-analytic at z_c .

A priori, there is no reason to expect the zeros to coalesce into lines. However, it is commonly believed that lines of zeros are more 'natural' than areas, in view of the Lee-Yang theorem that the zeros of the ferromagnetic Ising model lie on the unit circle $|z|=1$ (and so on the imaginary H axis). Later extensions of this theorem comprise the case of higher-order Ising spins (Griffiths 1969), Ising models with multiple spin interactions (Suzuki and Fisher 1971), the quantum Heisenberg model (Suzuki and Fisher 1971), the classical XY and Heisenberg model (Dunlop and Newman 1975) and some continuous spin models (Simon and Griffiths 1973, Newman 1974, 1976). Elvey (1974) has also established that, for a class of one-dimensional lattice gas models with finite-range, finite-order interactions, the zeros in the field or temperature plane are generally confined to lines. For a review of such results, see Kurtze (1979).

Consider now the low temperature expansion (see e.g. Thompson 1979) for the isotropic two-dimensional Ising model with nearest neighbour interactions J in zero field,

$$Z_N(H=0, T) = 2 \exp(\frac{1}{2}NJq/kT) \sum_{r=0}^{Q(N)} n_r (e^{-2J/kT})^r, \quad (4)$$

where q is the coordination number. As has been stressed in particular by Fisher (1965), the analogy of (4) with (1) shows that the Yang-Lee theory similarly describes the development of a singularity of $Z(H=0, T)$ in the complex temperature plane for an isotropic Ising model. Accordingly, it has often been tacitly assumed in the literature that zeros of the partition function in the complex T plane (Fisher 1965, Majumdar 1966, Jones 1966, Abe 1967, Abe and Katsura 1970) would also naturally fall in lines. This indeed happens to be the case for the isotropic Ising model (Fisher 1965), but it should be emphasised that the Lee-Yang theorem does *not* carry over to the complex temperature plane: the validity of the Lee-Yang theorem is a consequence of special properties of the coefficients P_n in (1) which the combinatorial factors n_r in (4) do *not* share.

It is the purpose of this paper to show that zeros in the complex temperature plane in fact generally fall in areas rather than in lines. As should be clear from the above,

this result is not all that surprising, as there is no *a priori* reason to expect a Lee–Yang theorem to hold in the complex temperature plane. It is therefore remarkable that the fact that the zeros in this plane generally fall in areas has not been realised before. In fact, a hint at differences between the isotropic and anisotropic Ising models is already obtained from the low temperature expansion of the anisotropic square Ising model with nearest neighbour interactions J and ΔJ ,

$$Z(H=0, T) = \sum_{k,l} m_{k,l} (e^{-2J/kT})^k (e^{-2\Delta J/kT})^l = \sum_{k,l} m_{k,l} (e^{-2J/kT})^{k+\Delta l}. \quad (5)$$

For $\Delta \neq 1$, this expansion is not of the same form as the one for the isotropic Ising model, cf (4), because Z is not a polynomial in $\exp(-2J/kT)$ for non-integer Δ . Though this does not necessarily imply that the zeros have to fall in areas (for example, the Ising model in an *anisotropic* field does obey a Lee–Yang theorem in the complex field plane (Suzuki and Fisher 1971) but is not a polynomial in $\exp(-2H/kT)$ either), it is nevertheless a warning to suspect qualitative differences in the location of zeros of anisotropic models from those of isotropic models.

In § 2 we investigate the location of the zeros of the exact expression for the partition function of the finite size two-dimensional Ising model in more detail. It is found that the zeros of the anisotropic model always fall in areas, and the behaviour of the density of zeros near the real axis is discussed. We also briefly investigate how the behaviour of the zeros differs for the two different phase transitions of the triangular Ising model, assuming that the expression for the partition function of the finite triangular lattice has a form analogous to that of the square Ising model. The paper closes with some concluding remarks regarding our results and their possible bearings on related quantum spin models in a magnetic field.

