Topological Correlations in Cellular Structures and Planar Graph Theory

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We study the topological properties of the ensemble of cells with trivalent vertices in the plane. The problem is equivalent to counting planar Feynman diagrams with a cubic interaction. This ensemble is also the equilibrium state of a topological model of cellular structure, obtained by applying repetitively a topological flip transformation to any initial configuration of cells with trivalent vertices. We give analytical expressions for two-cell correlations; in particular, we give the analytical form of the average number $m(n)$ of edges of cells adjacent to an n-sided cell. These results are confirmed by simulations.

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One finds many examples of random cellular structures in everyday life. Bones, wood, cork, foams, plants, food (bread, meringue, etc.), and soap froth, as a whole or partially, are cellular materials [1]. Since cellular structures exist on scales ranging from microscopic to geological, much work has been devoted to the search for universal geometrical characteristics. For instance, leaving aside their metric properties (e.g., sizes of cells), it is important to understand whether cellular structures obey some universal topological laws. It is therefore natural to study the probability distribution P_n of the number n of edges of a given cell, or correlations between the numbers of edges of adjacent cells. For example, Aboav noted a simple correlation between the number of edges n of a given cell and the average number of edges $m(n)$ of its n neighbors [2,3]: In all known cellular structures it is indeed usually found that $nm(n)$ is, to a very good approximation, linear in n.

In this Letter we present an analytical study of these correlations in the case of a very simple, purely topological model of cellular structure. We give the two-cell probability distribution Q_{ln} of finding an l-cell adjacent to a n-cell; we find also the exact form for the average total number of edges of cells adjacent to an n-sided cell:

$$nm(n)=7n+3+9/(n+1)\,. \tag{1}$$

Hence Aboav's law, stating that this quantity should be linear in n, is slightly violated. These results are in complete agreement with our numerical simulations.

We consider the following model. Starting from any configuration of $N+2$ cells with trivalent vertices (three edges meet at a vertex), one chooses randomly an edge between two cells and applies a topological transformation T_1 (cf. Fig. 1). Each configuration of cells generated in this way corresponds to a planar Feynman diagram of a ϕ^3 field theory with a fixed number of vertices. Such a process is ergodic, since any two graphs of fixed number of vertices may be related to each other through a sequence of transformations [4]; furthermore it is easy to show that it satisfies detailed balance. Hence, iterating this transformation leads to an equilibrium state. The ensemble of configurations thus obtained is also the ensemble of planar ϕ^3 diagrams with $2N$ vertices. We restrict the present study to a variant of this model where the class of diagrams considered does not contain tadpoles or self-energy parts; i.e., one cell cannot touch itself and two cells cannot touch more than once. In other words, T_1 is not applied to an edge such that cells c and d in Fig. 1 are already adjacent; in particular it is not applied to an edge belonging to a three-sided cell.

Consider a configuration of $N+2$ cells, labeled by $i=1,\ldots,N+2$, on the surface of a sphere, i.e., a graph G with the topology of the sphere. By the Euler relation one has

$$\mathcal{N}(\text{cells})-\mathcal{N}(\text{edges})+\mathcal{N}(\text{vertices})=2\,. \tag{2}$$

Since $2\mathcal{N}(\text{edges})=3\mathcal{N}(\text{vertices})$, one finds that $\mathcal{N}(\text{vertices})=2N$ and $\mathcal{N}(\text{edges})=3N$. The graph G is entirely described by its adjacency matrix,

$$G_{ij}=\begin{cases}1 & \text{if } i,j \text{ are adjacent,}\\ 0 & \text{otherwise,}\end{cases} \tag{3}$$

normalized such that $\sum_{i,j}G_{ij}=\sum_i n_i=6N$, where n_i is the number of edges of the ith cell.

