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RESIDUAL ENTROPIES OF THE ISING ANTIFERROMAGNETS ON FRACTALS

I. *d*-DIMENSIONAL SIERPINSKI GASKET TYPE OF FRACTALS

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We apply a new method to study the problem of the residual entropies of the antiferromagnetic Ising systems, in the maximum critical field, situated on Sierpinski gasket (SG) type of fractal lattices. The SG fractal lattices comprise a family, so that each member is labelled by an integer b $(2 \leq b < \infty)$ and is embedded in d-dimensional Euclidean space. In the two-dimensional (2D) and three-dimensional (3D) case, we find expressions for the residual entropy $\sigma(b)$ for arbitrary b, and show that in the limit $b \to \infty$ the calculated values should converge to the values pertinent to the corresponding Euclidean lattices. In particular, these results confirm recent findings concerning the residual entropy of the 2D Sierpinski gasket type of fractals, obtained by numerical fitting. We also study the d-dimensional case and find a general expression for $\sigma(b)$ for arbitrary $b \geq 3$.

1. Introduction

Numerous theoretical investigations performed in the past decade have confirmed that the laws of physics are modified when the underlying lattice is fractal instead of Euclidean. Thus one can judiciously ask how physical laws on fractal lattices cross over to known laws on the standard Euclidean lattices. A few answers to this question have been offered by studying electric resistances [1–3], self-avoiding random walks [4–6] and residual entropies of the Ising antiferromagnets [7] on the infinite family of Sierpinski gasket (SG) type of fractals. However, in order to achieve a general answer to the posed question, additional concrete studies are essential. For this reason, here we attack more comprehensively the problem of residual entropies of the Ising antiferromagnets on fractals.

In a previous paper [7] we have studied the specific problem of the residual entropies of the Ising antiferromagnets with the nearest-neighbor (nn) coupling J, in the maximum critical field. The Ising systems were situated on the family of the SG type of fractals embedded in the two-dimensional (2D) Euclidean space. Each member of the family is labelled by an integer b ($2 \leqslant b < \infty$), which appears to be the base of the corresponding fractal generator (see, for example, fig. 1 of ref. [7]). The general formula for the residual entropy $\sigma(b)$ for $b \geqslant 3$ has been expressed [7] in terms of only two parameters – the fractal generator base b and its ground state degeneracy Ω_G. We have calculated exactly [7] the values of $\sigma(b)$ for $3 \leqslant b \leqslant 21$, and by a *numerical* analysis we have established that $\sigma(b)$, in the limit $b \to \infty$, approaches the exact value $\sigma_{\text{Euclidean}} = 0.3332427219761\ldots$ (found for the standard triangular lattice [8, 9]) according to the crossover formula

$$\sigma(b) = \sigma_{\text{Euclidean}} - \frac{P}{b^{\alpha}}, \qquad b \to \infty, \tag{1}$$

where P and α are constants.

In section 2 of this paper we first report three additional values of $\sigma(b)$ ($b = 22, 23, 24$), for the 2D case. What is more important, we apply here the degeneracy factor method, introduced recently in ref. [10], to analyze the crossover behavior of $\sigma(b)$. Thus we confirm that formula (1) holds, with α being equal to one. In section 3 we find general expressions for the residual entropies $\sigma(b)$ for the SG fractal lattices embedded in the 3D Euclidean space, and calculate exact values of $\sigma(b)$ up to $b \leqslant 9$. Applying the degeneracy factor method we find a crossover formula for $\sigma(b)$ in the 3D case, which turns out to be also of the type (1). In section 4 we find general expressions for $\sigma(b)$ in the d-dimensional case, and then we provide an overall discussion of the obtained results.

2. Residual entropies of the 2D Sierpinski gasket type of fractals

The maximum critical field H_c and the concomitant residual entropies of the antiferromagnetic Ising systems depend on the maximum coordination number within a given lattice [11]. In the 2D case, the Sierpinski gasket ($b = 2$) and the other members of the SG family ($b \geq 3$) have maximum coordination numbers 4 and 6, respectively [12], and thereby the corresponding residual entropies have to be studied separately [7]. The case $b = 2$ was completed in ref. [7] and here we continue to study behavior of $\sigma(b)$ for large b.

The general expression for $\sigma(b)$ for $b \geq 3$ was found [7] to be of the form

$$\sigma(b) = \frac{2\{(b-1)(b-2)\ln 2 + [b(b+1)-2]\ln \Omega_G\}}{b(b+1)[(b+1)(b+2)-6]}, \qquad b \geq 3, \tag{2}$$

where b is the fractal generator base and Ω_G is the generator ground state degeneracy. Hence, one can see that in order to learn specific values of $\sigma(b)$ one should first determine Ω_G. In ref. [7] we have determined Ω_G for $3 \leq b \leq 21$. In order to find out the large b behavior of $\sigma(b)$, we have fitted [7] the obtained values of $\sigma(b)$ for $3 \leq b \leq 21$ to the formula

$$\sigma(b) = \sum_{i=0}^{m} a_i \left(\frac{1}{x}\right)^i, \tag{3}$$

where we have assumed the three possibilities $x = b$, $x = \ln b$ and $x = b^\alpha$, with α being a constant. It turned out that the best fit can be achieved for $x = b^\alpha$, and consequently for very large b the behavior of type (1) was suggested.

