

Topological correlations and asymptotic freedom in cellular aggregates

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Abstract

In random cellular systems, both observation and maximum entropy inference give a specific form to the topological pair correlation: it is bi-affine in the cells number of edges with coefficients depending on the distance between the two cells of the pair. Assuming this form for the pair correlations, we make explicit the conditions of statistical independence at large distance. When, on average, the defects do not contribute, the layer population and the enclosed topological charge both increase polynomially with distance. In dimension 2, the exponent of the leading terms depend on sum rules satisfied, or not, by the maximum entropy coefficients.

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1. Introduction

Foams are random but the precise probability distributions describing their structure are still largely unknown. Leaving aside the geometrical and energetic details, obviously dependent on the system considered, we focus on the topological characteristics, believed to be more universal. Only a few investigations have been devoted to correlations beyond nearest neighbours. Pair correlations at arbitrary distance were analysed by Fortes–Pina [1], Rivier et al. [2,3], Szeto et al. [4], and measured in Ref. [4].

Maximum entropy is one of the few methods able to predict some aspects of the probability distributions. Maximum entropy (maxent) arguments yield a specific form for the pair correlations at arbitrary distance [2,5].

Here, we examine the asymptotic behaviour of pair correlations and how the independence of occurrences at large distances constrains the parameters in the maxent formulae.

The present analysis is mostly devoted to bi-dimensional foams, subject to extensive theoretical and experimental investigations [1–21], and where the progresses are ahead of those on 3D foams.

2. Foam statistics

A foam \mathcal{F} divides space into $N = |\mathcal{F}|$ polygonal cells. Here \mathcal{F} is viewed as a set of cells and $|\mathcal{F}|$ represents the number of elements in the set.

2.1. One cell statistics

The local observable is n , the number of sides of each cell (“polygonality”), or the topological charge $q = 6 - n$. The fraction of n -sided cells is $p(n) = N(n)/N$.

The generic and physically stable vertex coordination (or degree) is $z = 3$. Euler’s theorem implies:

$$\langle q \rangle = \langle 6 - n \rangle = \sum_n (6 - n) p(n) = \frac{6\chi}{N} \quad (1)$$

where χ characterises the embedding space: $\chi = 2$ for the sphere, 0 for the torus.²

In the large N limit, $\langle q \rangle \rightarrow 0$. The second moment is $\mu_2 = \langle q^2 \rangle = \langle (n - 6)^2 \rangle$.

² As stated here, Eq. (1) only holds if the foam fills the 2D space, without boundary. Otherwise, the edges on the boundary must be counted only once in $\langle n \rangle N = 2E - E_{\text{boundary}}$, implying an additional boundary term in (1)[21]. E is the total number of edges, internal and on the boundary. In particular, this is so for a bounded cluster in the plane, where $\chi = 1$. In any reasonable case, $\langle q \rangle = \langle 6 - n \rangle \rightarrow 0$ as $N \rightarrow \infty$.

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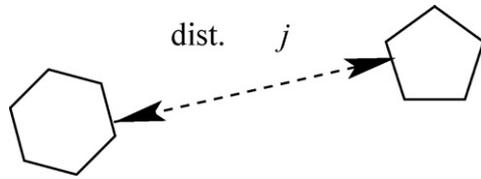


Fig. 1. A pair of cells, $(k, n) = (6, 5)$, at distance j .

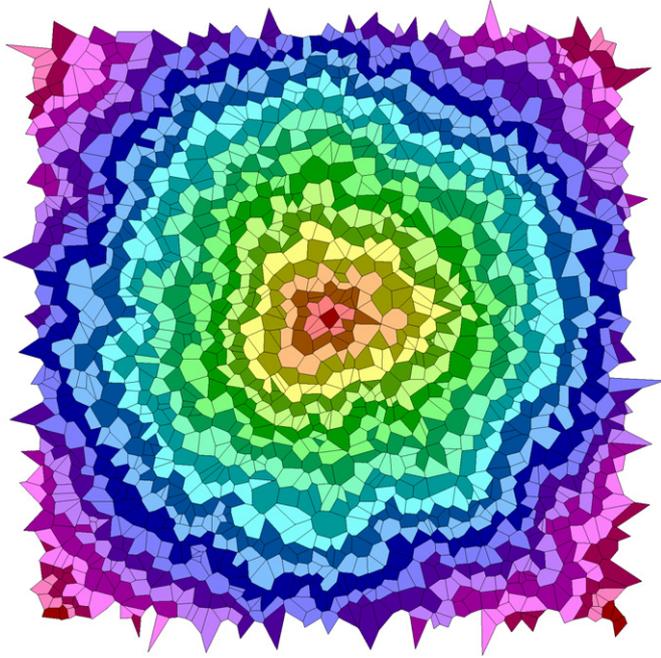


Fig. 2. Stratification of a Poisson–Voronoi froth into layers.

