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On the Aboav–Weaire law

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Abstract

The most general form of the Aboav–Weaire empirical topological law of random cellular networks is derived from conditions on local averages in two dimensions. We assume the average number of edges in a local cluster depends on the number of actual edges and its moments together with the probability distribution function. Based on this constitutive assumption we show that the Aboav–Weaire law depends only on the first and second moments of the distribution function. We show that the Aboav–Weaire law is a direct consequence of the existence of the well-known microscopic topological transformations. We study the effect of the constitutive equation's coefficients on the Aboav–Weaire law. The properties near to the equilibrium are also investigated to explain the role of the actual parameters of the network.
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1. Introduction

Numerous well-known theoretical and experimental studies show that the development of two-dimensional (2D) unbiased cellular patterns is not completely random.

Of numerous topological observations, the most basic is Euler's law [1], namely $\langle n \rangle = 6$ and $f - e + v - n = 1$, where n is the cell's number of sides, $\langle\,\rangle$ denotes averaging, e, v and f are the number of edges, the number of vertices and the number of cells, respectively. We assumed that in these patterns was assumed that three edges meet at

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every vertex. Lewis proposed that [2] the average area of a cell grows linearly with n. Later von Neuman [3] showed that the growth of a cell is proportional to $n - 6$ (for coarsening of foams). Therefore, the area of a cell with more than six sides increases, of a cell with less than six sides decreases, and of cells with exactly six sides remains the same. The Aboav law [4,5] relating the number of edges of neighboring clusters is

$$M_n = 6 - a + \frac{6a - \sigma_2}{n} = 6 + \frac{1}{n}(\sigma_2 - a\delta_n),$$

where we have substituted the first moment, the average number of edges, $\langle n \rangle = 6$, and the deviation from the average edge-number $\delta_n = (n - 6)$ as well as the second deviation $\sigma_2 = \sum_{i \geq 3} (i-6)^2 P(i)$ of $P(n)$, the probability distribution of number of edges. The average edges per cell for the neighbors of the actually chosen n-sided cell are M_n.

Consequently, the empirical law declares that the average number of the neighboring sides of a cell of a given n-sided cell in a random cellular network has one term, which is independent of n, and another, which is inversely proportional to n. This simple function contains three parameters: the first and second moments of the actual distribution function and a (a structure-specific parameter).

Weaire generalized the well proven Aboav law experimentally [1]. The original experimentally recognized law looks very general: it is valid that the randomly simulated cellular networks as well as for natural random networks like biological tissues, foams, crystallite surface patterns, self-organized pattern structures, etc. Stability distinguishes between natural and computer stimulated networks. The natural networks are actually non-equilibrium, evolving towards equilibrium. The equilibrium state is trivially a honeycomb lattice. However, its regular, defect-free form, derived from random networks only, is not shown yet. The evolution time scale depends on the specific material properties and physical and chemical states.

Numerous topological studies [6,7] and theoretical considerations [8,9] have been published as the Aboav law, but a general theoretical derivation is missing. The relatively few theoretical explanations fall into two groups:

- The first uses the second law of thermodynamics [6,10], stating the maximal entropy of the system at equilibrium. However, the experimentally realized physical random cellular networks are non-equilibrium, their entropy is time-dependent. Consequently, during the evolution of a random lattice (except the final equilibrium state) at the outmost the local entropy could be maximal, the global does not. Therefore, deriving the Aboav–Weaire law from the general entropy maximization does not point on the core of the law.
- The second approach derives the Aboav–Weaire law assuming a time-dependent variation of the difference of local- and global-average edge-numbers [11]. This assumption has a problem describing the Aboav–Weaire law for equilibrium networks.

We conclude that the correct explanation of the Aboav–Weaire law has to be compatible with both the above ideas, but more fundamental. We derive the Aboav law from a general probability function.