In this paper we first report three additional values for Ω_G (for $b = 22$, 23 and 24), obtained by using more powerful computer facilities than before (IBM 3090 instead of VAX 750). The values are

$$\begin{aligned} \Omega_G(22)_{\text{exact}} &= 7.857823608931616668 \times 10^{31}, \\ \Omega_G(23)_{\text{exact}} &= 1.017146461819327794 \times 10^{35}, \\ \Omega_G(24)_{\text{exact}} &= 1.837342709080040093 \times 10^{38}. \end{aligned} \tag{4}$$

Next, instead of the purely numerical fitting procedure mentioned above, we apply the degeneracy factor method (DFM), introduced in ref. [10], to determine the limiting behavior of $\sigma(b)$ for large b. The essence of the DFM is the scaling relation

$$\Omega_G(b) \approx c\omega^{b-2}\Omega_G(b-1), \qquad b > k, \tag{5}$$

which links the two successive Ω_G. Here c is a constant (characteristic for the entire SG family), and ω is the degeneracy constant (factor) that appears on adding a new spin to a fractal generator. Relation (5) is assumed to be valid, for a preset accuracy, beyond a certain value $b = k$.

If the values of $\Omega_G(b)$ are calculated up to some value b^*, then in order to learn (approximately) further values of $\Omega_G(b)$ one can assume that relation (5) holds starting with $b = b^* - 1$. This is equivalent to setting $k = b^* - 2$, that is, to presetting the accuracy of all subsequent formulas that involve $\Omega_G(b)$ with b larger than b^*. The constants c and ω can now be calculated from (5), according to

$$\omega \approx \frac{\Omega_G(b^*)\,\Omega_G(b^*-2)}{\Omega_G^2(b^*-1)} \tag{6a}$$

and

$$c \approx \frac{\Omega_G(b^*)}{\Omega_G(b^*-1)}\,\omega^{2-b^*}\,. \tag{6b}$$

Inserting (6) into (5), for $b = b^* + 1$, we find the expression for the unknown value $\Omega_G(b^* + 1)$,

$$\Omega_G(b^*+1) \approx \frac{\Omega_G^3(b^*)\,\Omega_G(b^*-2)}{\Omega_G^3(b^*-1)}\,, \tag{7}$$

in terms of the known values.

In order to verify this approach we use our data for $\Omega_G(b)$, and thus taking $b^* = 21$, $b^* = 22$ and $b^* = 23$ in (7) we obtain, respectively,

$$\begin{aligned} \Omega_G(22) &\approx 7.85782941 \times 10^{31}\,, \\ \Omega_G(23) &\approx 1.01714616 \times 10^{35}\,, \\ \Omega_G(24) &\approx 1.83734293 \times 10^{38}\,. \end{aligned} \tag{8}$$

By comparing these results with the exact results given in (4), one can see a rather good accuracy of the approximate approach. One can also see that the accuracy increases with increasing b^*, and in particular for $b^* = 23$ there are seven correct digits in the approximate value of $\Omega_G(24)$.

In what follows we adopt the above presented approach for obtaining $\Omega_G(b)$, for large b, and thereby we investigate the limiting behavior of $\sigma(b)$ when $b \to \infty$. First, by successive application of (5) we find

$$\Omega_G(b) \approx c^{b-k}\omega^{(b^2-3b-k^2+3k)/2}\Omega_G(k)\,, \tag{9}$$

and by inserting (9) into (2) we obtain

$$\sigma(b) \approx \ln \omega + \frac{1}{b}\,\frac{S_3 b^3 + S_2 b^2 + S_1 b + S_0}{b^3 + 4b^2 - b - 4}\,, \tag{10}$$

with

$$S_0 = 2k(k-3)\ln \omega - 4\ln \Omega_G(k) + 4k\ln c + 4\ln 2\,, \tag{11a}$$

$$S_1 = -(k^2 - 3k - 10)\ln \omega + 2\ln \Omega_G(k) - 2(k+2)\ln c - 6\ln 2\,, \tag{11b}$$

$$S_2 = -(k^2 - 3k + 4)\ln \omega + 2\ln \Omega_G(k) - 2(k-1)\ln c + 2\ln 2\,, \tag{11c}$$

$$S_3 = -6\ln \omega + 2\ln c\,. \tag{11d}$$

Now, choosing $b^* = 24$, from (6) we find

$$\ln \omega \approx 0.333242687\,, \tag{12a}$$

$$\ln c \approx 0.167735381\,, \tag{12b}$$

and using these values in (11), together with the choice $k = 24$, we achieve

$$\begin{aligned} S_0 &= 2.357598\,,\\ S_1 &= -1.289902\,,\\ S_2 &= 0.5962896\,,\\ S_3 &= -1.663985\,. \end{aligned} \tag{13}$$

Having confirmed that the constants which appear in (10) are finite, it becomes clear why the choice $x = b$ and $x = b^{\alpha}$ in (3) provided much better fitting [7] than the choice $x = \ln b$ (see fig. 6 in ref. [7]). For the same reason, it also follows from (10) that the leading term, for very large b, is of the order $1/b$. Thus, we can now claim that the asymptotic law (1) is true with $\alpha = 1$. Besides, comparing our limiting value of $\sigma(b)$ for $b \to \infty$, given by (12a), with the exactly known value [8, 9] of the residual entropy for the infinite triangular lattice $\sigma_{\mathrm{Euclidean}} = 0.3332427219761\ldots$, it becomes clear that the seven-digit accuracy initiated at $b = 24$ has been preserved. In fig. 1 we depict values of $\sigma(b)$ for $b \leqslant 1000$, calculated using (2) and (10), together with the residual entropies $\sigma'(b)$ of the corresponding fractal generators. Furthermore, one