The statistics of cells and edges—for a particular graph G—is given by the following probability distributions, defined in the thermodynamical limit. The probability distribution of cells with n edges is

$$P_n=\lim_{N\to\infty}\frac{1}{N+2}\sum_j\delta_{n,n_j}=\lim_{N\to\infty}\frac{N_n}{N+2}\,, \tag{4}$$

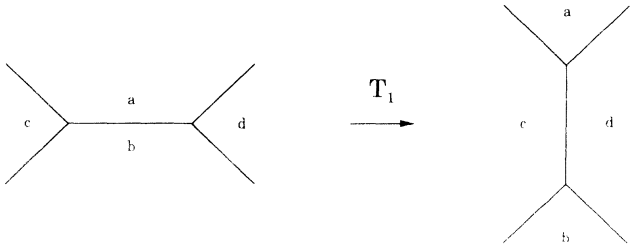

FIG. 1. The topological transformation T_1.

where N_n is the number of cells with n edges. P_n is normalized such that $\sum_n P_n = 1$ and $\sum_n nP_n = 6$. The probability of finding an edge common to two neighboring cells with numbers of edges l and n is defined as

$$Q_{ln} = \lim_{N\to\infty} \frac{1}{6N} \sum_{i,j} G_{ij}\delta_{l,n_i}\delta_{n,n_j} = \lim_{N\to\infty} \frac{N_{ln}}{6N}, \tag{5}$$

where N_{ln} is the number of such edges. Note that each edge is counted twice. Q_{ln} is normalized such that $\sum_l Q_{ln} \equiv Q_n = nP_n/6$ and $\sum_{l,n} Q_{ln} = 1$. Q_n is the probability of finding an edge belonging to a cell with n edges. The quantity $m(n)$ introduced above is the conditional expectation value,

$$m(n) = \sum_l l \frac{Q_{ln}}{Q_n} = \frac{6}{nP_n} \sum_l lQ_{ln}. \tag{6}$$

Note that if there were no correlations between cells, Q_{ln} would factorize into $Q_l Q_n$, and $m(n)$ would equal $\sum_l lQ_l = \sum_l l^2 P_l/6 = 6 + \mu_2/6$ where $\mu_2 = \sum_n P_n (n-6)^2$.

The probabilities considered hereafter will be obtained from the former ones, by averaging on the ensemble of diagrams with a fixed number of vertices—for simplicity we will keep the same notations for the averages. This implies attributing weights to each particular diagram.

The counting problem for planar diagrams has been well studied in the past [5]. Using these techniques, the authors of Ref. [4] have computed the probability distribution P_n. The calculation of Q_{ln}, sketched below, is in the same spirit, though more complicated. Consider the generating function $Z(g)$ for the number of connected planar graphs:

$$Z(g) = \sum_G \frac{1}{k(G)} g^{2N(G)} = \sum_{N=1}^{\infty} Z_{2N} g^{2N}. \tag{7}$$

Z_{2N} counts the number of (vacuum) graphs with $2N$ vertices, weighted by their symmetry factors. We define the quantities

$$Z_{ln}(g) = \sum_G \frac{N_{ln}(G)}{k(G)} g^{2N(G)} = \sum_{N=1}^{\infty} Z_{ln,2N} g^{2N}. \tag{8}$$

$Z_{ln,2N}$ counts, on the average, the number of edges of two adjacent l- and n-cells for graphs with $2N$ vertices. They are thus simply related to the probabilities Q_{ln}. In Fig. 2(a) such an edge is marked. By inversion one obtains a topologically equivalent graph; one may then decompose the rest of the graph into connected pieces, as illustrated by Fig. 2(b). This permits us to express $Z_{ln}(g)$ in terms of the Green functions $W_n(g) = \sum_{G_n} g^{M(G_n)}$, where the sum goes over all connected planar diagrams with n external legs and M vertices, without self-energy parts and tadpoles. Defining the generating functions

$$W(x) = 1 + x^2 + \sum_{n=3}^{\infty} W_n(g) x^n,$$
$$Z(x,y) = \sum_{l,n=2}^{\infty} Z_{ln}(g) x^l y^n, \tag{9}$$

