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Yang–Lee edge singularity on a class of tree-like lattices

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Abstract. The density of zeros of the partition function of the Ising model on a class of tree-like lattices is studied. An exact closed-form expression for the pertinent critical exponents is derived by using a couple of recursion relations which have a singular behaviour near the Yang–Lee edge.

It is well known that Ising model on finitely ramified fractal lattices [1, 2] cannot display a phase transition at any finite temperature. This means that the free energy density $f(T, H)$ of such a model provides an analytic function of temperature T ($T > 0$) and of a real magnetic field H. Yang and Lee [3, 4] were the first who pointed out that the free energy, even of a finite Ising system, can exhibit a singular behaviour if one allows the field H to become complex $H = H' + \mathrm{i}H''$. They showed that all of the zeros of the partition function of a nearest-neighbour ferromagnetic Ising model lie on the unit circle in the complex activity plane $y = \exp(-2H/k_B T) \equiv \exp(-2h)$. In the thermodynamic limit these zeros are expected to condense, yielding to a limiting density of zeros $g(h'', T)$. For any fixed temperature there exists a pair $\pm\mathrm{i}H_0(T)$ of zeros lying closest to the real H-axis, commonly referred to as the Yang–Lee (YL) edge singularities. These limiting nonanalytic points exert the most direct influence on the behaviour of $f(T, H)$ for real T and H, and it is very important, therefore, to understand the nature of the associated singularity in the density of zeros near the YL edge.

The calculation of the limiting density of zeros is generally a highly nontrivial problem and little is known about its behaviour near the YL edge, let alone about its actual form on the whole region of interest. It is widely accepted, however, that the density of zeros near the edge exhibits a power-law behaviour: $g \sim |h'' - h_0(T)|^{\sigma}$, as $h'' \to h_0(T)$, where σ is the YL edge singularity critical exponent. Since in this case there exists only a single relevant variable [5–8], all other YL critical exponents can be expressed in terms of σ. In particular, the correlation length critical exponent ν_c, which describes the spatial decay of the two-spin correlation function near the edge, $\xi_{YL} \sim |h'' - h_0(T)|^{-\nu_c}$, can be related to σ ($\sigma = d\nu_c - 1$, with d being the dimensionality of underlying lattice). It has been suggested [6–8] that the value of this exponent depends only on the dimensionality of the lattice and is independent of temperature for all T above the critical temperature. When $d = 1$, the problem can be solved exactly which yields to $\sigma = -\frac{1}{2}$ for $T > 0$. Despite the fact that $g(h'', T)$ is not known exactly for the two-dimensional Ising ferromagnet, it has been predicted $\sigma = -\frac{1}{6}$ in $d = 2$ [9, 10]. It is believed that σ maintains its mean-field value of $\sigma = \frac{1}{2}$ above the upper critical dimension $d = 6$ [7]. Only approximative analytical and numerical results are available for the intermediate values of space dimensionalities [7, 8].

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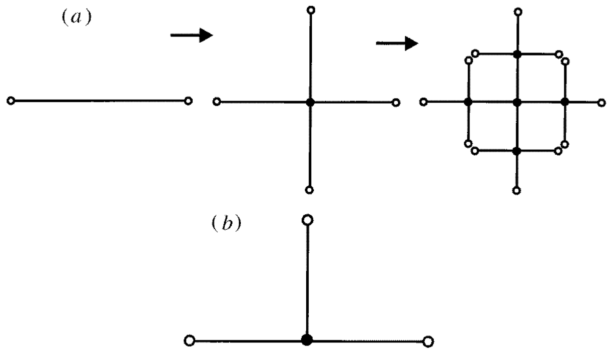

Figure 1. (a) First two stages in the iterative construction of a $p = 4$ tree-like fractal lattice. (b) A schematic representation of an rth stage $p = 3$ fractal lattice. In order to obtain a partition function $Z_i^{(r)}(S_1, S_2)$, $i = 1, 2, 3$, one has to fix the states of any two outer Ising spins S_1 and S_2 (open circles) and perform a summation over the states of all remaining spins (including the central spin (black circle))