2. Anisotropic two-dimensional Ising models

We first consider the square Ising model with reduced interactions K and K' . From Kaufman's (1949) exact solution, we have for a finite lattice†

$$Z_N = \prod_{r=1}^m \prod_{s=1}^{n/2} (\cosh 2K_1 \cosh 2K_2 - \alpha \sinh 2K_1 - \beta \sinh 2K_2), \quad (6)$$

with

$$\alpha = \cos 2\pi r/m, \quad \beta = \cos 2\pi s/n, \quad N = mn. \quad (7)$$

In the thermodynamic limit, (6) yields the well known Onsager (1944) solution for the free energy per spin f ,

$$\frac{f}{kT} = \frac{-1}{8\pi^2} \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \ln(\cosh 2K_1 \cosh 2K_2 - \sinh 2K_1 \cos \phi_1 - \sinh 2K_2 \cos \phi_2). \quad (8)$$

It can easily be checked that the zeros of (6) all satisfy $|\sinh 2K| = 1$ in the *isotropic* case $K_1 = K_2 = K$. We will therefore plot the zeros in the complex $\sinh 2K \equiv S$ plane.

† The expression for Z_N actually contains the sum of four terms like the one in (6). However, as remarked by Fisher (1965) and proven by Brascamp and Kunz (1974), the single term in (6) describes the asymptotic distribution of zeros in the thermodynamic limit.

Near $S = 1$, one finds for the density of zeros on this circle $g(S) \sim |\text{Im } S|$, consistent with the logarithmic singularity in the specific heat (see Fisher 1965). The behaviour near the antiferromagnetic intersection at $S = -1$ is similar.

In agreement with the arguments given in the introduction, (6) immediately shows that the zeros of Z fall in areas whenever $K_1 \neq K_2$: while the zeros depend only on the *single* parameter $\alpha + \beta$ in the isotropic case $K_1 = K_2$ (and so fall on lines), they depend on the two parameters α and β separately as soon as the symmetry is broken. Therefore lines bifurcate to areas in the anisotropic case. This can most easily be illustrated explicitly by investigating the case when $K_1 = K, K_2 = 3K$. Since $\sinh 6K = 3 \sinh 2K + 4 \sinh^3 2K$ and $\cosh 6K = -3 \cosh 2K + 4 \cosh^3 2K$, we have

$$\cosh 2K \cosh 6K - \alpha \sinh 2K - \beta \sinh 6K = 4S^4 - 4\beta S^3 + 5S^2 - (\alpha + 3\beta)S + 1. \quad (9)$$

Thus, for $K_1 = K = \frac{1}{3}K_2$, the partition function is a polynomial in $S \equiv \sinh 2K$ which can according to (6) and (9) be written as a product of factors of the form (9). For every value of α and β , there are therefore four zeros in the complex S plane, two in the upper half plane and two in the lower half plane. By varying α and β , one obtains the various locations of the zeros, and since $|\alpha| \leq 1$ and $|\beta| \leq 1$, the areas in which they fall are generally bounded. This is illustrated in figure 1, where the shaded areas

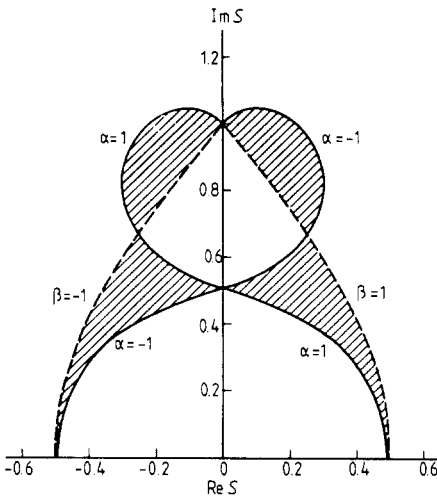


Figure 1. Location of the zeros in the upper half of the complex $S = \sinh 2K$ plane for the square Ising model with reduced interactions K and $3K$. The zeros are everywhere dense in the shaded areas, which touch the real axis at $S = \pm \frac{1}{2}$. At the boundaries of the areas, where $\alpha = \pm 1$ or $\beta = \pm 1$, the density of zeros diverges as $\rho^{-1/2}$ where ρ is the distance from the boundary.