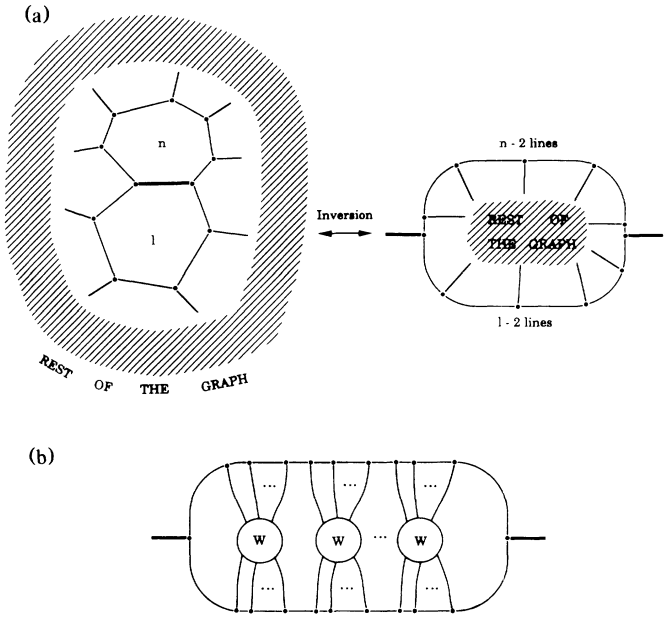

FIG. 2. (a) Representation of a graph with a marked line. (b) Decomposition of the hatched part of (a) into connected Green's functions.

$Z(x,y)$ can be expressed through $W(x)$ as

$$Z(x,y) = \frac{(x-y)(xyg)^2}{xW(yg) - yW(xg)}. \tag{10}$$

Searching the thermodynamical limit $N \to \infty$ of probabilities implies extracting the singular behavior of their generating functions. Around $g^2 = g_c^2 = 3^3/4^4$, the function $W(x)$ behaves as

$$W(x) = W(x)|_{g=g_c} + (g_c^2 - g^2)^{3/2} w(x) + \cdots. \tag{11}$$

Expanding $Z(x,y)$ in $(g^2 - g_c^2)^{3/2}$,

$$Z(x,y) = Z(x,y)|_{g=g_c} + (g_c^2 - g^2)^{3/2} z(x,y) + \cdots, \tag{12}$$

yields the generating function for the probabilities Q_{ln},

$$Q(x,y) = \frac{z(x,y)}{z(1,1)} = \sum_{l,n=2}^{\infty} x^l y^n Q_{ln}. \tag{13}$$

It reads

$$Q(x,y) = \frac{3^3}{4^4} x^2 y^2 (x-y) \frac{yQ(x) - xQ(y)}{[yF_0(x) - xF_0(y)]^2}, \tag{14}$$

where

$$Q(x) = \frac{f(x)}{f(1)} = \frac{1}{2} x \left[1 + \frac{9x-8}{(4-3x)^{3/2}} \right],$$
$$F_0(x) = \tfrac{1}{16} [9x + 8 + (4-3x)^{3/2}]. \tag{15}$$

f and F_0 are related to $W(x)$ by

$$F_0(x)=W(gx)|_{g=g_c},\quad f(x)=w(gx)\,. \tag{16}$$

Note the normalization conditions

$$Q(1,1)=1\,,$$
$$Q(1,x)=Q(x,1)=Q(x)=\sum Q_n x^n=\sum \frac{n}{6}P_n x^n\,, \tag{17}$$

where

$$P_n=16\frac{(n-2)(2n-2)!}{n!(n-1)!}\left(\frac{3}{16}\right)^n. \tag{18}$$

This equation was already given in Ref. [4]. Finally using the fact that

$$\sum_l lQ_{ln}=\frac{1}{n!}\frac{\partial^n}{\partial y^n}\frac{\partial}{\partial x}Q(x,y)\bigg|_{x=1,y=0}$$
$$=\frac{8}{3}(7n^2+10n+12)\frac{(n-2)(2n-2)!}{(n-1)!(n+1)!}\left(\frac{3}{16}\right)^n \tag{19}$$

yields the result for $nm(n)$ given in Eq. (1). Note that $\mu_2=6Q'(1)-36=10.5$.

