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RESIDUAL ENTROPIES OF THE ISING ANTIFERROMAGNETS ON FRACTALS

II. d-DIMENSIONAL CHECKERBOARD TYPE OF FRACTALS

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We study the residual entropies of the antiferromagnetic Ising systems, in the maximum critical field, situated on checkerboard (CB) type of fractals embedded in d-dimensional Euclidean space. For a given d, the CB fractals constitute a family, whose each member is labelled by b, where b is an odd integer ($3 \leqslant b < \infty$). Each family itself furnishes a crossover to the corresponding d-dimensional hypercubic lattice. By calculating explicitly residual entropies $\sigma(b)$ for finite b, and by using a specific method of extrapolating the obtained results, we were able to establish the crossover behavior of $\sigma(b)$. It turns out that the established crossover is of the same type as the one found in the case of fractal families of the Sierpinski gasket type.

1. Introduction

In the preceding paper [1] we have studied the residual entropies of the Ising antiferromagnetic systems, in the maximum critical field, situated on Sierpinski gasket (SG) type of fractals that are embedded in the d-dimensional Euclidean space. For a given d, the SG fractals comprise a family [2], so that each member is labelled by an integer b ($2 \leqslant b < \infty$) and the corresponding fractal dimensions d_f tend to d when $b \to \infty$. Thus, when $d = 2$, for instance, the SG fractal family furnishes a crossover to the Euclidean triangular lattice. In this case we have found [1] the following crossover formula for the residual entropy:

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

where P is a constant. It is interesting to observe that the correction term in (1) is not logarithmic and thus it is neither of the type that appears for the fractal dimension d_f, nor of the type that is pertinent to the spectral dimension d_s [2–4]. Besides, the crossover formula (1) was also found to be valid [1] in the case of SG fractals embedded in the three-dimensional (3D) Euclidean space, and thus one may conjecture that it could be valid for residual entropies in general. Indeed, in this paper we present a study of residual entropies for checkerboard (CB) type of fractals, and confirm that formula (1) is again valid both in the $d = 2$ and $d = 3$ cases.

This paper is organized as follows. In section 2 we survey general properties of the CB type of fractals, and elaborate the case of the CB fractal family embedded in the two-dimensional (2D) Euclidean space. The 3D case is elaborated in section 3. Finally, in section 4 we derive formulas valid in the case of arbitrary d, and conclude with a general discussion concerning the residual entropy behavior at the fractal to Euclidean crossover.

2. Residual entropies of the 2D checkerboard type of fractals

The CB fractals are, similarly to the SG fractals, of deterministic nature. All members of a checkerboard fractal family, embedded in a d-dimensional Euclidean space, may be obtained from an infinite set of d-dimensional generators $\mathrm{G}(b, d)$, where b is an odd integer ($b = 2k + 1$, $k = 1, 2, \ldots, \infty$). Each generator $\mathrm{G}(b, d)$ is a d-dimensional hypercube of side length b, composed of b layers of d-dimensional hypercubes of unit side length, so that within each layer and along each direction of alignment of the elementary hypercubes every other of them is removed (see fig. 1). A CB fractal lattice is grown in stages. The $(n + 1)$th stage of a fractal lattice is obtained by enlarging the generator by b^n and substituting each of the physically present elementary hypercubes by the nth stage structure. The complete fractal lattice is obtained in the limit $n \to \infty$. In fig. 1 we depict the first few steps of the above growing process in the $d = 2$ case, for $b = 3$ and $b = 5$. In the general case, it can be shown that the fractal dimension of a CB fractal lattice, for given d and b, has the form