2. Analysis of random cellular network

A 2D network containing N ($N \gg 1$) cells packs the plane properly. The position of the individual cells is characterized by pair of numbers (i, j). This is the so-called Voronoi construction [12], making the cell-edges by the perpendicular bisection of the polynomial-edges of the point-structure. The cells have a random integer number of sides not smaller than 3. If the number of n-sided cells is N_n then the definition is

$$P(n) = \lim_{N\to\infty} \frac{N_n}{N} \quad (n = 3, 4, \dots)$$

introduces a discrete distribution function. The average number of sides (the first moment of the distribution) is

$$\langle n \rangle = \sum_{n\geq 3} nP(n)$$

in every trivalent (three edges per vertex) random cellular network $\langle n \rangle = 6$ (Euler's rule) [13]. The higher moments are defined as

$$\langle n^k \rangle = \mu_k = \sum_{n\geq 3} n^k P(n)$$

and the generalized deviations are

$$\sigma_k = \sum_{n\geq 3} (n - \langle n \rangle)^k P(n).$$

Hence the second deviation of the distribution is

$$\sigma_2 = \sum_{n\geq 3} (n - \langle n \rangle)^2 P(n) = \sum_{n\geq 3} (n - 6)^2 P(n).$$

Introducing a probability density function

$$P(n^*) = P(n)\delta(n^* - n), \tag{1}$$

where δ is the Dirac delta-distribution. Instead of the discrete n variable we introduce continuous variable $n^* \in R^1$.

The random variable S_{ni} is the sum of the edges of the directly connected neighbors to an n-sided cell denoted N_n ($i = 1, 2, \dots, N_n$). Introduce the average of the edge-sums

$$S_n = \frac{1}{N_n} \sum_{i=1}^{N_n} S_{ni}$$

and so

$$\langle nM_n \rangle = \langle S_n \rangle = \langle n \rangle^2 + \sigma_2 = 36 + \sigma_2 = \mu_2 = \langle n^2 \rangle. \tag{2}$$

Referring to Edwards and Pithia's work [11] we introduce the local average of the number of sides. The n-sided cells and their neighbors form a cluster-subset of $n + 1$ units in the

network. The number of such subsets is N_n. The cluster has $N_n(nM_n + n)$ sides, while the number of cells in the subset is $N_n(n + 1)$, so the average edge-number is

$$n_{\text{lok}} = \frac{nM_n + n}{n + 1}. \tag{3}$$

This local average number of sides directly connects to M_n:

$$M_n = \frac{n + 1}{n} n_{\text{lok}} - 1. \tag{4}$$

3. The Aboav–Weaire law

Like Edwards and Pithia [4], we use the local average number of sides (Eq. (3)) to derive the Aboav–Weaire law. n_{lok} depends on the number of sides and is a function of $P(n^*)$

$$n_{\text{lok}} = f(n, [P(n^*)]), \tag{5}$$

where the rectangular bracket indicates the functional dependence which can be transformed into a function of the $P(n^*)$ moments (as shown in Appendix A), so

$$n_{\text{lok}} = g(n, \mu_0, \mu_1, \mu_2, \dots) \tag{6}$$

and similarly

$$n_{\text{lok}} = g(n, \sigma_0, \sigma_1, \sigma_2, \dots). \tag{7}$$

The zeroth deviation is 1 while the first is 0, so the dominant dependence of n_{lok} is on the second (standard) deviation. Consequently, from Eqs. (2), (3) and (5)

$$\sigma_2 + \langle n\rangle\langle n + 1\rangle = \langle (n + 1)g(n, \sigma_2, \dots)\rangle \tag{8}$$

and in 2D ($\langle n\rangle = 6$):

$$\sigma_2 + 42 = \langle (n + 1)g(n, \sigma_2, \dots)\rangle. \tag{9}$$

Let us use the McLauren-expansion of Eq. (8) to first order, then

$$\sigma_2 + \langle n\rangle\langle n + 1\rangle = \langle (n + 1)g(n, 0, \dots, 0, \dots)\rangle + \mu_2 \left\langle (n + 1) \left(\sum_{2\geq i} \left.\frac{\partial g}{\partial \sigma_j}\right|_0 \frac{\sigma_j}{\sigma_2} \right) \right\rangle. \tag{10}$$

Eq. (10) must hold for all values of σ_j so:

$$\langle (n + 1)g(n, 0, \dots, 0, \dots)\rangle = \langle n\rangle\langle n + 1\rangle = 42 \tag{11}$$

and in consequence

$$\left\langle (n + 1) \left(\sum_{2\geq i} \left.\frac{\partial g}{\partial \sigma_j}\right|_0 \frac{\sigma_j}{\sigma_2} \right) \right\rangle = 1 \tag{12}$$

for every j.