The Q_{ln} were obtained from Eq. (14) using MATHEMATICA. These probabilities are shown in Fig. 3(a) as functions of n for different values of l. An interesting quantity is Q_{ln}/P_lP_n. In a recent paper [6], it was claimed, on the basis of maximum-entropy arguments, that this quantity should be linear in n for each l, implying the linearity of $nm(n)$. In Fig. 3(b) we show Q_{ln}/P_lP_n as a function of n, for various l. Linearity is seen to be a good approximation for this quantity. For completeness, we show the plots of P_n and $nm(n)$ in Figs. 4(a) and 4(b).

Simulations.—We took as the initial condition a hexagonal network of 400×400 cells, with periodic boundary conditions. At each step, an edge is chosen at random. If this edge fulfills the constraints mentioned above—ensuring that no self-energy parts or tadpoles be generated—the topological transformation T_1 is applied to it. The points with error bars in Figs. 3 and 4 represent the average of Q_{ln}, Q_{ln}/P_lP_n, P_n, and $nm(n)$ at 100 different times, after equilibrium is reached. The error bars give the standard deviations of these quantities. All these numerical data agree perfectly with the analytical curves.

The cellular structure used in the simulations is defined on a torus, whereas the planar approximation uses the topology of the sphere. This is not contradictory since, though the partition function $Z(g)$ depends on the genus of the surface on which the cellular structure is defined, this is not the case for Q_{ln} or P_n which are local properties.

A number of other variants of this problem may be studied. We will present some of them elsewhere; in particular we will give the analytical study of correlations for the ensemble of diagrams with self-energy parts.

Other topological models implementing both the T_1 transformation and the topological transformation T_2 (suppression of triangles) may also be studied (see, e.g., Ref. [6]). In this case, the detailed balance property of the model is lost. Instead of an equilibrium state, a scaling regime is reached through the dynamics. The configurations thus obtained form a subset of all the possible configurations considered in this Letter. Analytical considerations on the correlations should be more difficult to elaborate.

