

## Fully frustrated Ising antiferromagnets at the fractal to Euclidean crossover

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Received 25 July 1991

We present a study of the residual entropies of the frustrated Ising antiferromagnets in a zero field, situated on the Sierpiński gasket type of fractals. Our results render it possible to establish the fractal residual entropy crossover towards Wannier's exact value for the Euclidean triangular lattice.

The exact residual entropy of the frustrated Ising antiferromagnet on the regular triangular lattice in zero field was calculated by Wannier in 1950 [1], whereas the residual entropy of the same model in the maximum critical field was found by Baxter in 1980 [2, 3]. The question as to how the residual entropy is modified when the underlying lattice is fractal has been recently addressed in both cases, that is, in the case of maximum critical field [4–6], where the corresponding fractal to Euclidean crossover formula was established, and in the case of zero field [7, 8], where so far no crossover formula has been found.

In this paper we study the zero field residual entropy  $\sigma$  of the Ising antiferromagnets situated on fractals that are members of the infinite Sierpiński gasket (SG) family [9]. Each member of the family is labelled by an integer  $b$  ( $2 \leq b < \infty$ ), and can be constructed in a self-similar way starting with a triangular generator of side length  $b$  (see fig. 1). Exact numerical values of the zero field residual entropy  $\sigma(b)$  have been calculated [7] for the first five members ( $2 \leq b \leq 6$ ) of the fractal family, but these results did not prove sufficient to explore possible convergence (crossover) of  $\sigma(b)$ , when  $b \rightarrow \infty$ , towards the value  $\sigma_{\text{Euclidean}} = 0.323066$  found for the infinite triangular lattice [1]. Here we first use the transfer matrix (TM) method [4] to calculate  $\sigma(b)$  for

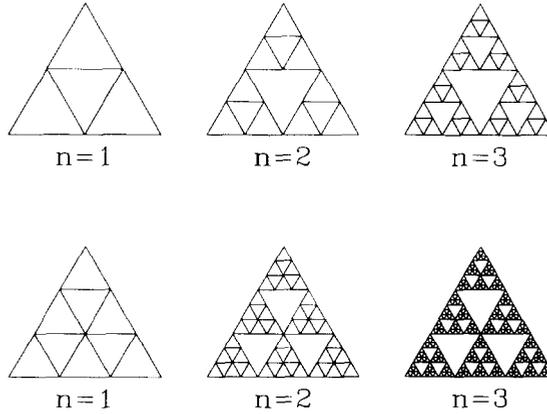


Fig. 1. The first three steps of construction ( $n = 1, 2, 3$ ) of the first two members ( $b = 2$  (upper) and  $b = 3$  (lower)) of the Sierpiński gasket fractal family.

$2 \leq b \leq 19$ , and then apply the recently introduced degeneracy factor method [10] to establish the crossover behavior of  $\sigma(b)$ . Finally, we make a comparison of the zero field entropy crossover behavior with the crossover behavior of the residual entropy in the maximum critical field [4, 5].

In zero external magnetic field, the Ising antiferromagnet on a SG fractal (with given  $b$ ) has a highly degenerate ground state energy level. A measure of this topological frustration is the residual entropy

$$\sigma(b) = \lim_{n \rightarrow \infty} \frac{\ln \Omega_{n,b}}{N_{n,b}}, \quad (1)$$

where  $\Omega_{n,b}$  is the ground state degeneracy of the system at the  $n$ th stage of construction of the fractal lattice, and  $N_{n,b}$  is the total number of spins [4], given by

$$N_{n,b} = C_b^{n-1} N_{G,b} - \frac{(b^2 - 1)(c_b^{n-1} - 1)}{c_b - 1}, \quad (2)$$

with

$$c_b = \frac{1}{2}b(b + 1) \quad (3)$$

being the number of  $n$ th stage structures that comprise the  $(n + 1)$ th stage structure, and with

$$N_{G,b} = \frac{1}{2}(b + 1)(b + 2) \quad (4)$$

being the number of spins in the fractal generator. To find the ground state degeneracy  $\Omega_{n,b}$  at different stages of construction of the lattice, we can use the fact that we are dealing with an exactly self-similar lattice and try to establish exact recursion relations between degeneracies of two successive stages. The details of this procedure are quite similar to the procedure implemented [4] for  $b = 2$  in the case of a nonzero field. However, to implement this procedure on SG fractals with larger  $b$  one would need to inspect  $2^{N_{G,b}}$  possible configurations of the  $N_{G,b} = \frac{1}{2}(b+1)(b+2)$  generator spins, which already for  $b = 7$  becomes a formidable task.