Eq. (12) also holds for all σ_j values, therefore

$$\left\langle (n+1)\left.\frac{\partial g}{\partial \sigma_2}\right|_0 \right\rangle = 1. \tag{13}$$

Let us assume a solution of Eqs. (11) and (13) in Aboav–Weaire form:

$$g(n,0,\dots,0,\dots) = A + \frac{B}{n+1}, \qquad \frac{\partial g}{\partial \sigma_2} = C + \frac{D}{n+1} \tag{14}$$

which by Eq. (6)

$$n_{\mathrm{lok}} \cong g(n,0,0,0,\dots) + \left.\frac{\partial g}{\partial \sigma_2}\right|_0 \sigma_2 \cong (A + C\sigma_2) + \frac{B + D\sigma_2}{n+1}. \tag{15}$$

Eq. (15) illustrates the statistical significance of both terms in the n_{lok} function.

In consequence of Eqs. (11) and (13)

$$7A + B = 42, \qquad 7C + D = 1. \tag{16}$$

In 2D when the Euler's rule holds:

$$A = 7 - \alpha, \qquad B = 7(\alpha - 1), \qquad C = \tfrac{1}{6}\beta, \qquad D = 1 - \tfrac{7}{6}\beta.$$

Substituting in Eq. (15) and recognizing that n_{lok} does not depend on moments higher than the second, for simplicity we can write σ instead of σ_2:

$$n_{\mathrm{lok}} \cong 7 - \alpha + \frac{\beta}{6}\sigma + \frac{7\alpha - 7 + (1 - (7\beta/6))\sigma}{n+1} \tag{17}$$

$$M_n = 6 - \alpha + \frac{\beta}{6}\sigma + \frac{6\alpha + (1-\beta)\sigma}{n}. \tag{18}$$

Generally, the equations have four independent parameters, the first and second moments and two fitting parameters (α and β). Parameters α and β weight the moments.

If we substitute

$$a = \alpha - \tfrac{1}{6}\beta\mu \tag{19}$$

we derive the well-known Aboav–Weaire law

$$M_n = 6 - a + \frac{6a + \sigma}{n}. \tag{20}$$

The law derives from the probability distribution function only. Remarkably, the independent probability distribution function parameters α and β connected.

After rearranging Eq. (20):

$$M_n = 6 + \frac{\sigma}{n} - \left(1 - \frac{6}{n}\right) a = 6 + \frac{\sigma}{n} - \left(\frac{a}{n}\delta_n\right), \tag{21}$$

M_n depends only on the first two moments of the actual distribution function, while a/n parameterizes the fit by the deviation from the average ($\delta_n = n - \langle n\rangle = n - 6$). Consequently, those cellular networks which have distribution functions identical in their

first two moments define the same Aboav–Weaire function. A further consequence is that every actual Aboav–Weaire function directly connects to a normal (Gaussian) distribution, which defined only by its two momenta. However, not every Aboav–Weaire law distribution is Gaussian. The a-parameter in the Aboav–Weaire law fits the actual distribution and causes deviation from the corresponding two-parameter Gaussian distribution.

4. Elementary transformations

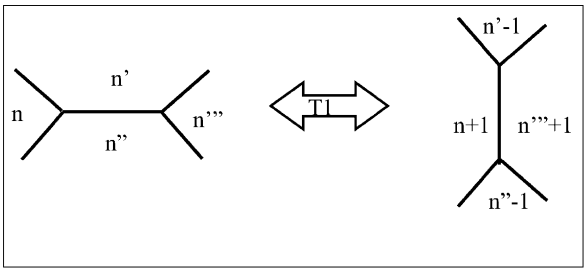
n_{lok} and nM_n are invariant under some elementary topological transformations (T1) [6]. (Meaning that the two first moments of the distribution function are invariant.) These transformations are microscopic, their symmetries and properties alone cannot describe the system.