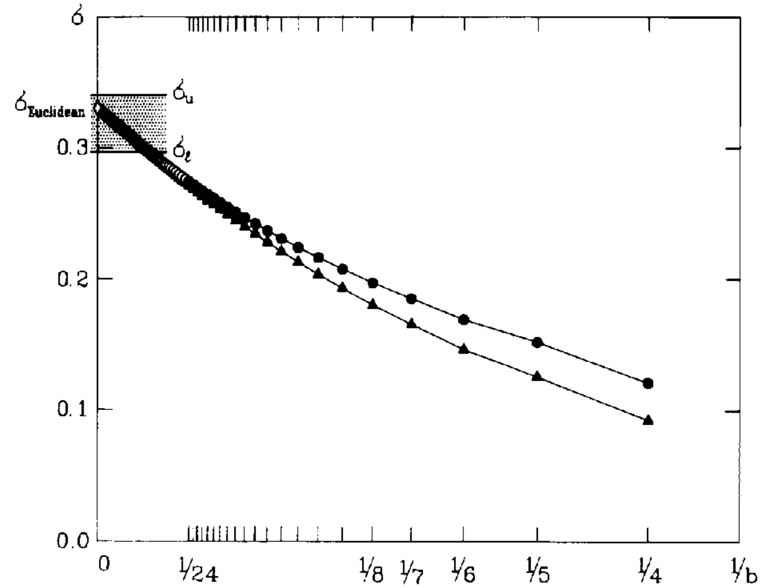

Fig. 1. Residual entropies $\sigma(b)$ and $\sigma'(b)$ of the 2D SG fractals and their generators, represented by circles and triangles, respectively. Exact values for $3 \leqslant b \leqslant 24$ are depicted by full circles and triangles, while the extrapolated values for $24 < b \leqslant 1000$ are depicted by open circles and triangles. Approximate values are obtained using eqs. (10)–(13), in the case of $\sigma(b)$, whereas extrapolated $\sigma'(b)$ are given by $\sigma'(b) = 2 \ln \Omega_G(b)/[(b+1)(b+2)]$ (here $\Omega_G(b)$ is determined by (9), and $(b+1)(b+2)/2$ is the total number of spins in the generator). The symbol ◇ represents the exactly known value [8, 9] of the residual entropy for the infinite triangular lattice $\sigma_{\text{Euclidean}} = 0.3332427219761\ldots$, and the shaded region corresponds to the upper and lower bound, $\sigma_u = 0.2970$ and $\sigma_\ell = 0.3403$, predicted for the Euclidean lattices with coordination number $z = 6$ in ref. [11]. The full lines serve as guides to the eye.

should notice that both residual entropies $\sigma(b)$ and $\sigma'(b)$, already for $b \geqslant 41$, enter the region of values determined by the corresponding upper and lower bound (σ_u and σ_ℓ) predicted for the Euclidean lattices with the coordination number $z = 6$ in ref. [11]. This means that already fractals with $b \geqslant 41$ (and their generators) have a sufficiently large ratio of number of spins with six nearest neighbors versus total number of spins [7].

3. Residual entropies of the 3D Sierpinski gasket type of fractals

Each member of the 3D SG fractal family is also labelled by an integer b ($2 \leqslant b \leqslant \infty$) and can be obtained from a generator G(b), which is an equilateral tetrahedron of side length b [12]. The generator G(b) is filled with b layers of smaller tetrahedra of unit side length (see fig. 2). Each layer consists of upward oriented unit tetrahedra (see fig. 3). A member of the 3D SG fractal family is

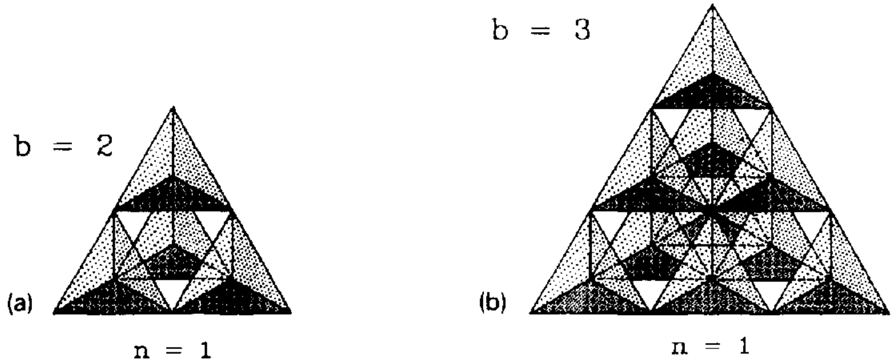

Fig. 2. The generators ($n=1$) of the 3D SG type of fractals. (a) The $b=2$ case. (b) The $b=3$ case. The darkest unit triangles should be conceived as horizontal bases of the four and ten upward oriented tetrahedra, respectively.

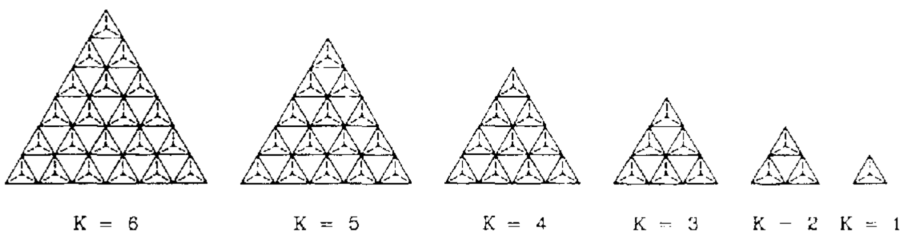

Fig. 3. Six successive layers of the $b=6$ 3D SG fractal generator. The largest triangle corresponds to the ground layer, which is composed of 21 upward oriented unit tetrahedra. In all layers, the edges of the unit tetrahedra that lie above the horizontal plane are represented by dashed lines.

also grown in stages. The structure of the $(n+1)$th stage is obtained by enlarging the generator (the $n=1$ stage) by b^n, and filling its all upward oriented tetrahedra with the nth stage structure. The complete fractal (lattice) is obtained in the limit $n \to \infty$.