We have found that it is possible to replace the necessary recursion relations with a simple approximate recursion formula which yields surprisingly accurate results. Indeed, one can assume that for a fractal structure, with given  $b$  and  $n$ , the eight different configurations of the three apex spins give identical contributions to the total ground state degeneracy. This assumption is certainly valid for any  $b$  if  $n$  is large enough, since an arbitrary configuration of merely three apex spins cannot significantly affect the ground state degeneracy of a large system. The question is whether the error introduced in this way for small both  $b$  and  $n$  can influence the result at later stages of recursion. It can be verified that the error is negligible even for  $b = 2$  (roughly, one part in  $10^5$ ). Thus, following the procedure expounded in ref. [4], the approximate recursion relations now acquire the form

$$\Omega_{n+1,b} \cong 2^{N_{G,b}} \left(\frac{1}{8} \Omega_{n,b}\right)^{C_b}. \tag{5}$$

Therefore, starting with the generator ( $n = 1$ ) ground state degeneracy  $\Omega_{G,b}$  and applying (5) iteratively  $n - 1$  times, we obtain

$$\Omega_{n,b} \cong \frac{[2^{(1-b^2)/(C_b-1)} \Omega_{G,b}]^{C_b^{n-1}}}{2^{(1-b^2)/(C_b-1)}}, \tag{6}$$

and inserting (6), together with (2)–(4), into (1), we find the following expression for the residual entropy:

$$\sigma(b) \cong \frac{4(1-b^2) \ln 2 + 2[b(b+1) - 2] \ln \Omega_{G,b}}{b(b^2-1)(b+4)}. \tag{7}$$

Hence we can see that the problem of calculating the residual entropy of an infinite fractal lattice is reduced to evaluation of the generator ground state degeneracy  $\Omega_{G,b}$ .

To find  $\Omega_{G,b}$  for fractals with a large generator base  $b$ , we use the transfer matrix approach elaborated in detail, for the nonzero field case, in ref. [4]. In

Table I

Generator ground state degeneracy  $\Omega_{G,b}$ , residual entropy  $\sigma(b)$  and the generator residual entropy  $\sigma'(b)$  for the Ising antiferromagnet situated on the Sierpiński gasket type of fractal lattices. The  $\sigma(b)$  values are calculated using (7), whereas the values of  $\sigma'(b)$  are found using (8).

$b$	$\Omega_{G,b}$	$\sigma(b)$	$\sigma'(b)$
2	26	0.492972	0.543016
3	160	0.472159	0.507517
4	1386	0.455920	0.482278
5	16814	0.442904	0.463332
6	284724	0.432239	0.448546
7	6715224	0.423340	0.436664
8	220240306	0.415800	0.426894
9	10032960146	0.409329	0.418712
10	634271091558	0.403714	0.411754
11	55607968072800	0.398794	0.405761
12	6757401238296446	0.394447	0.400543
13	1.137661035904122 $D + 18$	0.390578	0.395957
14	2.652656582154581 $D + 20$	0.387112	0.391894
15	8.563578021738200 $D + 22$	0.383989	0.388268
16	3.826727812041878 $D + 25$	0.381159	0.385011
17	2.366500329644923 $D + 28$	0.378584	0.382069
18	2.024949555917702 $D + 31$	0.376229	0.379398
19	2.397084420091121 $D + 34$	0.374068	0.376963

this way we have been able to obtain results up to  $b = 19$  (using the IBM personal computer with Intel 80386 processor and WEITEK coprocessor). The results are listed in table I. An inspection of the second column of table I can make one surprised that formula (7), obtained using an assumption which is rather crude for small  $b$  and  $n$ , gives results of such a high accuracy even for small values of  $b$ . Indeed, even for  $b = 2$  the value of  $\sigma(2)$  listed in table I differs from the exact result by one part in  $10^5$ . Besides, one should note that the first five values of  $\sigma(b)$  ( $2 \leq b \leq 6$ ) coincide with those recently reported in ref. [7]. Finally, we mention that the residual entropies of the fractal generators, listed in column three of table I, were calculated according to

$$\sigma'(b) = \ln \Omega_{G,b} / N_{G,b} . \quad (8)$$

Next we turn to the question as to how the residual entropies  $\sigma(b)$  converge to the value  $\sigma_{\text{Euclidean}} = 0.323066$  pertinent to the infinite triangular lattice [1]. To this end, we use the degeneracy factor method (DFM) introduced in ref. [10]. The essence of the DFM is the scaling relation

$$\Omega_{G,b} \approx \mathcal{L} c^{3(b-1)} \omega^{(b-1)(b-2)/2} , \quad b > k . \quad (9)$$