The original YL circle theorem [3, 4] is independent of the topological structure of the lattice and should also apply to the appropriate models of certain nonhomogeneous systems (diluted ferromagnets, for example). In order to understand certain aspects of their critical behaviour better, a few studies [11, 12] of the density of zeros of the Ising ferromagnets on a variety of deterministic fractals have been performed so far. It is shown that in this case the density of zeros exhibits a scaling form near the YL edge which is more complicated than a pure power law. Using the exact recursion relations nontrivial values of the edge exponents σ were found. Most of these values were estimated only numerically, due to the absence of a pertinent fixed point [12] when one uses the standard decimation transformation approach. To overcome this difficulty, one can try to construct a more reliable renormalization-group scheme possessing the appropriate YL fixed point—the block-spin transformation, for example. Unfortunately, such an approach is usually much more elaborate, and, as far as we know, only a few exact calculations are presented so far [11]. In this paper we develop an approach which allows us to obtain the exact closed-form expressions for the edge exponents of Ising models on finitely ramified fractal lattices. It turns out that relevant recursion relations themselves have a singular behaviour near the YL edge fixed point, which is reminiscent of a singular structure of corresponding mappings appearing in some recently studied Gaussian models [13–15].

Consider the nearest-neighbour ferromagnetic Ising model with a uniform magnetic field on a family of tree-like lattices shown in figure 1. Each lattice of this family can be labelled by an integer p, which represents the maximum coordination number of the lattice. This parameter can take all values from 2 to ∞, with $p = 2$ corresponding to a simple one-dimensional chain. Let us note that each of these lattices have a finite fractal dimension, $D = \ln p/\ln 2$, which make them very different from a Cayley tree lattice. The partition function of the Ising model of an rth order lattice can be written as a combination of only three partial partition functions: $Z_1^{(r)} = Z^{(r)}(+, +)$, $Z_2^{(r)} = Z^{(r)}(-, -)$, and $Z_3^{(r)} = Z^{(r)}(+, -)$, where $Z^{(r)}(+, +)$, for example, denotes the partial partition function with two outer Ising spins (see figure 1(b)) being fixed in the 'up state'. It is convenient to express the resulting recursion relations in terms of two reduced variables $z_2 = Z(+, -)/Z(+, +)$ and $z_3 = Z(-, -)/Z(+, +)$. Thus, for a lattice of index p, we have found

$$z_2' = \frac{z_2^2(z_2+z_3)^{p-2} + y^{p-1}z_3^2(1+z_3)^{p-2}}{z_3^2(z_2+z_3)^{p-2} + y^{p-1}(1+z_3)^{p-2}}$$
$$z_3' = z_3\frac{z_2(z_2+z_3)^{p-2} + y^{p-1}(1+z_3)^{p-2}}{z_3^2(z_2+z_3)^{p-2} + y^{p-1}(1+z_3)^{p-2}} \qquad (1)$$

with $y = \exp(-2h)$. To obtain an rth order partition function $z_i^{(r)}$ $(i = 1, 2)$ one has to iterate the above recursion relations r times, starting with the following initial conditions: $z_2^{(0)} = y^2$ and $z_3^{(0)} = xy$, where $x = \exp(-2K)$ (here $K = J/k_B T > 0$ stands for standard ferromagnetic interaction strength). It is easy now to express various derivatives of the free energy density in terms of these variables and their derivatives with respect to a suitable variable. For example, the average magnetization $M^{(r)}$ per spin is given by

$$\mathcal{N}^{(r)}M^{(r)} = \frac{t_1+t_2+2t_3}{1+z_2+2z_3} \qquad (2)$$

where we have omitted the iteration index r on the right-hand side of (2), and $\mathcal{N}^{(r)}$ represents the number of sites of the underlying lattice ($\mathcal{N}^{(r)} = p^r+1$, for a lattice of index p). In the above formula t_1, t_2, and t_3 denote the scaled derivatives $t_i^{(r)} = (\partial Z_i^{(r)}/\partial h)/Z_1^{(r)}$, $i = 1, 2, 3$, and they can also be calculated by a recursive procedure. In a similar way, one can express the two-point correlation function $G^{(r)}$ in terms of $z_2^{(r)}$ and $z_3^{(r)}$

$$G^{(r)} = \langle S_1S_2\rangle - \langle S_1\rangle\langle S_2\rangle = \frac{4(z_2-z_3^2)}{(1+z_2+2z_3)^2}. \qquad (3)$$

The density of zeros $g(h'', T)$ is known [3] to be given by the limiting behaviour of the real part of M/π as $h' \to 0$, so that we may focus our attention here on the asymptotic behaviour of the above variables near the edge.