One elementary topological transformation is neighbor switching (Fig. 1) [6], rearranging the edges of a cluster, keeping the total edge-number constant.

Study the effect of a T1 on the Aboav–Weaire law. Hence, before the transformation:

$$nM_n = n' + n'' + \text{SON} = (6 - \alpha + \tfrac{1}{6}\beta\sigma)n + 6\alpha + (1 - \beta)\sigma \tag{22}$$

(a)



(b)

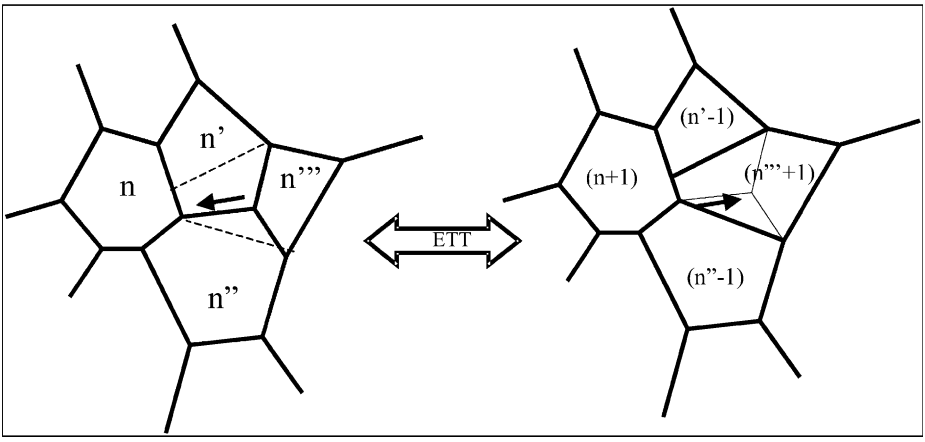


Fig. 1. Neighbor switching (T1): (a) concept and (b) example.

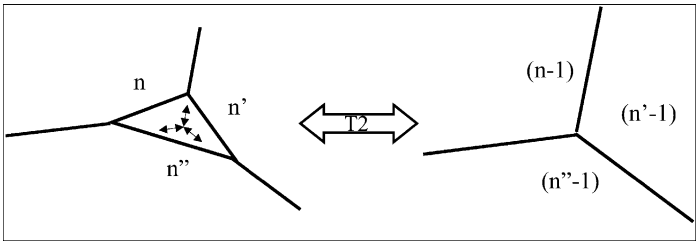


Fig. 2. Formation and disappearance of a three-sided cell.

after the transformation:

$$(n+1)M_{n+1} = (n' - 1) + (n'' - 1) + (n''' + 1) + \text{SON} = (6 - \alpha + \tfrac{1}{6}\beta\sigma)(n+1) + 6\alpha + (1-\beta)\sigma, \tag{23}$$

where SON means the untransformed edges of the other neighbors of an n-sided cell.

Consequently,

$$6 - \alpha + \tfrac{1}{6}\beta\sigma = n''' - 1. \tag{24}$$

Averaging assuming of the non-correlated next-neighbors:

$$6 - \alpha + \tfrac{1}{6}\beta\sigma = \langle n''' \rangle - 1 = 5. \tag{25}$$

Hence

$$nM_n = 5n + (6 + \sigma) \tag{26}$$

which corresponds to the $\alpha = 1$ and $\beta = 0$ ($a = 1$) case.

A slightly more complex transformation connects to three-, four- and five-sided polygons, shown in Figs. 2–4. (These are "breathing" like distortions in the cellular cluster.)