In fig. 3 one can, in fact, see all layers from which the SG fractal generators with $2 \leq b \leq 6$ are formed. Hence, one can notice that the maximum coordination number z is equal to 6, 9 and 12, for $b=2$, $b=3$ and $b \geq 4$, respectively. Therefore, the maximum critical fields [7, 11] are $H_c = 6J$, $H_c = 9J$, and $H_c = 12J$ in the three cases, respectively. The three different critical fields necessitate separate studies, and we will start with the $b \geq 4$ case, as it is relevant for the study of fractal to Euclidean crossover.

3.1. The case $b \geq 4$

In the maximum critical field $H_c = 12J$, the configuration with all spins oriented up has the same energy (the ground state energy) as all configurations with an arbitrary number of spins oriented down, provided that each of the latter is surrounded by 12 upward oriented neighbors. In order to find the corresponding residual entropy $\sigma(b)$ of the infinite 3D SG fractal, we shall first study degeneracies of the intermediate stages of the fractal construction.

It can be deduced from fig. 3 that the number of the SG generator spins surrounded by 12 nearest neighbors is given by

$$B = \tfrac{1}{6}(b-1)(b-2)(b-3)\,. \tag{14}$$

We will hereafter call these spins the bulk spins. Furthermore, it is important to observe that spins at the apexes of the SG fractal, at any stage of the self-similar construction, are not nearest neighbors of the bulk spins. When the $(n+1)$th stage fractal structure is formed out of the nth stage structures, B of the apex spins of the latter become surrounded by twelve nearest neighbors oriented up and (since the nth stage apex spins cannot be nearest neighbors to each other) they may be arbitrarily oriented. Hence, the degeneracy Ω_{n+1} of the $(n+1)$th stage fractal structure is related to the degeneracy Ω_n of the nth stage structure via

$$\Omega_{n+1} = 2^B \Omega_n^C\,, \tag{15}$$

where

$$C = \tfrac{1}{6}b(b+1)(b+2)\,. \tag{16}$$

This is the number of the nth stage structures that comprise the $(n+1)$th stage structure (this is also the number of upward oriented equilateral tetrahedra in the SG generator). Starting with the ground state degeneracy Ω_G of the SG generator, we apply (15) $(n-1)$ times and thereby we obtain the following relation:

$$\Omega_n = \frac{[2^{B/(C-1)}\Omega_G]^{C^{n-1}}}{2^{B/(C-1)}}\,. \tag{17}$$

The residual entropy of the infinite 3D SG fractal is defined by

$$\sigma = \lim_{n\to\infty} \frac{\ln \Omega_n}{N_n}\,, \tag{18}$$

where N_n is the total number of spins of the nth stage structure,

$$N_n = \frac{C[(b+3)(C^n - 1) - 4b(C^{n-1} - 1)]}{b(C-1)} \,. \tag{19}$$

Inserting (17) and (19) into (18) we obtain

$$\sigma = \frac{b[B \ln 2 + (C-1) \ln \Omega_{\mathrm{G}}]}{C[C(b+3) - 4b]} \,, \tag{20}$$

which, upon using (14) and (16), acquires the form

$$\sigma(b) = \frac{6\{(b-1)(b-2)(b-3)\ln 2 + [b(b+1)(b+2) - 6] \ln \Omega_{\mathrm{G}}\}}{b(b+1)(b+2)[(b+1)(b+2)(b+3) - 24]} \,, \quad b \geqslant 4 \,. \tag{21}$$

Therefore, the residual entropy $\sigma(b)$ as a function of b appears to depend explicitly on the fractal generator ground state degeneracy Ω_{G}. To determine Ω_{G} we use a special numerical technique, similar to the one used in the two-dimensional case [7], and thus we obtain the values of $\sigma(b)$, for $4 \leqslant b \leqslant 9$, presented in table I (even using the most powerful present-day computers, instead of the IBM 3090, can hardly provide results for $b \geqslant 11$).

For the purpose of learning the crossover behavior of $\sigma(b)$, we apply the DFM method [10]. In this case it provides the following recursion relation for the ground state degeneracies:

$$\Omega_{\mathrm{G}}(b) \approx c^{b-3} \omega^{(b-2)(b-3)/2} \Omega_{\mathrm{G}}(b-1) \,, \qquad b > k \,. \tag{22}$$

Table I
Residual entropies $\sigma(b)$ and $\sigma'(b)$ of the Ising antiferromagnet situated on the 3D Sierpinski gasket type of fractals and on the corresponding finite size generators, respectively. Values $\sigma(b)$ are calculated using (21), whereas values $\sigma'(b)$ are determined by $\sigma'(b) - 6 \ln \Omega_{\mathrm{G}}(b)/[(b+1)(b-2)(b+3)]$ (here $(b+1)(b+2)(b+3)/6$ is the total number of spins in the generator).