2.2. Two cells, correlations

The topological distance j between cells is measured in nearest neighbour steps (Fig. 1). The j th layer around a given cell o , $\text{lay}(j|o)$, is the set of cells at distance j from o (Fig. 2). It has population $K_j(o) = |\text{lay}(j|o)|$. The average over n -sided central cells is $\langle K_j(n) \rangle$ and the overall average is $\langle\langle K_j \rangle\rangle$.

The joint distribution $p_j^{(2)}(k, n)$ – the probability that a (k, n) -sided pair of cells occur at mutual distance j – and the corresponding marginal distribution $s_j(n) = \sum_k p_j^{(2)}(k, n)$ – the probability that a cell is at distance j from an n -sided one³ – satisfy $s_j(n) = \langle\langle K_j(n) \rangle\rangle / \langle\langle K_j \rangle\rangle p(n)$.

The correlator $A_j(k, n)$ and correlation function $g_j(k, n)$ are defined by

$$p_j^{(2)}(k, n) = A_j(k, n) \frac{p(k) p(n)}{\langle\langle K_j \rangle\rangle}, \quad (2)$$

$$p_j^{(2)}(k, n) = g_j(k, n) s_j(k) s_j(n). \quad (3)$$

Both account for the statistical dependence of the concurrent occurrence of a k and a n -sided cell at distance j . They only dif-

fer in the way they are normalised: the correlation function is 1 whereas the correlator is the mean population $\langle\langle K_j \rangle\rangle$ in independent situations. The correlator is related to the layer population by [1,2]:

$$\sum_k p(k) A_j(k, n) = \langle K_j(n) \rangle. \quad (4)$$

A similar identity follows from counting the edges ('polygonality' P_j of layer j) [1]:

$$\sum_k k p(k) A_j(k, n) = \langle P_j(n) \rangle. \quad (5)$$

The polygonality of a set is the sum of the individual polygonalities n . Because charges are additive, and simply related to n by $q = 6 - n$, it is more natural to consider the total charge⁴ of layer j , $Q(\text{lay}(j|o)) = 6K_j(o) - P_j(o)$. Here we are getting closer to Ref. [2]. Then averaging over n -sided central cells o yields, according to (4) and (5):

$$\langle Q(\text{lay}(j|n)) \rangle = \sum_k (6 - k) p(k) A_j(k, n). \quad (6)$$

3. Maximum entropy

Maximum entropy arguments (maxent) and the recursion relation to be described in Section 5 give the following expressions, also observed in numerical simulations [2]:

$$A_j(k, n) = \sigma_j(k - 6)(n - 6) + a_j(n + k - 12) + b_j, \quad (7)$$

$$\langle K_j(n) \rangle = a_j(n - 6) + b_j, \quad (8)$$

σ_j, a_j, b_j are real parameters for $j = 1, 2, \dots$. The contributions from defects have been neglected. In the infinite foam limit, the average of (8) gives $\langle\langle K_j \rangle\rangle = b_j$.

4. Asymptotic freedom

In normal systems of statistical physics, spatially distant events become uncorrelated. In foams, this was first measured by [4]. As $j \rightarrow \infty$:

$$p_j^{(2)}(k, n) \rightarrow s_j(k) s_j(n) \Leftrightarrow g_j(k, n) \rightarrow 1. \quad (9)$$

With

$$g_j(k, n) = \frac{A_j(k, n) \langle\langle K_j \rangle\rangle}{\langle K_j(k) \rangle \langle K_j(n) \rangle}, \quad (10)$$

$$g_j(k, n) = 1 + \left(\frac{\sigma_j}{b_j} - \left(\frac{a_j}{b_j} \right)^2 \right) (k - 6)(n - 6) \quad (11)$$

and maxent, asymptotic de-correlation holds if and only if

$$\frac{\sigma_j}{b_j} - \left(\frac{a_j}{b_j} \right)^2 \rightarrow 0. \quad (12)$$

³ This is also the probability that an n -sided cell is at distance j from another one.