In the three-sided case, before the transformation:

$$nM_n = n' + n'' + 3 + \text{SON} = (6 - \alpha + \tfrac{1}{6}\beta\sigma)n + 6\alpha + (1-\beta)\sigma \tag{27}$$

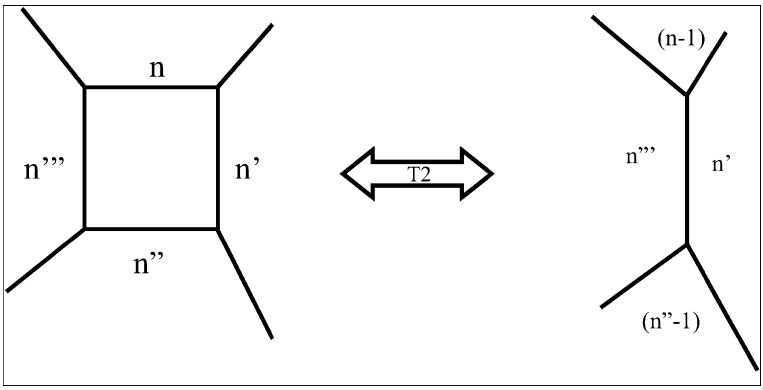


Fig. 3. Formation and disappearance of a four-sided cell.

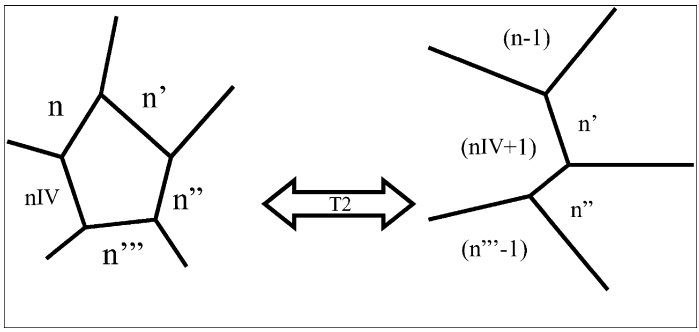


Fig. 4. Formation and disappearance of a five-sided cell.

and after

$$(n-1)M_{n-1} = (n'-1) + (n''-1) + \text{SON} = (6 - \alpha + \tfrac{1}{6}\beta\sigma)(n-1) + 6\alpha + (1-\beta)\sigma. \tag{28}$$

Consequently,

$$6 - \alpha + \tfrac{1}{6}\beta\sigma = 5 \tag{29}$$

which is identical to the T1 case.

We apply the method to cells with *xxx*. In the four-sided case:

$$nM_n = n' + n''' + 4 + \text{SON} = (6 - \alpha + \tfrac{1}{6}\beta\sigma)n + 6\alpha + (1-\beta)\sigma \tag{30}$$

and

$$(n-1)M_{n-1} = n' + n''' + \text{SON} = (6 - \alpha + \tfrac{1}{6}\beta\sigma)(n-1) + 6\alpha + (1-\beta)\sigma \tag{31}$$

so

$$6 - \alpha + \tfrac{1}{6}\beta\sigma = 4 \quad (\alpha = 2, \beta = 0 \Rightarrow a = 2). \tag{32}$$

In the five-sided case:

$$nM_n = n' + n^{\text{iv}} + 5 + \text{SON} = (6 - \alpha + \tfrac{1}{6}\beta\sigma)n + 6\alpha + (1-\beta)\sigma \tag{33}$$

and

$$(n-1)M_{n-1} = n' + n^{\text{iv}} + 1 + \text{SON} = (6 - \alpha + \tfrac{1}{6}\beta\sigma)(n+1) + 6\alpha + (1-\beta)\sigma \tag{34}$$

so

$$6 - \alpha + \tfrac{1}{6}\beta\sigma = 4 \tag{35}$$

which is identical to the previous result.