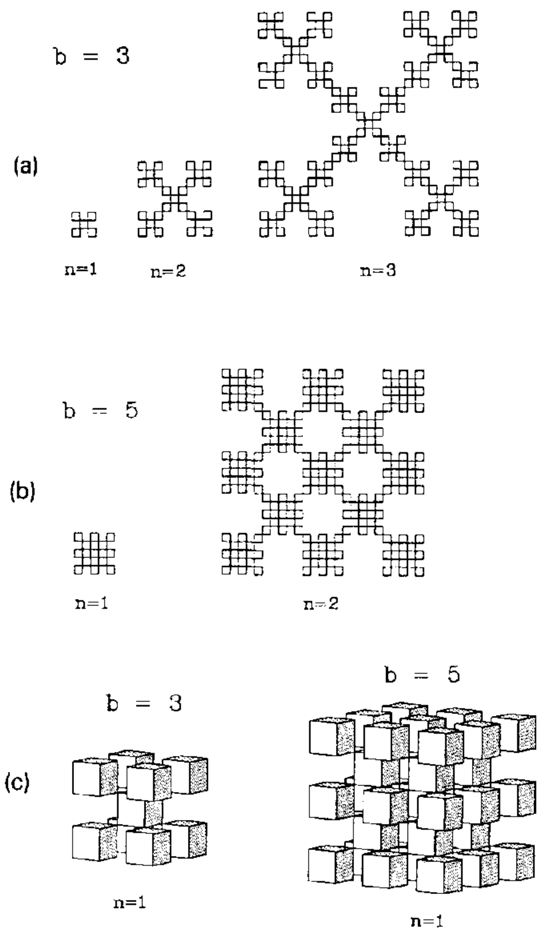

Fig. 1. (a) The first three steps of construction ($n = 1, 2, 3$) of the 2D CB fractal lattice with $b = 3$. (b) The first two steps of construction ($n = 1, 2$) of the 2D CB fractal with $b = 5$. (c) The generators ($n = 1$) of the 3D CB fractals with $b = 3$ and $b = 5$.

$$d_{\mathrm{f}} = \frac{\ln\{[\frac{1}{2}(b+1)]^d + [\frac{1}{2}(b-1)]^d\}}{\ln b} . \tag{2}$$

Hence one can notice that, in analogy with the SG case [2], the fractal dimension of the CB fractals approaches, for large b, the Euclidean value d with a logarithmic correction of the form $(1-d)\ln 2/\ln b$.

In what follows we study the antiferromagnetic Ising systems, with the nearest-neighbor (nn) interaction J, in the maximum critical field H_{c}. The value of H_{c} is determined by the maximum coordination number z of the lattice the Ising system is situated on [5]. In the case of the CB fractal lattices, the relation

$z = 2d$ holds (for each b) and thereby it follows [5] that $H_c = 2d|J|$. Here it should be emphasized that, contrary to the SG case, within one CB fractal family (for a given d) the maximum critical field H_c does not depend on b. Consequently, in investigating the residual entropies $\sigma(b)$ one does not have to study separate cases defined by some particular values of b. This will be first demonstrated in the case of the CB fractal family in the $d = 2$ space.

In the maximum critical field $H_c = 4J$, 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 4 upward oriented neighbors. Hereafter, we will use the term bulk spins for those spins which have the maximum number of nearest neighbors. When the $(n + 1)$th stage fractal structure is formed out of the nth stage structures, some of the apex spins of the latter become bulk spins. However, they may take arbitrary orientations since they are not neighbors to the other bulk spins. Therefore, the recursion relation between the nth stage ground state degeneracy Ω_n and the $(n + 1)$th stage degeneracy Ω_{n+1}, is given by

$$\Omega_{n+1} = 2^B \Omega_n^C , \tag{3}$$

where

$$B = (b - 1)^2 \tag{4}$$

is the number of bulk spins in the generator, and

$$C = [\tfrac{1}{2}(b + 1)]^2 + [\tfrac{1}{2}(b - 1)]^2 \tag{5}$$

is the number of nth stage structures that comprise the $(n + 1)$th stage structure (this is also the number of elementary squares in the generator). By iterative application of (3), starting from the generator ground state degeneracy Ω_G, we obtain the expression for the nth stage ground state degeneracy

$$\Omega_n = \frac{(2^{B/(C-1)}\Omega_G)^{C^{n-1}}}{C - 1} . \tag{6}$$

The number of spins in the nth stage of construction of the fractal is obtained using the recursion relation

$$N_{n+1} = CN_n - B , \tag{7}$$

and thereby it is found that

$$N_n = \frac{C^{n-1}[(C-1)N_G - B] + B}{C-1}, \tag{8}$$

where

$$N_G = (b+1)^2 \tag{9}$$

is the number of spins in the generator.