b	$\sigma(b)$	$\sigma'(b)$
4	0.023477566	0.019804205
5	0.032474129	0.028739963
6	0.048562205	0.044776192
7	0.060159307	0.056778705
8	0.071981208	0.069010949
9	0.082206607	0.079642623

where c is a constant (characteristic of the trigonal Euclidean lattice), ω is the degeneracy factor that appears on adding a new spin to the system, and k is an integer which is, in general, determined by the preset accuracy. By successive application ($(b-k)$ times) of (22) we find

$$\Omega_G(b) \approx c^{(b^2-5b-k^2+5k)/2} \omega^{(b^3-6b^2+11b-k^3+6k^2-11k)/6} \Omega_G(k) , \tag{23}$$

and by inserting (23) into (21) we obtain

$$\sigma(b) \approx \ln \omega + \frac{1}{b} \frac{S_5 b^5 + S_4 b^4 + S_3 b^3 + S_2 b^2 + S_1 b + S_0}{b^5 + 9b^4 + 31b^3 + 27b^2 - 32b - 36} , \tag{24}$$

with

$$S_0 = 6k(k^2 - 6k + 11) \ln \omega + 18k(k-5) \ln c - 36 \ln 2 - 36 \ln \Omega_G(k) , \tag{25a}$$

$$S_1 = -2(k^3 - 6k^2 + 11k + 15) \ln \omega - 6(k^2 - 5k - 15) \ln c + 66 \ln 2 + 12 \ln \Omega_G(k) , \tag{25b}$$

$$S_2 = -3(k^3 - 6k^2 + 11k - 30) \ln \omega - 3(3k^2 - 15k + 16) \ln c - 36 \ln 2 + 18 \ln \Omega_G(k) , \tag{25c}$$

$$S_3 = -(k^3 - 6k^2 + 11k + 12) \ln \omega - 3(k^2 - 5k + 13) \ln c + 6 \ln 2 + 6 \ln \Omega_G(k) , \tag{25d}$$

$$S_4 = -36 \ln \omega - 6 \ln c , \tag{25e}$$

$$S_5 = -12 \ln \omega + 3 \ln c . \tag{25f}$$

Formula (24) for the residual entropy is similar to formula (10) obtained in the 2D case. The values $\Omega_G(b)$ that we have found in the 3D case (see table I) do not seem to be sufficient for a very accurate evaluation of the constants S_0, S_1, S_2, S_3, S_4, S_5, c and ω. Nevertheless, extrapolation of data given in table I, performed in the same spirit as in the 2D case, provides such values $\sigma(b)$ which in the limit $b \to \infty$ approach the value $\sigma(\infty) \approx 0.22$, well within the region determined [11] for the Euclidean lattices with coordination number $z = 12$ (see fig. 4). In fact, the extrapolated values $\sigma(b)$ already for $b \geqslant 138$ surpass the lower Euclidean boundary $\sigma_\ell = 0.2030$ [11]. It may be of interest to note that this surpassing at $b = 138$ corresponds to fractals which contain more than

92% of the bulk spins, which is close to the percentage of bulk spins at which the 2D fractal residual entropies $\sigma(b)$ surpass the corresponding lower Euclidean bound σ_ℓ (see the discussion at the end of section 2). Finally, since the constants S_0, S_1, S_2, S_3, S_4, S_5 and ω are finite, one can see from (24) that in the 3D case the crossover formula of the type (1) (with $\alpha = 1$) is again valid.

3.2. The case $b = 3$

The above considerations (for $b \geq 4$) are valid in the case $b = 3$. The only difference is that in the case $b = 3$ the maximum coordination number is $z = 9$. The number of generator spins with nine nearest neighbors is $B = 4$ (these spins belong to the generator surfaces). Inserting $B = 4$, and (16), into (20), we obtain

$$\sigma(b = 3) = \tfrac{1}{160}(4 \ln 2 + 9 \ln \Omega_G) . \qquad (26)$$

Since the four spins with nine nearest neighbors, within the $b = 3$ generator, are nearest neighbors to each other, the ground state degeneracy is $\Omega_G = 4 + 1$, and from (26) it follows the exact residual entropy value

$$\sigma(b = 3) = 0.10785956 . \qquad (27)$$

The obtained value does not lie between the lower bound $\sigma_\ell = 0.2400$ and the upper bound $\sigma_u = 0.2799$ predicted in ref. [11] for systems with coordination number $z = 9$. This is conceivable since the $b = 3$ fractal generator has altogether 20 spins, out of which only 4 have 9 nearest neighbors, and since the ratio of bulk versus total number of spins does not change substantially for higher stages of the fractal construction.

3.3. The case $b = 2$

In the maximum critical field $H_c = 6J$, the configuration with all spins oriented up has the same energy (the ground state energy) as all other configurations with an arbitrary number of spins oriented down, provided that each of the latter is surrounded by 6 upward oriented neighbors (in what follows it is useful to call bulk spins those spins which have 6 nearest neighbors). Keeping in mind this constraint, we will first determine the ground state degeneracies of the nth stage fractal structure for $b = 2$ that correspond to different apex spin configurations.

The apex spins of the nth stage fractal structure (when it is considered alone) must be oriented up because they are surrounded by 3 nearest neighbors.