The corresponding Aboav–Weaire law is

$$nM_n = 4n + (12 + \sigma).$$

In these calculations the averaging assumed uncorrelated next-neighbors. However, the cells with more edges have more possibility to connect to their next-neighbor, so we use weighting:

$$\langle n''' \rangle = \frac{\sum_n n^2 P(n)}{\sum_n nP(n)} = 6 + \frac{\sigma}{6} \tag{36}$$

hence

$(6 - \alpha + (\beta\sigma/6)) = 5 + (\sigma/6)$ ($a = 1 - (\sigma/6)$) and $(6 - \alpha + (\beta\sigma/6)) = 4 + (\sigma/6)$ ($a = 2 - (\sigma/6)$). The corresponding Aboav functions are:

$$nM_n = (5 + \tfrac{1}{6}\sigma)n + 6 \quad (\alpha = 1 \text{ and } \beta = 1) \tag{37}$$

and

$$nM_n = (4 + \tfrac{1}{6}\sigma)n + 12 \quad (\alpha = 2 \text{ and } \beta = 1), \tag{38}$$

respectively.

The allowed topological changes in various clusters a given n-sided cell define the microscopic behavior of the network, so we can call these functions microscopic Aboav functions (Table 1).

The difference in both cases between the first and second coordination number interactions is $((\sigma/n) - (\sigma/6) = -(\sigma\delta_n/6n))$.

Many microscopic topological transformations exist. Let us denote their number by N_T. The number of n-sided cells, which are involved in the jth microscopic reversible topological transformation is $N_{\mathrm{T}j}$ and the ratio of such cells is

$$p^{(j)} = \frac{N_{\mathrm{T}j}}{N_n}. \tag{39}$$

The actual Aboav function for this transformation is

$$M_n n^{(j)} = E^{(j)} n + F^{(j)}, \tag{40}$$

Table 1
Special cases of the Aboav–Weaire function

Case	Parameters	Actual microscopic Aboav–Weaire law
$a = 1$	$\alpha = 1, \beta = 0$	$M_n = 5 + \dfrac{6+\sigma}{n}$
$a = 1 - \frac{1}{6}\sigma$	$\alpha = 1, \beta = 1$	$M_n = 5 + \dfrac{\sigma}{6} + \dfrac{6}{n}$
$a = 2$	$\alpha = 2, \beta = 0$	$M_n = 4 + \dfrac{12+\sigma}{n}$
$a = 2 - \frac{1}{6}\sigma$	$\alpha = 2, \beta = 1$	$M_n = 4 + \dfrac{\sigma}{6} + \dfrac{12}{n}$

where

$$E^{(j)} = \langle n \rangle - a^{(j)} \tag{41}$$

and

$$F^{(j)} = \langle n \rangle a^{(j)} + \sigma^{(j)}. \tag{42}$$

Taking into account all the possible microscopic transformations:

$$M_n n = \sum_{j=1}^{N_T} p^{(j)} M_n n^{(j)} = n \sum_{j=1}^{N_T} p^{(j)} E^{(j)} + \sum_{j=1}^{N_T} p^{(j)} F^{(j)} = nE + F, \tag{43}$$

where

$$E = \langle n \rangle - a = \sum_{j=1}^{N_T} p^{(j)} E^{(j)} \tag{44}$$

and

$$F = \langle n \rangle a + \sigma = \sum_{j=1}^{N_T} p^{(j)} F^{(j)}. \tag{45}$$

This is the macroscopic Aboav law, with parameters averages of the distribution-functions of microscopic topological transformations.

5. Equilibrium states

If the potential energy (interaction) of the cells is not negligible, the cells can relax toward to equilibrium [14]. This case was investigated by computer simulation [14], fol-