contain the zeros. Obviously, the zeros become everywhere dense within these areas in the thermodynamic limit. However, since according to (7) $\alpha = \cos \phi_1$ and $\beta = \cos \phi_2$ with ϕ_1 and ϕ_2 equally distributed on the interval $[0, 2\pi]$, the density of zeros per unit area g diverges at the boundaries of the areas, where $\alpha = \pm 1$ or $\beta = \pm 1$. This is also apparent from the explicit behaviour of g near the point where the areas 'pinch off' the real axis. This occurs at the critical values of the square Ising model where $\sinh 2K_1 \sinh 2K_2 = 1$ (in the case $K_1 = \frac{1}{3}K_2 = K$, this yields $S_c = \frac{1}{2}$). For small $\delta S = S - S_c$

and arbitrary anisotropy $\Delta = K_2/K_1 > 0$, g behaves as (see appendix, equation (A19))

$$g(S) \sim \frac{|\delta S''|}{\{[-\delta S' - c_2(\delta S'')^2][\delta S' + c_1(\delta S'')^2]\}^{1/2}}, \quad (10)$$

with $\delta S' \equiv \text{Re } \delta S$ and $\delta S'' \equiv \text{Im } \delta S$ satisfying (see (A16))

$$\begin{aligned} c_2(\delta S'')^2 \leq -\delta S' \leq c_1(\delta S'')^2 & \quad \text{if } \Delta < 1, \\ c_1(\delta S'')^2 \leq -\delta S' \leq c_2(\delta S'')^2 & \quad \text{if } \Delta > 1, \end{aligned} \quad (11)$$

and the coefficients c_1 and c_2 depending on Δ through (A15). Equation (10) shows that $g(S)$ has square root singularities at the boundaries of the area. As is well known, of course, the critical behaviour of the Ising model is unaltered by the presence of anisotropy. Thus the density of zeros (10) should still in some sense show the same qualitative behaviour as the density of zeros of the isotropic model on the circle. This is in fact the case because the critical behaviour is determined by the density h which is proportional to the number of zeros with $\text{Im} S$ in a given interval. For $\Delta < 1$, we have

$$h \equiv \int_{-c_1(\delta S'')^2}^{-c_2(\delta S'')^2} dS' g(S) \sim |\delta S''| \int_{-c_1}^{-c_2} dx [(-x - c_2)(x + c_1)]^{-1/2}. \quad (12)$$

Since the integral is independent of $\delta S''$, we have $h \sim |\delta S''|$, just like what is found for the isotropic Ising model (see after (8)). Accordingly, $g(S)$ in (10) gives rise to the same logarithmic singularity in the specific heat.

In the appendix, we also show that for $|\Delta - 1| \ll 1$

$$c_1 - c_2 = -0.188(\Delta - 1), \quad (13)$$

so that the width of the areas vanishes linearly in Δ if $\Delta \rightarrow 1$.

It seems virtually impossible to derive general properties of the shapes of the areas, since these depend quite sensitively on Δ . This can most easily be seen by investigating the location of zeros along part of the imaginary axis. When $S = ix$ with x real and $|x| \leq 1$, we have $2K = i \sin^{-1} x \equiv iy$. According to (6), along this part of the imaginary axis the zeros are therefore the solutions of

$$\cos y \cos y\Delta - i\alpha \sin y - i\beta \sin y\Delta = 0. \quad (14)$$

Since the imaginary part is always zero when $\alpha = \beta = 0$, and since $\cos y \neq 0$ whenever $\sinh 2K \neq i$ the zeros on the imaginary axis are determined by the equation