The residual entropy of an infinite fractal lattice is given by

$$\sigma = \lim_{n\to\infty} \frac{\ln \Omega_n}{N_n}, \tag{10}$$

so that by inserting (6) and (8) into (10) we find

$$\sigma(b) = \frac{B \ln 2 + (C-1) \ln \Omega_G(b)}{(c-1)N_G - B}. \tag{11}$$

Finally, inserting (4), (5) and (9) into (11) we obtain

$$\sigma(b) = \frac{4(b-1)^2 \ln 2 + [(b+1)^2 + (b-1)^2 - 4] \ln \Omega_G(b)}{(b+1)^2[(b+1)^2 + (b-1)^2 - 4] - 4(b-1)^2}. \tag{12}$$

Thus, the residual entropy of 2D CB fractals depends explicitly on the generator side length b and the generator ground state degeneracy Ω_G. In order to evaluate the explicit values of σ from (12) it remains to find the generator ground state degeneracies Ω_G. Keeping in mind that we want to study the crossover behavior of $\sigma(b)$, it is preferable to learn Ω_G for as large generators as possible. To accomplish this task we have used a special numerical technique, similar to the one used in the case of Sierpinski gasket type of fractals [1, 6], and have calculated $\Omega_G(b)$ for $b \leq 17$. In table I we present the calculated values of $\sigma(b)$, as well as the values of the residual entropies $\sigma'(b)$ of the corresponding generators. The values $\sigma'(b)$ were calculated according to the formula

$$\sigma'(b) = \frac{\ln \Omega_G(b)}{N_G}. \tag{13}$$

With the goal to establish the limiting behavior of $\sigma(b)$ when $b \to \infty$, we apply the degeneracy factor method (DFM) introduced in ref. [7]. The essence

Table I
Residual entropies $\sigma(b)$ and $\sigma'(b)$ of the Ising antiferromagnet in the maximum critical field, situated on the 2D checkerboard fractal lattices and on the corresponding finite size generators, respectively. Values $\sigma(b)$ are calculated using (12), whereas values $\sigma'(b)$ are obtained using (13) and (9).

b	$\sigma(b)$	$\sigma'(b)$
3	0.17593716	0.12161938
4		0.16572539
5	0.23198690	0.19772267
6		0.22292210
7	0.26524471	0.24278240
8		0.25889169
9	0.28786100	0.27216487
10		0.28329028
11	0.30428457	0.29274022
12		0.30086461
13	0.31675443	0.30792147
14		0.31410711
15	0.32654310	0.31957256
16		0.32443614
17	0.33442996	0.32879168

of the DFM is the scaling relation

$$\Omega_{\mathrm{G}}(b) \approx c^2 \omega^{(b-1)^2-(b-2)^2} \Omega_{\mathrm{G}}(b-1)\,, \qquad b \geq k\,, \tag{14}$$

where c is a constant (characteristic for the square lattice), and ω is the degeneracy factor that appears on adding a new spin to a fractal generator. The relation (14) is assumed to be valid, for a preset accuracy, beyond a certain value $b = k$. By successive application of (14) we find

$$\Omega_{\mathrm{G}}(b) \approx c^{2(b-k)} \omega^{b^2-k^2-2b+2k} \Omega_{\mathrm{G}}(k)\,, \tag{15}$$

and inserting (15) into (12) we obtain

$$\sigma(b) \approx \ln \omega + \frac{S_2 b^2 + S_1 b + S_0}{b^3 + 3b^2 + b + 3}\,, \tag{16}$$

with

$$S_2 = 2 \ln c - 4 \ln \omega\,, \tag{17a}$$

$$S_1 = 2 \ln 2 - 2(k-1) \ln c - (k^2 - 2k + 3) \ln \omega + \ln \Omega_{\mathrm{G}}(k)\,, \tag{17b}$$

$$S_0 = -2 \ln 2 - 2k \ln c - (k^2 - 2k + 3) \ln \omega + \ln \Omega_{\mathrm{G}}(k)\,. \tag{17c}$$

To evaluate the numerical values of these coefficients we assume that (14) is valid beyond $k = 16$, and use the calculated values of $\Omega_G(b)$ ($b \leqslant 17$) to obtain