As it has been emphasized, for any $T > 0$ there exists a strip $|H''| < H_0(T)$ inside of which the density of zeros vanishes. The limiting value $H_0(T)$ can be determined numerically, by a study of the magnetization (2) and the correlation function (3). Such an analysis reveals that, for $H' = 0$ and $H'' \to H_0(T)$, z_2 and z_3 iterate toward the fixed point

$$z_2^* = (-y_0)^{\frac{2(p-1)}{p}} \qquad z_3^* = -(-y_0)^{\frac{p-1}{p}} \qquad (4)$$

where $y_0 = \exp(-2\mathrm{i}h_0)$ depends on x (for $x = \frac{1}{2}$, we have found $h_0 = 0.328\,648\,956\ldots$ and $h_0 = 0.152\,769\,589\ldots$ for $p = 3$ and $p = 5$, respectively). As it can be verified, however, recursion relations (1) become singular at this point, leading to a failing of the common fixed-point analysis. This puzzle is quite similar to the one encountered recently in the studies of critical properties of ideal polymer chains on fractal space [13–15]. In particular, both a numerical and an analytical examination of the above recursion relations reveals the existence of an invariant 'line' $z_3 = z_3(z_2)$, all points of which are attracted by (4). An asymptotic equation of this line, evaluated near the fixed point, can be expressed as an expansion over the small variable $\delta z = z_3^2 - z_2$ (note that at the fixed point one has $z_2 = z_3^2$). Thus, we obtain

$$z_3 = z_3^* + c_1\sqrt{z_3^2 - z_2} + c_2(z_3^2 - z_2) + \mathrm{O}[(z_3^2 - z_2)^{3/2}] \qquad (5)$$

where the coefficients c_1 and c_2 are given by

$$c_1 = \frac{1+\sqrt{1+4p}}{2p}$$
$$c_2 = \frac{p^2-2p-1+(3p^2-6p-1)z_3^* + [p^3-3p-1+(3p^3-2p^2-7p-1)z_3^*]c_1}{2p^2z_3^*(1+z_3^*)(2+c_1+2pc_1)}. \qquad (6)$$

Using the above formulae one can show that along the invariant line, near the fixed point, δz renormalizes according to the law: $\delta z' = 2\delta z/(1+2p+\sqrt{1+4p})$. This enables us to describe the way in which $z_3^{(r)}$ approaches its fixed point value:

$$z_3^{(r)} - z_3^* \sim \left(\frac{2}{1+\sqrt{1+4p}}\right)^r \qquad r \gg 1. \tag{7}$$

In a similar way we can extract the leading asymptotic behaviour of $\partial z_2^{(r)}/\partial h$ and $\partial z_3^{(r)}/\partial h$ at the edge. Indeed, it is easy to see that these derivatives satisfy a couple of linear recursion relations, an analysis of which reveals the following behaviour

$$\left.\frac{\partial z_2^{(r)}}{\partial h}\right|_{h=\mathrm{i}h_0} \sim \left.\frac{\partial z_3^{(r)}}{\partial h}\right|_{h=\mathrm{i}h_0} \sim 2^r. \tag{8}$$

In the above established asymptotic relations we have supposed $h = \mathrm{i}h_0$. In fact, they also hold for a finite but very small value of $\delta h = h'' - h_0$ $(0 < \delta h \ll 1)$, provided $r \lesssim r_0$, where $r_0 \gg 1$ is the number of iterations one can make along the invariant line before going away from it (starting with the initial conditions in which $y = y_0 \exp(-2\mathrm{i}\delta h)$). This number depends on the value of δh and can be estimated from the following obvious relation: $z_3^{(r_0)}(\delta h) \approx z_3^* + \frac{\partial z_3^{(r_0)}}{\partial h}|_{\delta h=0}\delta h$. Thus, taking into account (7) and (8), we find $\lambda^{r_0} \sim (\delta h)^{-1}$, where $\lambda = 1+\sqrt{1+4p}$. This enables us to express the YL correlation length as a function of δh: $\xi_{YL} \sim 2^{r_0} \sim \exp(-\ln 2 \ln(\delta h)/\ln\lambda)$, i.e.

$$\xi_{YL} \sim \delta h^{-\nu_c} \quad \text{with} \quad \nu_c = \frac{\ln 2}{\ln\lambda} = \frac{\ln 2}{\ln(1+\sqrt{1+4p})} \tag{9}$$

independent of the temperature. We have also calculated the critical exponent ν_c for several values of p, by using a numerical study of the correlation function (3), and we have found an excellent agreement with (9). Let us note further that for $p = 2$ the value of ν_c ($\nu_c = \frac{1}{2}$) coincides with the known value for the Ising ferromagnetic chain, while for $p = 3$ our exact value of ν_c is very close to the one that was obtained earlier by using a somewhat different numerical approach [12]. What is perhaps more interesting is that our values of ν_c for $p = 2, 3$ are the same as those found for the correlation length critical exponent ν_G of a simple zero-field Gaussian model on the same lattices [13–15]. It is tempting, therefore, to see whether this coincidence persists for all values of p. The calculation of [16], which follows along the lines of [13], shows that this is, really, the case ($\nu_c = \nu_G$).