$$y = \pm (\pi/2\Delta)(1 + 2k), \quad k = 0, 1, 2, 3, \dots, \quad (15)$$

or

$$\sinh 2K = \pm i \sin[(\pi/2\Delta)(1 + 2k)]. \quad (16)$$

If Δ is an integer or a rational number, there are according to this equation only a finite number of points where the areas of zeros touch the imaginary axis with $|\sinh 2K| < 1$, and if $\Delta = 1/l$ with l an integer, then there are no solutions other than $\sinh 2K = 0$ or $\sinh 2K = i$. On the other hand, if Δ is an irrational number, there are infinitely many solutions of (16), so that the areas of zeros probably comprise this part of the imaginary axis completely.

It should be stressed that the general conclusion that the zeros fill areas is *not* an artifact of our choice of the S plane; it holds in the K plane or in any other plane as well. The differences between the locations of the zeros for the various choices are, however, most pronounced for zeros that have large imaginary parts and hence have little influence on the real behaviour of the system.

In the above analysis of the square Ising model we found that while the location of the zeros depends quite sensitively on the anisotropy away from the real axis, the behaviour of $g(S)$ is always of the form (10) near the real axis. In the triangular Ising model, on the other hand, the behaviour of the density of zeros is more exciting since anisotropy does change the critical behaviour of the antiferromagnetic lattice: for the triangular Ising model with reduced interactions K_1, K_2 and K_3 , the ferromagnetic phase transition is essentially the same as the one on the square Ising lattice, but the antiferromagnetic transition is different because of frustration effects. In the isotropic antiferromagnetic case, the ground state is degenerate so that there is a finite entropy even at $T = 0$ (Wannier 1950, Stephenson 1964). This suppresses the phase transition to $T = 0$. However, since anisotropy breaks the ground state degeneracy, it becomes a relevant operator (Forgacs and Fradkin 1981) at this transition. Triangular lattices with reduced antiferromagnetic interactions $|K_1| = |K_2| > |K_3|$ have a finite temperature phase transition, but if $|K_1| = |K_2| < |K_3|$ the ground state degeneracy is still present and no finite temperature phase transition exists (Stephenson 1969, 1970, Peschel 1982). To demonstrate how these effects show up in the context of the location of the zeros, we now briefly report results for the triangular Ising model.

The solution of the free energy per spin of the triangular Ising model reads (Houtappel 1950)

$$\ln \frac{1}{2} Z_T = \frac{1}{8\pi^2} \int_0^{2\pi} d\phi_1 \int_0^{2\pi} d\phi_2 \ln [C_1 C_2 C_3 + S_1 S_2 S_3 - S_1 \cos \phi_1 - S_2 \cos \phi_2 - S_3 \cos(\phi_1 + \phi_2)], \tag{17}$$

where

$$S_i \equiv \sinh 2K_i, \quad C_i \equiv \cosh 2K_i. \tag{18}$$

To our knowledge there exists no derivation of the partition function for a finite triangular lattice. However, comparison with (6) and (8) suggests that we may obtain the zeros of the triangular partition function as the solutions of

$$C_1 C_2 C_3 + S_1 S_2 S_3 - S_1 \cos \phi_1 - S_2 \cos \phi_2 - S_3 \cos(\phi_1 + \phi_2) = 0. \tag{19}$$

Let us introduce the variable

$$X \equiv (\sinh 2K)/(2 \cosh 2K - \sinh 2K), \tag{20}$$

so that the positive real X axis with $0 < X < 1$ corresponds to ferromagnetic interactions and the negative real axis for $-\frac{1}{3} < X < 0$ to antiferromagnetic interactions. The point $X = -\frac{1}{3}$ is the $K = -\infty$ antiferromagnetic point. In the isotropic case $K_1 = K_2 = K_3 = K$, equation (19) reduces to

$$(3 + 2\mu + 2\nu)X^2 - 2(\mu + \nu)X + 1 = 0. \tag{21}$$

From the definition of μ and ν ,

$$\mu \equiv \cos \phi_1 + \cos \phi_2, \quad \nu \equiv \cos(\phi_1 + \phi_2), \tag{22}$$