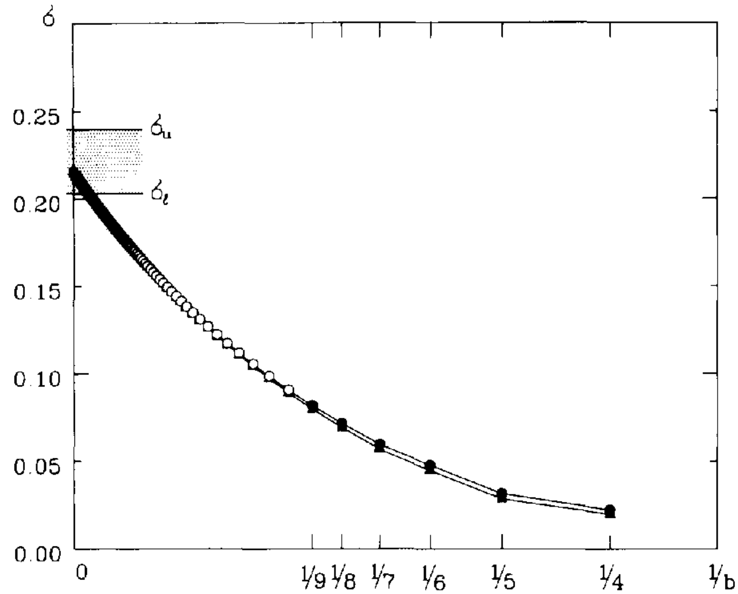

Fig. 4. Residual entropies $\sigma(b)$ and $\sigma'(b)$ of the 3D SG fractals and their generators, represented by circles and triangles, respectively. The notation is the same as in fig. 1. The exact values are given for $4 \leqslant b \leqslant 9$ (these values are listed in table I), and the extrapolated values are shown for $9 < b < 1000$. The exact value of the residual entropy for the infinite trigonal lattice is not known, and the shaded region here corresponds to the upper and lower bounds, $\sigma_u = 0.2030$ and $\sigma_\ell = 0.2398$, predicted for the Euclidean lattices, with the coordination number $z = 12$, in ref. [11].

However, when the $(n+1)$th stage structure is formed out of the nth stage structure, some of the nth stage apex spins become $(n+1)$th stage bulk spins neighboring the former nth stage bulk spins (see fig. 2a). For this reason, we must consider all possible configurations of the nth stage apex spins and find corresponding contributions to the different $(n+1)$th stage apex spin configurations. Thus, we introduce quantities (partial degeneracies) Ω_i $(i = 1, 2, 3, 4, 5)$ that correspond to the five different apex spin configurations $(++++)$, $(+++-)$, $(++--)$, $(+---)$ and $(----)$, respectively. In fig. 4 we depict all the nth stage apex spin configurations which contribute to the $(n+1)$th apex spin configuration of the type $(++++)$. From fig. 4 we obtain the first partial degeneracy recursion relation

$$\Omega_1' = \Omega_1^4 + \Omega_4^4 + 3(\Omega_2^4 + \Omega_3^4) + 4(\Omega_2^3\Omega_4 + \Omega_1\Omega_3^3) + 6(\Omega_1^2\Omega_2^2 + \Omega_3^2\Omega_4^2) + 12(\Omega_1\Omega_2^2\Omega_3 + \Omega_2^2\Omega_3^2 + \Omega_2\Omega_3^2\Omega_4) . \tag{28a}$$

Similarly, we obtain the other four recursion relations,

$$\Omega_2' = \Omega_1^3 \Omega_2 + \Omega_2^3 \Omega_5 + \Omega_4^3 \Omega_5 + 3(\Omega_1 \Omega_2^3 + \Omega_3 \Omega_4^3 + \Omega_1^2 \Omega_2 \Omega_3 + \Omega_1 \Omega_2^2 \Omega_4 + \Omega_1 \Omega_3^2 \Omega_4 + \Omega_2 \Omega_3^2 \Omega_5 + \Omega_3^2 \Omega_4 \Omega_5) + 6(\Omega_2^3 \Omega_3 + \Omega_3^3 \Omega_4 + \Omega_1 \Omega_2 \Omega_3^2 + \Omega_2 \Omega_3 \Omega_4^2) + 7\Omega_2 \Omega_3^3 + 9\Omega_2^2 \Omega_3 \Omega_4 , \tag{28b}$$

$$\Omega_3' = \Omega_2^4 + \Omega_4^4 + \Omega_1^2 \Omega_2^2 + \Omega_1^2 \Omega_3^2 + \Omega_3^2 \Omega_5^2 + \Omega_4^2 \Omega_5^2 + 2(\Omega_3^4 + \Omega_2^3 \Omega_4 + \Omega_1 \Omega_3^3 + \Omega_3^3 \Omega_5 + \Omega_2 \Omega_4^3 + \Omega_2^2 \Omega_4^2 + \Omega_2^2 \Omega_3 \Omega_5 + \Omega_1 \Omega_3 \Omega_4^2) + 4(\Omega_1 \Omega_2^2 \Omega_3 + \Omega_3 \Omega_4^2 \Omega_5 + \Omega_1 \Omega_2 \Omega_3 \Omega_4 + \Omega_2 \Omega_3 \Omega_4 \Omega_5) + 7(\Omega_2^2 \Omega_3^2 + \Omega_3^2 \Omega_4^2) + 12\Omega_2 \Omega_3^2 \Omega_4 , \tag{28c}$$

$$\Omega_4' = \Omega_1 \Omega_2^3 + \Omega_1 \Omega_4^3 + \Omega_4 \Omega_5^3 + 3(\Omega_2^3 \Omega_3 + \Omega_4^3 \Omega_5 + \Omega_1 \Omega_2 \Omega_3^2 + \Omega_1 \Omega_3^2 \Omega_4 + \Omega_2 \Omega_3^2 \Omega_5 + \Omega_2 \Omega_4^2 \Omega_5 + \Omega_3 \Omega_4 \Omega_5^2) + 6(\Omega_2 \Omega_3^3 + \Omega_3 \Omega_4^3 + \Omega_2^2 \Omega_3 \Omega_4 + \Omega_3^2 \Omega_4 \Omega_5) + 7\Omega_3^3 \Omega_4 + 9\Omega_2 \Omega_3 \Omega_4^2 , \tag{28d}$$

$$\Omega_5' = \Omega_2^4 + \Omega_5^4 + 3(\Omega_3^4 + \Omega_4^4) + 4(\Omega_3^3 \Omega_5 + \Omega_2 \Omega_4^3) + 6(\Omega_2^2 \Omega_3^2 + \Omega_4^2 \Omega_5^2) + 12(\Omega_3^2 \Omega_4^2 + \Omega_2 \Omega_3^2 \Omega_4 + \Omega_3 \Omega_4^2 \Omega_5) . \tag{28e}$$