Here  $\mathcal{S}$  is a constant (characteristic of the infinite triangular lattice),  $c$  is the degeneracy factor that appears on adding a new border spin (i.e. a spin with four nearest neighbors) to a fractal generator, and  $\omega$  is the degeneracy factor that appears on adding a new bulk spin (a spin with six nearest neighbors). For a preset accuracy, the relation (9) is assumed to be valid beyond a certain value  $b = k$ . From (9) it follows that

$$Y(b) \equiv \frac{1}{b-2} \ln \left( \frac{\Omega_{G,b}}{\Omega_{G,b-1}} \right) \approx \ln \omega + \frac{3 \ln c}{b-2}, \quad b > k, \quad (10a)$$

and

$$z(b) \equiv \ln \left( \frac{\Omega_{G,b} \Omega_{G,b-2}}{\Omega_{G,b-1}^2} \right) \approx \ln \omega, \quad b > k. \quad (10b)$$

To test whether our set of data (cf. table I) allows application of the DFM, in fig. 2 we plot quantities  $y(b)$  and  $z(b)$ . We can see that our exact data for  $y(b)$ , in accordance with (10a), nicely follow a straight line, whereas we notice a systematic deviation of the points  $z(b)$  from the constant  $\ln \omega$ , which suggests that higher order correction terms should be taken into account in (10b). Therefore, we have fitted the quantities  $z(b)$  to a polynomial in  $1/(b+1)$  (here  $b+1$  is the linear dimension of the fractal generator), with the result

$$z(b) = 0.3228 + \frac{0.01035}{b+1} + \frac{0.5170}{(b+1)^2} + \frac{0.4553}{(b+1)^3}. \quad (11)$$

The generator ground state degeneracies  $\Omega_{G,b}$  for arbitrary  $b > 19$  can now be found, with a higher accuracy, by iterative application of (10) and (11), and then they can be used in (7) and (8) to find the residual entropies of fractals and their generators, respectively. The values calculated in this way for  $b \leq 1000$  are shown in fig. 3, together with Wannier's exact value for  $b = \omega$ . This figure suggests that one should expect a smooth fractal to Euclidean crossover in the case of the zero field residual entropies.

The explicit form of the fractal to Euclidean crossover,

$$\sigma(b) = \ln \omega + \frac{6 \ln c}{b}, \quad (12)$$

follows after inserting (9) into (7) and neglecting higher order terms in  $1/b$ . The same type of crossover can be found, for the generator residual entropies, by inserting (9) into (8). This should not be surprising if one takes into account that we are dealing with finitely ramified fractals, which means that each

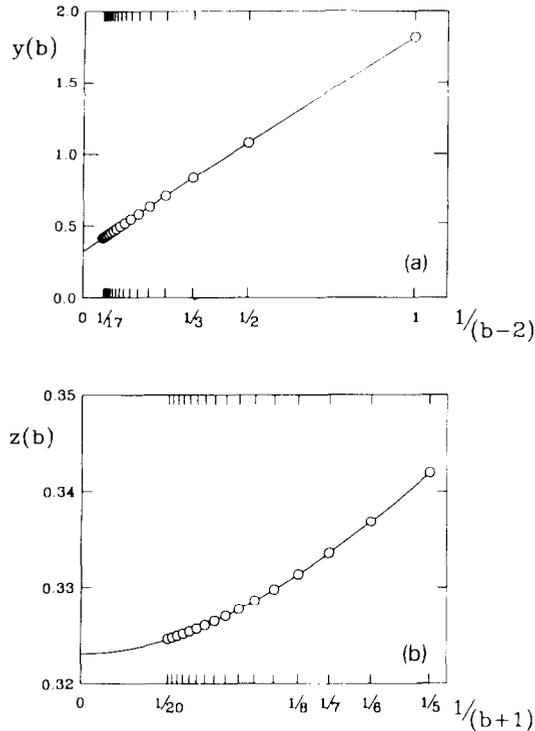


Fig. 2. (a) Quantity  $y(b)$  defined by eq. (10a) versus  $1/(b-2)$ . The solid straight line represents the best fit of the exact data (obtained for  $b \approx 19$ ) using the variable  $1/(b-2)$ . (b) Quantity  $z(b)$  defined by (10b) versus  $1/(b+1)$ . The solid curve represents the best fit of the exact data to a third order polynomial in  $1/(b+1)$ .

generator of a fractal can be separated from the rest of the fractal lattice by cutting only six bonds.