it follows that

$$\mu^2 = 2(\nu + 1) \cos^2[\frac{1}{2}(\phi_1 - \phi_2)]. \tag{23}$$

Hence, because $\phi_1 - \phi_2$ can take on arbitrary values for fixed ν , μ lies in the range

$$-[2(\nu + 1)]^{1/2} \leq \mu \leq [2(\nu + 1)]^{1/2}. \tag{24}$$

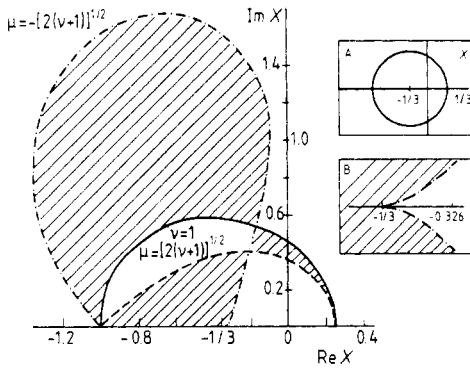


Figure 2. Location of the zeros in the complex X plane for the triangular Ising model with interactions K, K and $2K$. There is no finite temperature antiferromagnetic phase transition for $-\frac{1}{3} < X < 0$. Inset A: location of the zeros of the isotropic model in the complex X plane. Inset B: enlargement of the figure near the point $X = -\frac{1}{3}$. This antiferromagnetic zero temperature point is the endpoint of the cusp-like region without zeros.

As shown in inset A of figure 2, the solutions of (21) lie on a circle with radius $\frac{2}{3}$ and centre at $X = -\frac{1}{3}$, and on the negative real axis $X < -\frac{1}{3}$. Thus, the zeros do not intersect the antiferromagnetic interval $-\frac{1}{3} < X < 0$ in agreement with the result that there is no finite temperature phase transition, but they just touch the $K = -\infty, X = -\frac{1}{3}$ point.

Figure 2 shows the location of the zeros in the complex X plane for a triangular lattice with interactions $K_1 = K_2 = \frac{1}{2}K_3 = K$. As discussed above, there should be no finite temperature antiferromagnetic phase transition in this case. Indeed, the zeros do not pinch the negative real axis between $X = -\frac{1}{3}$ ($K = -\infty$) and $X = 0$ ($K = 0$), but nevertheless the location of the zeros near the point $X = -\frac{1}{3}$ is quite different from the one in the isotropic case of inset A. As shown in inset B, this point is the endpoint of a ‘zero-free’ cusp penetrating the area of zeros. However, in the opposite case with interactions $\frac{1}{2}K_1 = \frac{1}{2}K_2 = K_3 = K$ shown in figure 3, the zeros near $X = -\frac{1}{3}$ disappear, while a new intersection now shows up on the negative real axis. This is in agreement with the general behaviour of the antiferromagnetic triangular lattice described above.

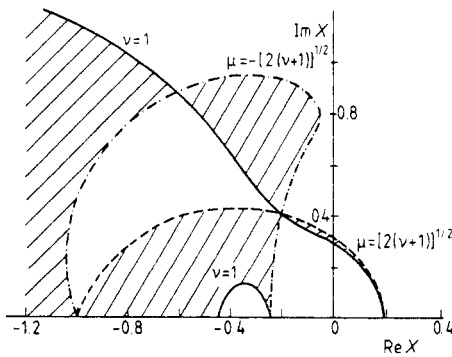


Figure 3. Location of the zeros in the complex X plane for the triangular Ising model with interactions $2K, 2K$ and K . The points where the areas of zeros touch the real temperature axis for $-\frac{1}{3} < X < 1$ mark one antiferromagnetic and one ferromagnetic phase transition. The shaded area on the left is bounded since the $\nu = 1$ boundary (full line) finally bends over and intersects the negative real axis at about $X = -2.8$.