In fig. 5 we have assumed that all elementary tetrahedra have an interior structure. To determine the initial conditions for the recursion relations (28) we should consider the situation when elementary tetrahedra do not have a substructure, that is, we should find the partial degeneracies of the fractal generator that correspond to different apex spin configurations. In fig. 6 we show all possible configurations of the generator spins (grouped according to the possible apex spin configurations) that appear in the $n = 2$ fractal stage ground state configurations. Thereby, we obtain the following initial conditions for relations (28):

$$\Omega_1^{(1)} = 10 , \qquad \Omega_2^{(1)} = 4 , \qquad \Omega_3^{(1)} = 2 , \qquad \Omega_4^{(1)} = 1 , \qquad \Omega_5^{(1)} = 1 . \tag{29}$$

If we introduce the superscript (n) for the nth stage partial degeneracies, the

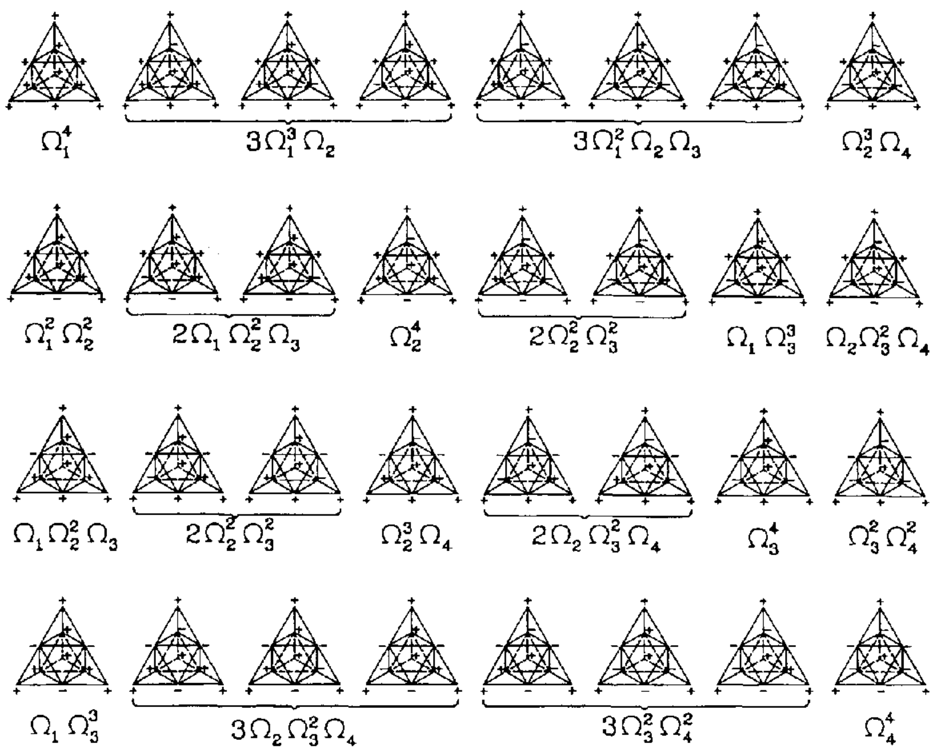

Fig. 5. All the apex spin configurations of the nth stage fractal structure ($b=2$, $d=3$) that contribute to the ground state degeneracy of the $(n+1)$th stage apex spin configuration of the type $(++++)$. The elementary tetrahedra are assumed to have interior structure, which means that their apex spins are not nearest neighbors to each other.

residual entropy of the infinite fractal lattice can be determined by

$$\sigma = \lim_{n\to\infty} \frac{\ln \Omega_1^{(n)}}{N_n}\,, \tag{30}$$

where i can be any of the integers (1, 2, 3, 4, 5) since the differences between the five quantities $\Omega_i^{(n)}$, scaled by the number of spins $N_n = (4^{n+1}+4)/2$, approaches zero when $n\to\infty$. Indeed, for each i, we find after 15 iterative applications of (28), the following value of $\sigma(b)$:

$$\sigma(b=2,\, d=3) = 0.32859960\,. \tag{31}$$

This value lies between the lower bound $\sigma_\ell = 0.2971$ and the upper bound $\sigma_\mu = 0.3403$ predicted by Hajduković and Milošević [11] for systems with coordination number $z=6$.