It remains to compare the crossover behavior of the zero field residual entropy studied in this work with the crossover behavior of the residual entropy in the maximum critical field  $H_c$  (cf. refs. [4, 5]). First, we should point out that the crossover formula of the type (12), that is with the correction term proportional to  $1/b$ , appears to be quite general. Indeed, the same type of crossover has been established [4–6] for the maximum critical field residual entropies of the Ising antiferromagnets situated on different families of fractal lattices. Next, in fig. 4 we compare the overall behavior of the residual entropies (in a zero field and in the maximum critical field) in the case of the Sierpiński gasket family of fractals. One can note that the  $H=0$  and the  $H \neq 0$  residual entropy curves cross each other at  $b \cong 270$ , that is, before entering the fractal to Euclidean crossover region that occurs at  $b \rightarrow \infty$ . This interesting

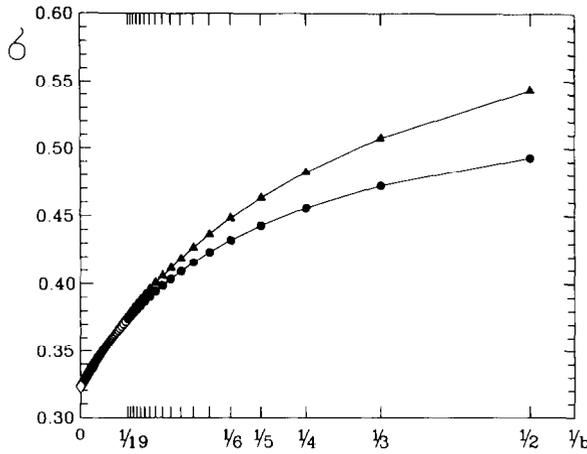


Fig. 3. Residual entropies  $\sigma(b)$  and  $\sigma'(b)$  of the SG fractals and their generators represented by circles and triangles, respectively. Exact results for  $2 \leq b \leq 19$  are depicted by full circles and triangles, while the extrapolated values for  $19 < b \leq 1000$  are depicted by open circles and triangles. The symbol  $\diamond$  represents the known exact value [1] of the zero field residual entropy for the infinite triangular lattice  $\sigma_{\text{Euclidean}} = 0.323066$ . The full lines serve as guide to the eye.

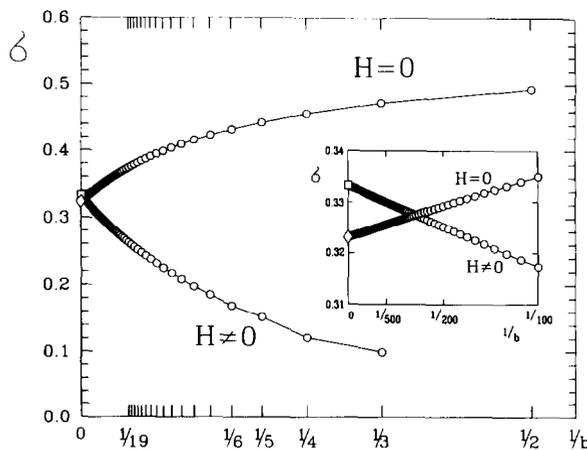


Fig. 4. Comparison of the crossover behavior of the zero field residual entropy  $\sigma(b, H = 0)$  of the SG fractals (same data as in fig. 3), and the residual entropy  $\sigma(b, H = H_c)$  of the SG fractals in the maximum critical field  $H_c$  (same data as in fig. 1 of ref. [5]). The symbol  $\diamond$  represents the known exact value [1] of the zero field residual entropy for the infinite triangular lattice  $\sigma_{\text{Euclidean}}(H = 0) = 0.323066$ , whereas the symbol  $\square$  represents the known exact value [2, 3] of the residual entropy in the maximum critical field for the infinite triangular lattice  $\sigma_{\text{Euclidean}}(H = H_c) = 0.333243$ . The full lines serve as guides to the eye. The inset depicts a magnification of the region (close to  $b \cong 270$ ) where the two sets of data cross each other.

result implies that beyond  $b \cong 270$  the frustration associated with the bulk spins starts to dominate over the border spin frustration. In other words, the finite-size effects of the fractal generators dominate up to  $b \cong 270$ .

### **Acknowledgements**

This work has been supported in part by the Yugoslav–USA Joint Scientific Board under the project JF900 (NSF), by the Yugoslav Federal Science Funds under the project P-26, and by the Serbian Science Foundation under the project 1.27.

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