$$\ln \omega = 0.4074945\,, \tag{18a}$$

$$\ln c = 0.0670637\,. \tag{18b}$$

For the coefficients in (16) we now find

$$S_2 = -1.49585\,, \tag{19a}$$

$$S_1 = 0.635168\,, \tag{19b}$$

$$S_0 = -2.27155\,. \tag{19c}$$

Since the constants (19) are finite, it follows that the leading term in (16) is of the order $1/b$ for large b, and we can now claim that the asymptotic law (1) is true in the case of the 2D CB fractals as well. Also, comparing our limiting value of $\sigma(b)$ for $b \to \infty$, given by (18a), with the value of the residual entropy found in ref. [7] for the infinite square lattice $\sigma_{\text{Euclidean}} = 0.40749510126068$, we see that knowledge of exact data up to $b = 17$ provides a six digit accuracy of the approximate formulas for larger b. In fig. 2 we depict values of $\sigma(b)$ for $b \leqslant 1000$, calculated using (16), together with the residual entropies $\sigma'(b)$ of the corresponding fractal generators, calculated using (13) and (15). Thus we can see that the limiting value of $\sigma(b)$, when $b \to \infty$, lies slightly above the region predicted [5] for the Euclidean lattices with coordination number $z = 4$. On the other hand, the extrapolated values $\sigma(b)$ surpass the lower Euclidean boundary $\sigma_\ell = 0.3584$ [5] for $b \geqslant 26$, corresponding to fractals containing more than 86% of the bulk spins, which is the same percentage of bulk spins at which the residual entropies of 2D Sierpinski gasket type of fractals surpass the corresponding lower Euclidean bound (see ref. [1]).

3. Residual entropies of the 3D checkerboard type of fractals

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 bulk spins oriented down, provided that they are not nearest neighbors to each other. Argumentation similar to that used in the 2D case (see section 2) shows that now eq. (11) is also valid, except for the fact that B, C and N_G are here different. The number of bulk

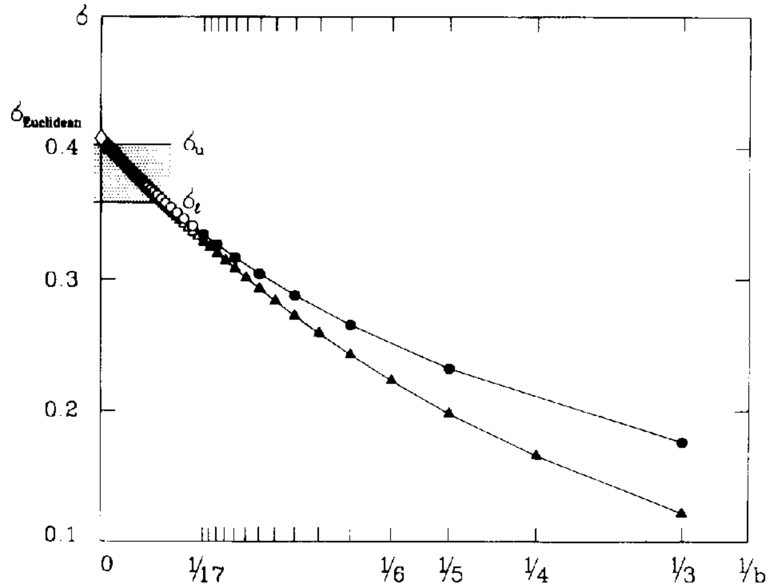

Fig. 2. Residual entropies $\sigma(b)$ and $\sigma'(b)$ of the 2D CB fractals and their generators, represented by circles and triangles, respectively. Exact values for $3 \leqslant b \leqslant 17$ are depicted by full circles and triangles, while the extrapolated values for $18 \leqslant b \leqslant 1000$ are depicted by the corresponding open geometrical shapes. The extrapolated values of $\sigma(b)$ are obtained using eqs. (16)–(19), whereas the extrapolated values $\sigma'(b)$ are found using (13) and (14). The symbol ◇ represents the value found [7] for the residual entropy of the infinite square lattice $\sigma_{\text{Euclidean}} = 0.40749510126068$, and the nearby shaded region corresponds to the upper and lower bounds, $\sigma_u = 0.4024$ and $\sigma_\ell = 0.3584$, predicted [5] for the Euclidean lattices with the coordination number $z = 4$. The full lines serve as guides to the eye.

spins in the generator is here given by

$$B = (b-1)^3 , \tag{20}$$

whereas the number of nth stage structures that comprise the $(n+1)$th stage structure (this is also the number of elementary cubes in the generator) is

$$C = [\tfrac{1}{2}(b+1)]^3 + [\tfrac{1}{2}(b-1)]^3 , \tag{21}$$

and finally the total number of spins in the generator is

$$N_G = (b+1)^3 . \tag{22}$$

Inserting (20), (21) and (22) into (11) we find

$$\sigma(b) = \frac{8(b-1)^3 \ln 2 + [(b+1)^3 + (b-1)^3 - 8] \ln \Omega_G(b)}{(b+1)^3[(b+1)^3 + (b-1)^3 - 8] - 8(b-1)^3} . \tag{23}$$

Again, the residual entropy $\sigma(b)$ depends explicitly on the generator side length b and on the generator ground state degeneracy Ω_G. To determine Ω_G, we have used a numerical technique similar to that used in the 2D case, and thus we have calculated Ω_G exactly up to $b \leq 6$. In table II we present the values of $\sigma(b)$ calculated using (23), as well as the values of the residual entropies $\sigma'(b)$ of the corresponding generators, calculated according to (13) and (22).