3. Concluding remarks

In the preceding sections we have seen that the extension of the Yang–Lee approach to the case of complex temperatures is less obvious and beneficial than had been assumed until now. It is rather surprising that this fact has not been appreciated before, and our analysis indicates that one should rather turn the question around and ask: why *do* the zeros fall on lines in the isotropic case? Or, is the fact that the temperature zeros of the isotropic square Ising model lie on the unit circle $|\sinh 2K|=1$ related to the self-duality of the model? Another interesting point that might deserve further attention is the curious fact that even an imaginary temperature can have a ‘physical’ meaning: by means of the star–triangle relation (Syozzi 1972) the hexagonal Ising lattice with purely imaginary interactions iK , $K \in [0, \pi/6]$ can be transformed into the antiferromagnetic triangular Ising lattice. Consequently, in the complex temperature plane the hexagonal Ising lattice has the two different phase transitions of the triangular lattice: an ordinary Ising transition at real temperatures and one at imaginary temperatures corresponding to the one in the frustrated antiferromagnetic triangular Ising lattice, discussed above.

Our findings may also have their bearings on the zeros in the complex field plane of the class of d -dimensional quantum models whose behaviour at zero temperature Suzuki (1976) has related to the behaviour of a $(d+1)$ -dimensional zero field Ising model in the extreme anisotropy limit. (These quantum models are not covered by the theorem of Suzuki and Fisher (1971).) According to this relation the quantum Ising chain in a transverse field at zero temperature can be obtained from the square Ising model in the extreme anisotropy limit $K_1 \rightarrow 0$, $K_2 \rightarrow \infty$, $K_1 \exp 2K_2$ fixed, and this quantum chain (solved exactly by Pfeuty (1970)) has indeed a zero temperature phase transition at finite values of the field. Thus, at $T=0$ the zeros in the complex transverse field plane should at least come off the imaginary axis and may possibly fall in areas. Though the first does happen for the quantum Ising chain, the zeros fall on a set of circle segments instead of in areas. It may be of interest to analyse explicitly how the zeros condense again into lines in the extreme anisotropy limit in this model, in order to get an indication of the possible behaviour of the quantum models obeying Suzuki’s relation in higher dimensions.

Acknowledgment

One of us (WvS) is grateful to Professor M E Fisher for a discussion that motivated the work described in this paper.

Appendix

In this appendix, we calculate the density of zeros of the square lattice near the real axis. We first have to calculate the location of the zeros near the real axis. According to (6) the zeros are the solutions of

$$\cosh 2K \cosh 2K\Delta - \sinh 2K \cos \phi_1 - \sinh 2K\Delta \cos \phi_2 = 0. \quad (\text{A1})$$

We take $\Delta > 0$, so that the solutions of (A1) touch the real axis for $\phi_1 \rightarrow 0$, $\phi_2 \rightarrow 0$ and satisfy $\sinh 2K_c \sinh 2K_c\Delta = 1$, the criticality condition for the two dimensional square

Ising model (if $\Delta < 0$, this happens if $\phi_1 = 0$, $\phi_2 = \pi$). In expanding around this point, we use the fact that

$$d \sinh 2K \Delta / dS = \Delta / S_c, \quad (\text{A2})$$

$$d^2 \sinh 2K \Delta / dS^2 = \Delta^2 / S_c C_c^2 - \Delta / C_c^2, \quad (\text{A3})$$

$$\frac{d^3 \sinh 2K \Delta}{dS^3} = \frac{\Delta^3}{S_c C_c^2} - \frac{3\Delta^2}{C_c^4} - \Delta \left(\frac{1}{S_c C_c^2} - \frac{3S_c}{C_c^4} \right), \quad (\text{A4})$$

$$d \cosh 2K \Delta \cosh 2K / dS = \Delta / S_c + 1, \quad (\text{A5})$$

$$\frac{d^2 \cosh 2K \Delta \cosh 2K}{dS^2} = \frac{\Delta^2}{S_c} + \frac{\Delta}{C_c^2} + \frac{1}{S_c C_c^2}, \quad (\text{A6})$$