In a similar way we have found: $t_1^{(r)}|_{h=\mathrm{i}h_0} \sim t_2^{(r)}|_{h=\mathrm{i}h_0} \sim t_3^{(r)}|_{h=\mathrm{i}h_0} \sim \lambda^r$. Taking into account these results and (2), we can write $M^{(r_0)} \sim t_1^{(r_0)}/\mathcal{N}^{(r_0)} \sim (\lambda/p)^{r_0}$, which yields to

$$M \sim g \sim \delta h^{\sigma} \qquad \sigma = \frac{\ln p}{\ln(1+\sqrt{1+4p})} - 1. \tag{10}$$

It is interesting to note that this expression can be rewritten in the form of an expected scaling relation: $\sigma = D\nu_c - 1$. As it can be seen from the above formula, $\sigma = \sigma(p)$ is an increasing function of p and its limiting value, $\sigma(p \to \infty) = 1$, exceeds the above mentioned mean-field value of $\sigma = \frac{1}{2}$ for the homogeneous lattices. Note that $\sigma(p)$ changes its sign at $p = 6$, which means that the singular part of the density of zeros diverges near the edge if $p < 6$, whereas it vanishes for all $p > 6$. As can be noticed in figure 2, where we plotted the density of zeros as a function of h'' for several values of the lattice parameter p, the zeros are not homogeneously distributed on the unit circle but instead have a striking Cantor-set structure with many gaps, especially for the low values of p (except, of course, for $p = 2$). As p increases, this fractal pattern become less and less pronounced, and it

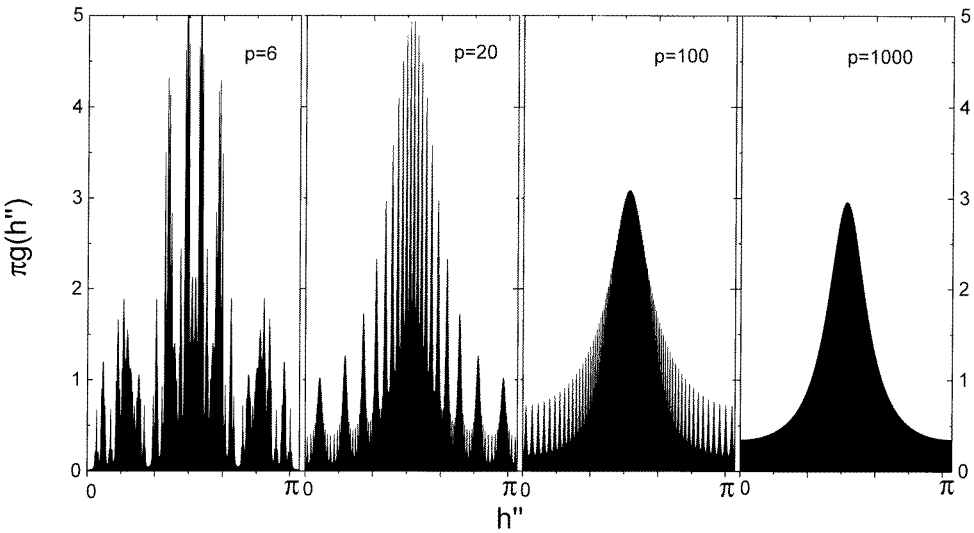

Figure 2. Density of zeros $g(h'', T)$ as a function of the imaginary field h'' for several values of p. In all cases temperature corresponds to $x = \frac{1}{2}$ and the real part of the field is $h' = 0.005$.

seems that, for any small but finite h', it acquires a rather regular limiting form (see figure 2 for $p \gg 1$). For a fixed and finite temperature, the value of the YL edge decreases with p and one can show that $h_0 \sim 1/p$ when $p \gg 1$, corresponding to the absence of any gap in the density of zeros, in the limit when the lattice coordination number tends to infinity. On the other hand, for a finite p the density of zeros exhibits a scaling form near the edge, similar to the one that has been discussed in details in [11, 12].

In conclusion, we have presented exact results for the density of zeros in the complex activity plane for a family of tree-like lattices. We have found that our recursion relations have a singular behaviour near the edge. The technique we have used here to extract the leading singularity can be, in principle, extended to all other finitely ramified fractal lattices and to other classical spin models.

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