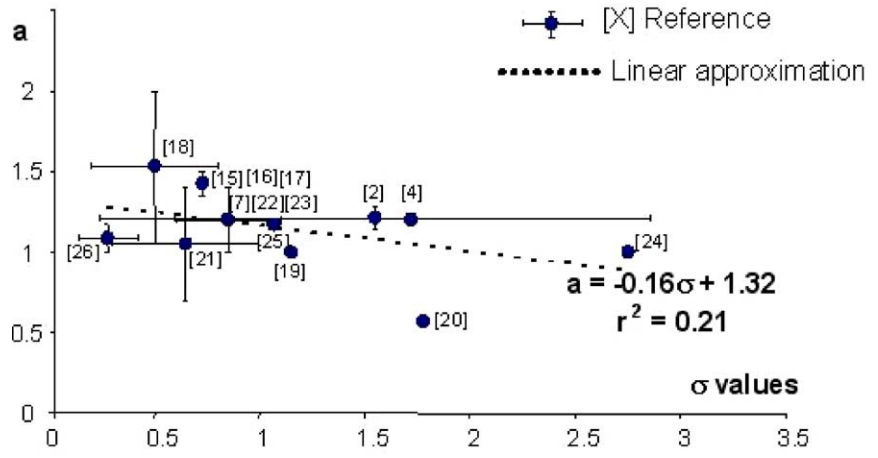


Fig. 5. The parameter a versus parameter σ from the literature [2,4,7,15–26].

lowed the entirely random system in its relaxation to equilibrium due to the switched on interaction.

In the relaxed cellular structures the pattern is near to the honeycomb lattice, and $n \to 6$ consequently

$$M_n \to 6 + \tfrac{1}{6}\sigma. \tag{46}$$

However, as we see from the micro-transformations, far from equilibrium the parameter a depends on σ forming a linear function with slope $-1/6$.

Collect the data from the literature on various cellular systems, the parameter a versus parameter σ is linear, with a best-fit slope of (1/6.3) (Fig. 5). Note that the intersection at the y-axis is larger than 1, indicating the existence of the four and higher folded transformations.

6. Conclusion

This paper derived the Aboav–Weaire law using very general constitutive assumptions. Every probability distribution function with identical first and second moments connects the equivalent Aboav–Weaire law. Consequently, in every random cellular network the distribution of the cells is not entirely random. In general, a deviation from mean six does not depend on only the second moment. Therefore, there could exist such "old" patterns, where the large cells are surrounded only by five-fold polygons. We presented, that the Aboav–Weaire law could be directly derived from the microscopic topological transformations.

It could be such case as well, when the local average is independent from the edge-number of cells. In this case, the second moment alone determines the deviation of the number of sides from five.

Appendix A

Theorem. *In every case, when the $P(n^*)$ probability density function has the form*:

$$\int_{-\infty}^{\infty} f(n^*)\, P(n^*)\, \mathrm{d}n^*, \tag{A.1}$$

it can be represented as:

$$P(n^*) = \sum_{i=0}^{\infty} \frac{(-1)^i}{i!} \sigma_i \delta^{(i)}(n^* - 6), \tag{A.2}$$

where $\delta^{(i)}$ is the ith derivative of the δ Dirac delta-distribution, and

$$\sigma_i = \int_{-\infty}^{\infty} (n^* - 6)^i\, P(n^*)\, \mathrm{d}n^* \tag{A.3}$$

is its ith moment. We know $\sigma_0 = 1$ and $\sigma_1 = 0$.

Use the Taylor expansion of $f(n^*)$ *in* Eq. (A.1) *at* $n^* = 6$ *and use the identity*:

$$\int_{-\infty}^{\infty} f(n^*)\delta^{(i)}(n^* - 6)\,\mathrm{d}n^* = (-1)^i f^{(i)}(n^* = 6). \tag{A.4}$$

Thus

$$\begin{aligned}\int_{-\infty}^{\infty} f(n^*)\,P(n^*)\,\mathrm{d}n^* &= \sum_{i=0}^{\infty}\frac{1}{i!}f^{(i)}(n^* = 6)\int_{-\infty}^{\infty}(n^* - 6)^i P(n^*)\,\mathrm{d}n^* \\ &= \sum_{i=0}^{\infty}\frac{1}{i!}f^{(i)}(n^* = 6)\sigma_i = \int_{-\infty}^{\infty} f(n^*)\sum_{i=0}^{\infty}\frac{(-1)^i}{i!}\sigma_i\delta^{(i)}(n^* - 6)\,\mathrm{d}n^*\end{aligned} \tag{A.5}$$

which proves the theorem.

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