$$\frac{d^3 \cosh 2K \Delta \cosh 2K}{dS^3} = \frac{\Delta^3}{S_c C_c^2} + \frac{\Delta(2 - S_c^2)}{S_c C_c^4} - \frac{3}{C_c^4}, \quad (\text{A7})$$

where

$$S \equiv \sinh 2K, \quad S_c \equiv \sinh 2K_c, \quad C_c \equiv \cosh 2K_c. \quad (\text{A8})$$

Expanding (A1) with the aid of these results, we obtain for $\delta S \equiv S - S_c$ the equation

$$(1 + \Delta S_c)(\Delta - S_c)(\delta S)^3 + C_c^2(1 + \Delta S_c)^2(\delta S)^2 + C_c^4(\phi_1^2 S_c + \phi_2^2 \Delta)\delta S + C_c^4(\phi_1^2 S_c^2 + \phi_2^2) = 0. \quad (\text{A9})$$

Writing the solution in terms of the real and imaginary part, $\delta S = \delta S' + i\delta S''$, we get from (A9)

$$-\delta S' = A_{11}\phi_1^2 + A_{21}\phi_2^2, \quad (\delta S'')^2 = A_{21}\phi_1^2 + A_{22}\phi_2^2, \quad (\text{A10})$$

where

$$A_{11} = \frac{S_c}{2(1 + \Delta S_c)^3} (S_c^2(1 + \Delta S_c) + C_c^2), \quad A_{12} = \frac{S_c}{2(1 + \Delta S_c)^3} (\Delta^2 C_c^2 + \Delta S_c + 1), \\ A_{21} = C_c^2 S_c^2 / (1 + \Delta S_c)^2, \quad A_{22} = C_c^2 / (1 + \Delta S_c)^2. \quad (\text{A11})$$

Note that all matrix elements A_{ij} are positive, so that $\delta S'$ is always negative.

Since (6) is unchanged under the transformations $\phi_1 \rightarrow 2\pi - \phi_1$, $\phi_2 \rightarrow 2\pi - \phi_2$, we can restrict ϕ_1 and ϕ_2 to the interval $[0, \pi]$ rather than $[0, 2\pi]$ as is obtained from (6). If there are N zeros, the density of zeros in the ϕ_1, ϕ_2 plane is then N/π^2 . Defining the density of zeros $g(S)$ so that $Ng(S) dS' dS''$ approaches in the thermodynamic limit the number of zeros having $S' \leq \text{Re} S \leq S' + dS'$ and $S'' \leq \text{Im} S \leq S'' + dS''$, we get

$$g(S) = \pi^{-2} |\partial(S', S'') / \partial(\phi_1, \phi_2)|^{-1}. \quad (\text{A12})$$

In the neighbourhood of the real axis, this becomes with the aid of (A10)

$$g(S) = |\delta S''| / (2\pi^2 |\det A| \phi_1 \phi_2). \quad (\text{A13})$$

From (A10), it also follows that

$$\phi_1 = [(\det A)^{-1} (-A_{22}\delta S' - A_{12}(\delta S'')^2)]^{1/2}, \\ \phi_2 = [(\det A)^{-1} (A_{21}\delta S' + A_{11}(\delta S'')^2)]^{1/2}. \quad (\text{A14})$$

We define the positive coefficients c_1 and c_2 by

$$\begin{aligned} c_1 &\equiv A_{11}/A_{21} = (S_c^2(1 + \Delta S_c) + C_c^2)(2S_c C_c^2(1 + \Delta S_c))^{-1}, \\ c_2 &\equiv A_{12}/A_{22} = S_c(\Delta^2 C_c^2 + \Delta S_c + 1)(2C_c^2(1 + \Delta S_c))^{-1}. \end{aligned} \quad (\text{A15})$$