⁴ The charge of a set of cells is the sum of the individual charges $q = 6 - n$.

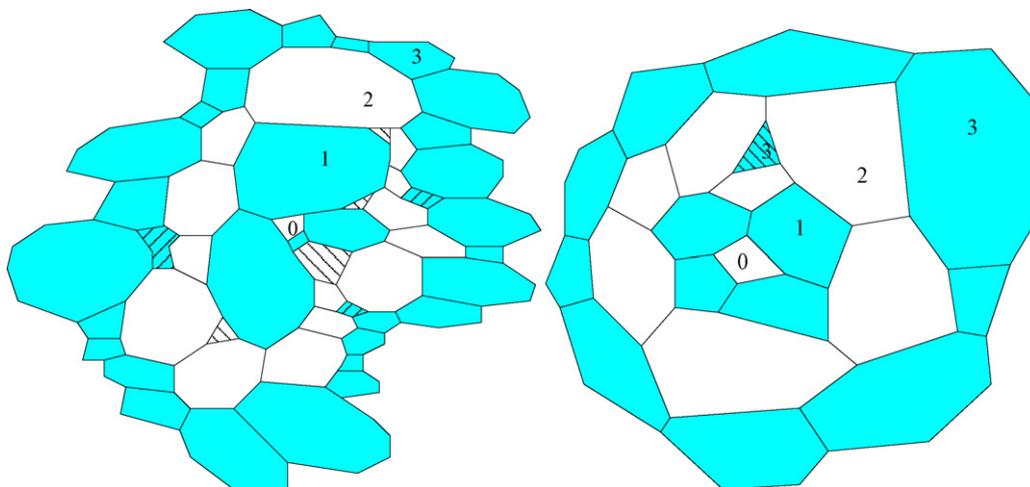


Fig. 3. Defects (left) and an inclusion (right), marked hatched.

A sufficient condition is that the ratios $\sigma_j/b_j \rightarrow 0$ and $a_j/b_j \rightarrow 0$, meaning that, in both A_j and K_j , the n dependent terms would be dominated by the constant one (b_j) at large j , a sensible result. In this limit, (8) implies $\langle K_j(n) \rangle \rightarrow \langle \langle K_j \rangle \rangle$ and then $s_j(n) \rightarrow p(n)$; the effect of the central condition vanishes, another manifestation of asymptotic de-correlation. In (9), s_j can then be replaced by p .

5. Recursion equation

The following equation was derived in Ref. [1] and in Refs. [2,22]:

$$\Delta \langle K_j(n) \rangle + \langle q_j(n) \rangle \langle K_j(n) \rangle = \langle I_j(n) \rangle \simeq 0. \quad (13)$$

The curly bracket quantities $\langle q_j(n) \rangle$ (resp. $\langle m_j(n) \rangle$) are the cellular charge (resp. sidedness) averaged over the neighbours at topological distance j to an n -side cell. They are defined by $\langle q_j(n) \rangle = 6 - \langle m_j(n) \rangle = \langle Q(\text{lay}(j|n)) \rangle / \langle K_j(n) \rangle$. $\Delta K_j = K_{j+1} - 2K_j + K_{j-1}$ is the discrete laplacian.

The right hand side is due to the presence of defects, the cells of layer j which have no edge in common with the next layer, $j + 1$ (Fig. 3). It is assumed that, on average, this contribution vanishes: $\langle I_j(n) \rangle = 0$.

Using (6) for the total charge $\langle Q(\text{lay}(j|n)) \rangle = \langle q_j(n) \rangle \langle K_j(n) \rangle$ allows to put the recursion relation (13) in the following form:

$$\Delta \langle K_j(n) \rangle = \sum_k (k - 6) p(k) A_j(k, n). \quad (14)$$

6. Asymptotic behaviour and sum rules

With the maxent form (7) and (8) of the correlator $A_j(k, n)$ and population $\langle K_j(n) \rangle$, the recursion relation implies the following system, with $\alpha_j = a_j$ and $\beta_j = b_j - 6a_j$:

$$\Delta \begin{pmatrix} \alpha_j \\ \beta_j \end{pmatrix} = \mu_2 \begin{pmatrix} \sigma_j \\ \alpha_j - 6\sigma_j \end{pmatrix}, \quad (15)$$

$$\begin{pmatrix} \alpha_0 \\ \beta_0 \end{pmatrix} = 0, \quad \begin{pmatrix} \alpha_1 \\ \beta_1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix}. \quad (16)$$

The initial conditions follow from $\langle K_0(n) \rangle = 0$ and $\langle K_1(n) \rangle = n$; μ_2 was defined in Section 2.1.