To study the crossover behavior of $\sigma(b)$ when $b \to \infty$, we apply the DFM method [7]. In this case it provides the following recursion relation for the ground state degeneracies:

$$\Omega_G(b) \approx c^{3(b-1)} \omega^{(b-1)^3-(b-2)^3} \Omega_G(b-1)\,, \qquad b \geq k\,, \tag{24}$$

where c is a constant (characteristic for the simple cubic lattice), and ω is the degeneracy factor that appears on adding a new spin to a fractal generator. The relation (24) is assumed to be valid, for a preset accuracy, beyond a certain value $b = k$. By successive application of (24) we find

$$\Omega_G(b) \approx c^{(3/2)[b(b-1)-k(k-1)]} \omega^{b^3-3b^2+3b-k^3+3k^2-3k} \Omega_G(k)\,, \tag{25}$$

and inserting this expression into (23) we obtain

$$\sigma(b) \approx \ln \omega + \frac{1}{b} \frac{S_5 b^5 + S_4 b^4 + S_3 b^3 + S_2 b^2 + S_1 b + S_0}{b^5 + 3b^4 + 6b^3 + 2b^2 + 9b - 21}\,, \tag{26}$$

with

$$S_5 = -6 \ln \omega + \tfrac{3}{2} \ln c\,, \tag{27a}$$

$$S_4 = -\tfrac{3}{2} \ln c\,, \tag{27b}$$

Table II
Residual entropies $\sigma(b)$ and $\sigma'(b)$ of the Ising antiferromagnet situated on the 3D CB fractals and on the corresponding finite size generators, respectively. Values $\sigma(b)$ are calculated using formula (23), while values $\sigma'(b)$ are found using (13) and (22).

b	$\sigma(b)$	$\sigma'(b)$
3	0.06743643	0.05555231
4		0.08932202
5	0.12527753	0.11814529
6		0.14238375

$$S_3 = 4\ln 2 - \tfrac{3}{2}(k^2 - k - 3)\ln c - (k^3 - 3k^2 + 3k + 15)\ln \omega + \ln \Omega_G(k)\,, \tag{27c}$$

$$S_2 = -12\ln 2 + \tfrac{21}{2}\ln c + 12\ln \omega\,, \tag{27d}$$

$$S_1 = 12\ln 2 - \tfrac{3}{2}(3k^2 - 3k - 4)\ln c - 3(k^3 - 3k^2 + 3k - 3)\ln \omega + 3\ln \Omega_G(k)\,, \tag{27e}$$

$$S_0 = -4\ln 2 + 6k(k-1)\ln c + 4(k^3 - 3k^2 + 3k)\ln \omega - 4\ln \Omega_G(k)\,. \tag{27f}$$

The obtained approximate formula for the residual entropy (26) is similar to formula (16) obtained in section 2 for the 2D CB fractal family, as well as to the corresponding formulas obtained [1] for the 2D and 3D SG fractal families. Similarly to the 3D SG fractal case [1], the exact values $\Omega_G(b)$ $(3 \leq b \leq 6)$ that we have calculated 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. Still, the extrapolation of data given in table II, according to (24), (26) and (27), provides values $\sigma(b)$, shown in fig. 3, that, in the limit $b \to \infty$, approach the value $\sigma(\infty) \approx 0.36$. This value