Because ϕ_1 and ϕ_2 are real, the solutions of (A14) only exist for

$$\begin{aligned} c_2(\delta S'')^2 \leq -\delta S' \leq c_1(\delta S'')^2 &\quad \text{if } c_1 > c_2 \text{ (i.e. } \det A > 0), \\ c_1(\delta S'')^2 \leq -\delta S' \leq c_2(\delta S'')^2 &\quad \text{if } c_2 > c_1 \text{ (i.e. } \det A < 0). \end{aligned} \quad (\text{A16})$$

From the explicit expressions (A15), one may show that

$$\begin{aligned} c_1 > c_2 &\quad \text{if } \Delta < 1, \\ c_2 > c_1 &\quad \text{if } \Delta > 1, \end{aligned} \quad (\text{A17})$$

and that for $|\Delta - 1| \ll 1$

$$c_1 - c_2 \approx -\frac{1}{2}[1 - (1/\sqrt{2}) \ln(1 + \sqrt{2})](\Delta - 1) \approx -0.188(\Delta - 1). \quad (\text{A18})$$

The latter result shows again that the width of the areas shrinks to zero linearly in the isotropy limit $\Delta \rightarrow 1$.

For $g(S)$ in (A13), we finally get in the region where (A16) is obeyed

$$g(S) = \frac{|\delta S''|(1 + \Delta S_c)^2}{2\pi^2 C_c^2 S_c \{[-\delta S' - c_2(\delta S'')^2][\delta S' + c_1(\delta S'')^2]\}^{1/2}}. \quad (\text{A19})$$

References

- Abe R 1967 *Prog. Theor. Phys.* **37** 1070
 Abe Y and Katsura S 1970 *Prog. Theor. Phys.* **43** 1402
 Brascamp H J and Kunz H 1974 *J. Math. Phys.* **15** 65
 Dunlop F and Newman C M 1975 *Commun. Math. Phys.* **44** 223
 Elvey J S N 1974 *Commun. Math. Phys.* **35** 101
 Fisher M E 1965 in *Boulder Lectures in Theoretical Physics* (University of Colorado, Boulder) vol 7
 Forgacs G and Fradkin E 1981 *Phys. Rev. B* **23** 3442
 Griffiths R B 1969 *J. Math. Phys.* **10** 1559
 Houtappel R M F 1950 *Physica* **16** 425
 Jones G L 1966 *J. Math. Phys.* **7** 2000
 Kaufman B 1949 *Phys. Rev.* **76** 1232
 Kurtze D A 1979 *Yang-Lee Edge Singularities in Ferromagnetic Systems*, MSC Report No 4184, Cornell University, unpublished
 Lee T D and Yang C N 1952 *Phys. Rev.* **87** 410
 Majumdar C K 1966 *Phys. Rev.* **145** 158
 Newman C M 1974 *Commun. Pure Appl. Math.* **27** 143
 ——— 1976 *J. Stat. Phys.* **15** 399
 Onsager L 1944 *Phys. Rev.* **65** 117
 Peschel I 1982 *Z. Phys. B* **45** 339
 Pfeuty P 1970 *Ann. Phys.* **57** 79
 Simon B and Griffiths R B 1973 *Commun. Math. Phys.* **33** 145
 Stephenson J 1964 *J. Math. Phys.* **5** 1009
 ——— 1969 *Can. J. Phys.* **47** 2621
 ——— 1970 *Phys. Rev. B* **11** 4405
 Suzuki M 1976 *Prog. Theor. Phys.* **56** 1454

Suzuki M and Fisher M E 1971 *J. Math. Phys.* **12** 235

Syozi I 1972 in *Phase Transitions and Critical Phenomena* ed C Domb and M S Green (London: Academic)
vol 1

Thompson C J 1979 *Mathematical Statistical Mechanics* (Princeton: PUP)

Wannier G M 1950 *Phys. Rev.* **79** 357

Yang C N and Lee T D 1952 *Phys. Rev.* **87** 404