The solutions involve $f_k = -\mu_2 \sigma_k$, conjectured to decrease fast at large k . Then, $\sum_{k=1}^{j-1} f_k \rightarrow S$ as $j \rightarrow \infty$, so that f/S defines a normalised distribution (like probabilities except that some f_k may be negative). Let M_n be the moments of this distribution:

$$S = \sum_{k \geq 1} f_k, \quad M_n = \frac{1}{S} \sum_{k \geq 1} k^n f_k. \quad (17)$$

The solutions to (15) and (16) are

$$\alpha_j = \sum_{k=1}^{j-1} k f_k + j \left(1 - \sum_{k=1}^{j-1} f_k \right), \quad (18)$$

$$\beta_j = \frac{\mu_2}{6} \left[(j+1)j(j-1) \left(1 - \sum f_k \right) + (3j^2 - 1) \sum k f_k - 3j \sum k^2 f_k + \sum k^3 f_k \right] + 6 \sum (j-k) f_k \quad (19)$$

where the sums run from $k = 1$ to $j - 1$. As $j \rightarrow \infty$, they behave like

$$\alpha_j \rightarrow j(1 - S) + S M_1, \quad (20)$$

$$\beta_j \rightarrow \frac{\mu_2}{6} S [(j+1)j(j-1)(1/S - 1) + (3j^2 - 1)M_1 - 3jM_2 + M_3] + 6S(j - M_1). \quad (21)$$

The leading order will be lower if the $\{f_k = -\mu_2 \sigma_k\}$ satisfy certain sum rules. Indeed, if $S = 1$, the estimates become

$$\alpha_j \rightarrow M_1 \quad (22)$$

$$\beta_j \rightarrow \frac{\mu_2}{6} [(3j^2 - 1)M_1 - 3jM_2 + M_3] + 6(j - M_1), \quad (23)$$

so that the average population $\langle K_j(n) \rangle$ would not grow faster than j^2 .

The so-called Euclidean scaling [3,23], $\langle K_j(n) \rangle \sim j$ in 2D, requires a second condition:

$$M_1 = -\mu_2 \sum_{k \geq 1} k \sigma_k = 0.$$

7. Topological charge

The purpose of this section is to relate the moments S and M_k to the average charge contained in a ball or in a layer. It does not enforce the precise values found in the previous section, as we first hoped; but it shows that the sum rules and asymptotes, for charges and populations, are compatible.

7.1. Charge enclosed in a ball

Let $B_j(o)$ be the union of the cells at distance at most j from an arbitrarily chosen cell o . The total charge enclosed in the cluster $B_j(o)$ satisfies, averaging over n -sided origins o :

$$\begin{aligned} \langle Q(B_j(n)) \rangle &= \left(6 - n - \mu_2 \frac{j(j+1)}{2} \right) \left[1 - \sum_{k=1}^j f_k \right] \\ &+ \frac{\mu_2}{2} \left[\sum_{k=1}^j k^2 f_k - (2j+1) \sum_{k=1}^j k f_k \right]. \end{aligned} \quad (24)$$

This expression follows from inserting the solutions α_j, β_j into (7) and (8) and either summing the layer charges (6) from 0 to j or integrating the difference equation (13). It is consistent with (21). Indeed, if the individual charges are normal random variables, averaging to zero by Euler equation (1), their sum should behave like fluctuations:

$$|\langle Q(B_j(n)) \rangle| \leq \text{const} \langle |B_j(n)| \rangle^{1/2}. \quad (25)$$

Now, if $S \neq 1$, the population $\langle |B_j(n)| \rangle \propto \sum_{l=0}^j \langle K_l(n) \rangle \sim j^4$ and $\langle Q(B_j(n)) \rangle \sim j^2$, as in (24) without further condition.

If, on the other hand, the charge fluctuations are less, $\langle Q(B_j(n)) \rangle = o(j^2)$, then $S = 1$ must hold, predicting a layer population $\sim j^2$, according to (23).