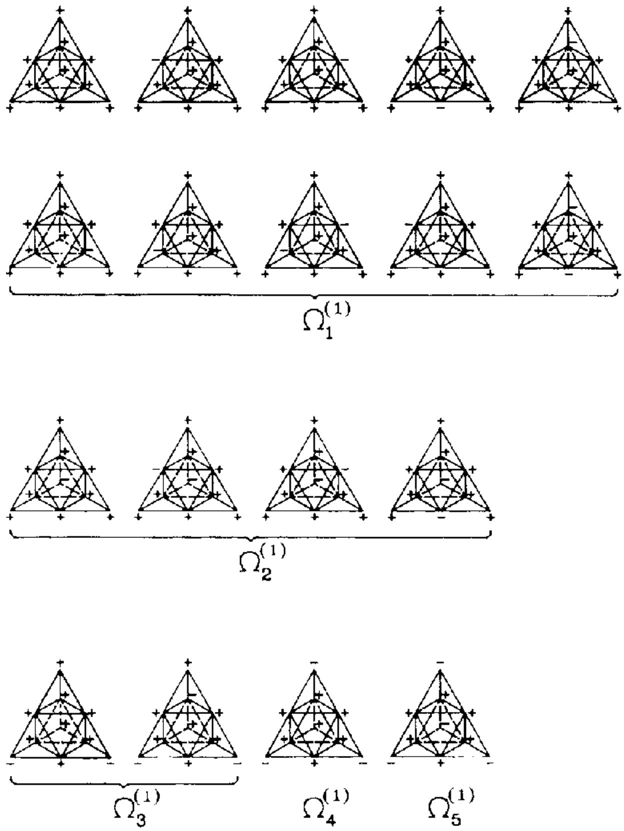

Fig. 6. All spin configurations of the SG fractal generator ($b=2$, $d=3$) that contribute to the ground state degeneracy of the $n=2$ stage structure, grouped according to the different possible apex spin configurations. In contrast to fig. 5, the elementary tetrahedra here do not have substructure, which means that their apex spins neighbor each other.

4. Summary

In this section we first derive, for the sake of completeness, formulas for the residual entropy $\sigma(b)$ of the Sierpinski gasket family of fractals embedded in the d-dimensional Euclidean space. It will be found that these new results contain as special cases formulas obtained in previous sections for $d=2$ and $d=3$.

We start this general case by noting that all members of the SG fractal family can be obtained from the infinite set of d-dimensional generators $G(b,d)$, where b is an integer that runs from 2 to infinity. The generator $G(b,d)$ is a d-dimensional hypertetrahedron of side length b, which is itself filled with b layers of smaller hypertetrahedra of unit side length [12]. For a given d and b, the maximum coordination number is $z = bd$ [12], in the case $b \leqslant d$, and $z = d(d+1)$, in the case $b \geqslant d+1$, yielding the maximum critical fields $H_c = bdJ$ and $H_c = d(d+1)J$, respectively.

The reasoning that led to formula (20), in the case $d = 3$, can be repeated here for $b \geqslant 3$. Thus we obtain the following formula for the residual entropy:

$$\sigma = \frac{b[B \ln 2 + (C-1) \ln \Omega_G]}{C[C(b+d) - b(d+1)]}, \qquad b \geqslant 3, \tag{32}$$

where C is the number of hypertetrahedra with unit side length in a generator,

$$C(b,d) = \binom{b+d-1}{d}, \tag{33}$$

and B is the number of bulk spins in the generator (bulk spins are spins with $z = bd$ nearest neighbors), that is

$$B = \prod_{k=b}^{d} (k+1), \tag{34a}$$

for $3 \leqslant b \leqslant d$, and

$$B = \binom{b-1}{d}, \tag{34b}$$

for $b \geqslant d+1$. Inserting (33), (34a) and (34b) into (32) we obtain

$$\sigma = \frac{d!\left[d!\left(\prod_{k=b}^{d} (k+1)\right) \ln 2 + \left(\prod_{k=0}^{d-1} (b+k) - d!\right) \ln \Omega_G\right]}{\prod_{k=0}^{d-1} (b+k)\left(\prod_{k=1}^{d} (b+k) - (d+1)!\right)}, \tag{35}$$

for $3 \leqslant b \leqslant d$, and

$$\sigma = \frac{d!\left[\left(\prod_{k=b}^{d} (b-k)\right) \ln 2 + \left(\prod_{k=0}^{d-1} (b+k) - d!\right) \ln \Omega_G\right]}{\prod_{k=0}^{d-1} (b+k)\left(\prod_{k=1}^{d} (b+k) - (d+1)!\right)}, \tag{36}$$

for $b \geqslant d+1$. The last two formulas are quite general. Indeed, inserting $d = 2$ into (36) we obtain expression (2), while inserting $d = 3$ into (35) and (36) we obtain (26) and (21), respectively.

In the case $b = 2$ (and arbitrary d), in contrast to the above cases, we cannot present a general formula, since it would imply to generalize the complex recursion relations (12), which certainly is a formidable task. Besides, the case $b=2$ is irrelevant for the fractal to Euclidean crossover analysis, which is one of the primary objectives of this paper.

As regards behavior of the residual entropy at the fractal to Euclidean crossover, we have confirmed that the crossover formula (1) (anticipated in ref. [7], in the case $d=2$) is valid in both cases $d=2$ and $d=3$, with α being equal to 1. The confirmation of formula (1) was achieved by calculating additional data, in the case $d=2$, and by creating a new set of data ($b \leqslant 9$), in the case $d=3$, which were analyzed using the recently introduced degeneracy factor method (DFM) [11]. In addition to the validation of (1), the extrapolated values of $\sigma(b)$ obtained by the DFM lie well in the regions determined by the corresponding lower, σ_ℓ, and upper bounds, σ_u, for the residual entropies of the Euclidean lattices [11]. We can expect that the crossover law (1) is valid also for the SG fractals embedded in higher-dimensional spaces ($d>3$). However, it is certainly more challenging to see whether (1) is to some extent universal, that is, whether, for instance, it stays valid for other families of fractals which furnish the crossover to Euclidean lattices. An answer to this question will be elaborated in the adjoined paper II.

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