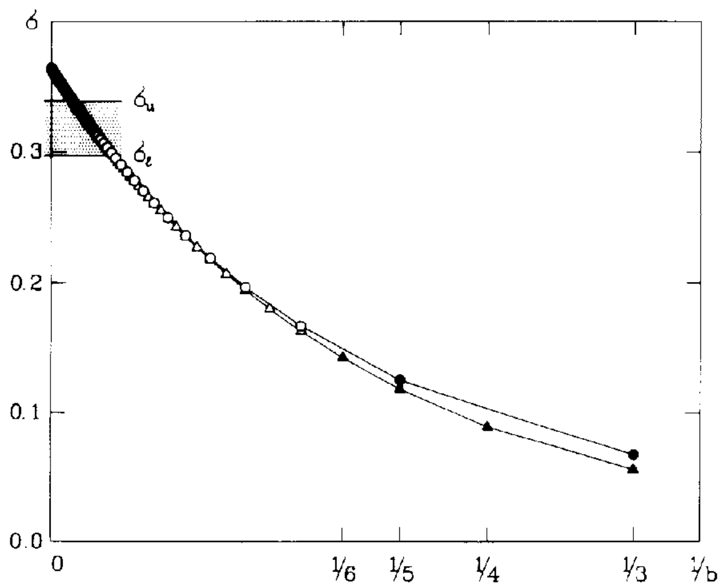

Fig. 3. Residual entropies $\sigma(b)$ and $\sigma'(b)$ of the 3D CB fractals and their generators, represented by circles and triangles, respectively. The notation is the same as in fig. 2. The exact values are depicted for $3 \leq b \leq 6$, and the extrapolated values are shown for $7 \leq b \leq 1000$. The shaded region corresponds to the upper and lower bounds, $\sigma_u = 0.3403$ and $\sigma_l = 0.2971$, predicted [5] for the Euclidean lattices with the coordination number $z = 6$.

(similarly to the 2D CB fractal family case presented in section 2) lies above the region predicted [5] for the Euclidean lattices with coordination number $z = 6$. Besides, the extrapolated values $\sigma(b)$ surpass the lower Euclidean boundary $\sigma_{\mathcal{E}} = 0.2971$ [5] for $b \geqslant 28$, which corresponds to fractals with more than 81% of bulk spins. Although the accuracy of the above approximations is not very high (to improve the accuracy one would need a new generation of computers), it provides sufficiently firm ground to infer that the constants which appear in (26) are finite. Consequently, we can conclude that the crossover formula of type (1) is again valid.

4. Summary

At the beginning of section 2 we have surveyed some general properties of CB fractals embedded in d-dimensional Euclidean space. We start this section by deriving formulas for the residual entropy in the maximum critical field for arbitrary d. It will turn out that formulas derived in previous sections, for the 2D and 3D CB fractal families, represent special cases of the new general results.

In the maximum critical field $H_c = 2dJ$, the configuration with all spins parallel to the field has the same energy (the ground state energy) as all other configurations with an arbitrary number of bulk spins antiparallel to the field, provided that they are not nearest neighbors to each other. Applying arguments similar to those used in the 2D CB fractal family case in section 2, it can be shown that the residual entropy $\sigma(b)$ is again given by (11), while the expressions for B, C, and N_G are different. For the number of bulk spins in the generator here we find

$$B = (b-1)^d , \tag{28}$$

for the number of nth stage structures that comprise the $(n+1)$th stage structure (this is also the number of elementary hypercubes in the generator) we obtain

$$C = [\tfrac{1}{2}(b+1)]^d + [\tfrac{1}{2}(b-1)]^d , \tag{29}$$

and finally for the total number of generator spins we find

$$N_G = (b+1)^d . \tag{30}$$

Inserting (28), (29) and (30) into (11), we obtain the following general formula for the residual entropy of CB fractals:

$$\sigma(b, d) = \frac{2^d(b-1)^d \ln 2 + [(b+1)^d + (b-1)^d - 2^d] \ln \Omega_G(b)}{(b+1)^d[(b+1)^d + (b-1)^d - 2^d] - 2^d(b-1)^d}, \tag{31}$$

in terms of the Euclidean dimension d of the space in which the fractal is embedded, fractal generator side length b, and the generator ground state degeneracy Ω_G. Inserting $d = 2$ and $d = 3$ into (31), expressions (12) and (23) are retrieved, respectively.

Therefore, we have captured formulas for residual entropies for the 2D and 3D CB fractals within the single formula (31) valid for arbitrary d. Formula (31) itself (without additional explicit calculations of Ω_G) does not provide sufficient information to make general conclusions about the crossover behavior of the residual entropy of fractals embedded in higher dimensional Euclidean spaces. However, the specific results of sections 2 and 3 make us conclude that in the 2D and 3D CB fractal family case the behavior of the residual entropy at the fractal to Euclidean crossover is governed by formula (1). It should be emphasized that the validity of (1) has been checked by calculating exact data for the finite sequences of fractals ($b \leq 17$ for $d = 2$, and $b \leq 6$ for $d = 3$), and by analyzing data via the recently introduced degeneracy factor method (DFM) [7]. Since it was shown [1] that formula (1) is also valid for the residual entropy crossover behavior of 2D and 3D Sierpinski gasket fractal families, we can conclude that (1) is to some extent universal. In other words, we may expect that (1) will stay valid for other families of fractals which furnish the crossover to Euclidean lattices.

Acknowledgements

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