A possible interpretation of $S = 1$ can be deduced from (24). Define the average $\langle \langle Q_j \rangle \rangle = \sum_n p(n) \langle Q(B_j(n)) \rangle$. It coincides with the mean charge of a ball centred at a neutral cell: $\langle Q(B_j(6)) \rangle$. Then, using (24), we can calculate the mean excess charge in the ball due to conditioning on n -sided central cells:

$$\langle Q(B_j(n)) \rangle - \langle \langle Q_j \rangle \rangle = (6 - n) \left[1 - \sum_{k=1}^j f_k \right]. \quad (26)$$

As $j \rightarrow \infty$, this excess charge becomes $(6 - n)(1 - S)$; then $S = 1$ means global neutrality: the central charge $q = 6 - n$ is exactly screened by the excess charge $(6 - n)S$ in the layers around.

7.2. Layer charge and Aboav–Weaire’s law

Inserting the maxent formula (8) for $\langle K_j(n) \rangle$ into (13) and using (15) gives an expression for the average charge in layer j :

$$\langle Q(\text{lay}(j|n)) \rangle = (n - 6)f_j - \mu_2 \alpha_j, \quad (27)$$

or, dividing by the mean layer population:

$$\langle q_j(n) \rangle = \frac{\langle Q(\text{lay}(j|n)) \rangle}{\langle K_j(n) \rangle} = \frac{(n - 6)f_j - \mu_2 \alpha_j}{\alpha_j n + \beta_j}. \quad (28)$$

This is a fractional linear function of n as in Aboav–Weaire’s law [24], which is in fact the first case, $j = 1$, of this sequence labelled by j . Because double contacts are negligible in foams, the first layer population is just the number of sides of the central cell: $K_1(n) = \langle K_1(n) \rangle = n$ and $\langle q_1(n) \rangle = \langle q_1(n) \rangle = 6 - \langle m_1(n) \rangle$, where $\langle m_1(n) \rangle$ is the mean number of sides (the polygonality) of the first neighbours of n -sided cells. So, with (16), Eq. (28) for $j = 1$ specialises to

$$\langle q_1(n) \rangle = \frac{(n - 6)f_1 - \mu_2}{n} = f_1 - \frac{6f_1 + \mu_2}{n}. \quad (29)$$

Compared to the usual form of Aboav–Weaire’s law [24,25]: $\langle m_1(n) \rangle = 6 - a + (6a + \mu_2)/n$, Eq. (29) gives an interpretation of the parameter a as the n k coefficient in the pair correlator: $a = f_1 = -\mu_2 \sigma_1$.

8. Conclusion

To summarise, the major part of this article is a brief review of what is known, so far, on correlations in foams beyond first neighbours. This includes the definitions and sum rules in Section 2, the (bi)affine form of the correlations in Section 3, the recursion equation in Section 5 and the solutions in Section 6. Except for the affine ansatz, controversially [25] justified by maximum entropy arguments [2,5], and the related hypothesis that defects do not contribute on average, which we assumed from the start, our purpose has been to restrain approximations or ad hoc substitutions to a minimum. Some approximations (factorisations, etc.) give interesting perspectives and will be treated in an other article [26].

The new results are mainly contained in Sections 4, 6 and 7. First, we have shown that the maxent affine ansatz is compatible with asymptotic freedom, and how the correlation decay affects the affine coefficients.

Next, the decay of the correlations, or the rate of increase of the layer populations, at large distance are tightly related to sum rules for the coefficients σ_j in Eq. (7), specifying the screening of (topological) charges. Charge neutrality means that a given charge is surrounded by a cloud of total opposite charge. In electrostatics, charge neutrality results from energy bounds and shielding the long range Coulomb field. This strong Debye screening implies subnormal charge fluctuations [27].

In foams, as far as we can see, no electric field constrains the topological charge. Global neutrality is a consequence of Euler equation (1). Neutrality seems also true at an intermediate scale. The charge fluctuations result from a strange compromise

between statistical disorder and geometrical constraints [28]. In Section 6, the order of the asymptotic polynomial behaviour of the layer population is related to specific sum rules satisfied by the correlation coefficients. In turn, these sum rules command the overall charge (fluctuations) in large domains.

The conclusion is that both populations and charges are consistently related. The next question is what do we need to get more precise, or more predictive, estimates.

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