To conclude, we believe that the exactly soluble model

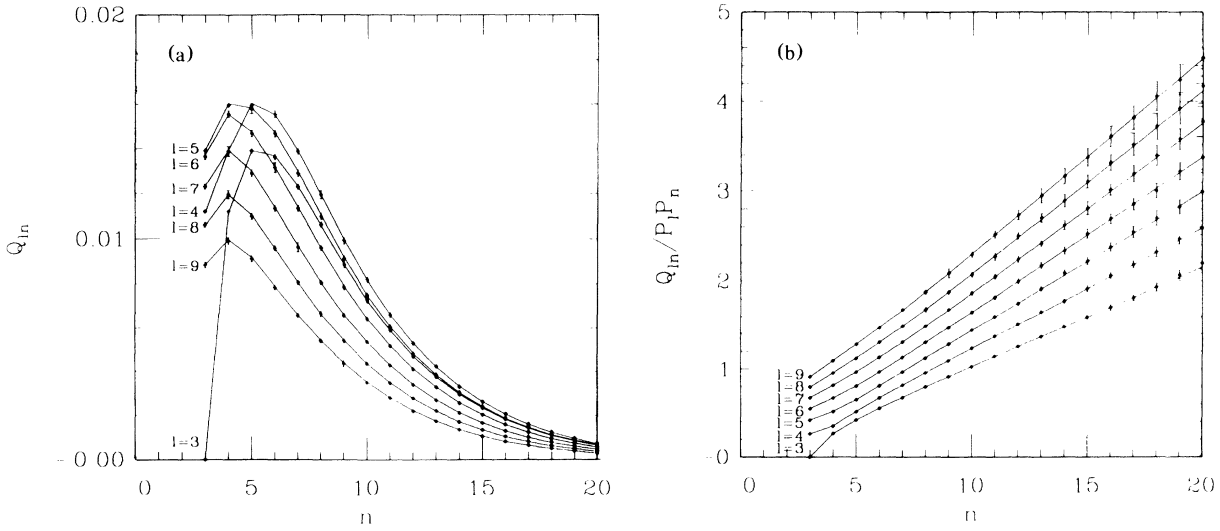

FIG. 3. (a) The joint probabilities Q_{ln} vs n, for $l=3,\ldots,9$. (b) Plot of Q_{ln}/P_lP_n vs n, for $l=3,\ldots,9$. The continuous curves are the theoretical predictions. Points with error bars are results of simulations, averaged on 100 different times.

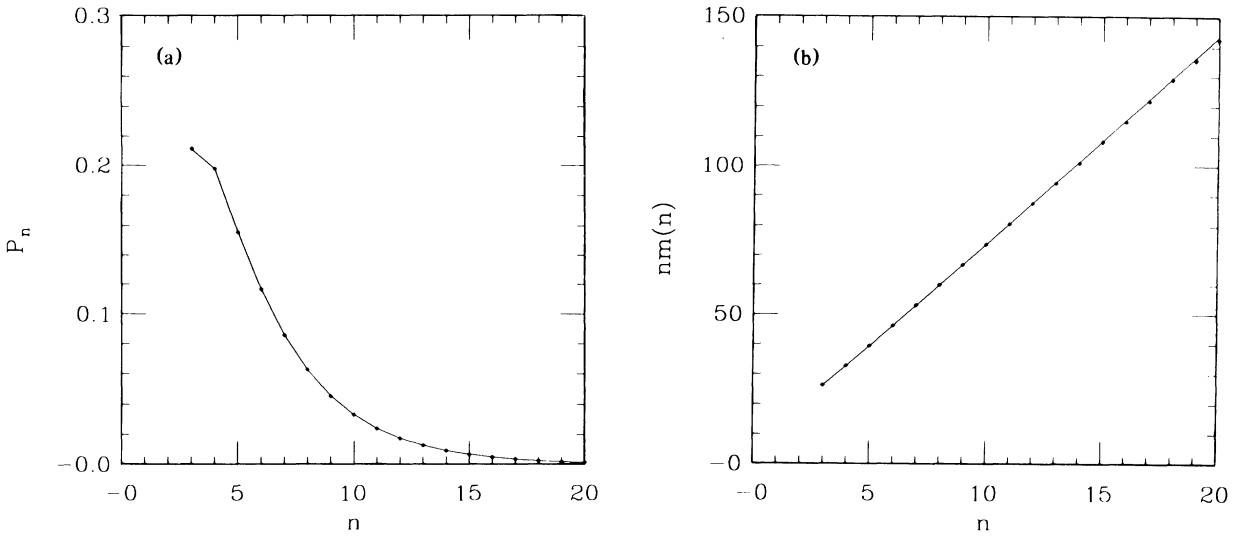

FIG. 4. (a) Probability distribution P_n of cells with n edges. (b) Plot of $nm(n)$. Same representation as Fig. 3.

presented in this Letter may serve as a template for more complicated cellular structures. In particular the results given here may help to understand the theoretical status of maximum-entropy arguments.

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[1] L. J. Gibson and M. F. Ashby, *Cellular Solids* (Pergamon, New York, 1988).

[2] D. A. Aboav, Metallography **3**, 383 (1970); **13**, 43 (1980).

[3] D. Weaire and N. Rivier, Contemp. Phys. **25**, 59 (1984).

[4] D. V. Boulatov, V. A. Kazakov, I. K. Kostov, and A. A. Migdal, Nucl. Phys. **B275**, 641 (1986).

[5] E. Brézin, C. Itzykson, G. Parisi, and J. B. Zuber, Commun. Math. Phys. **59**, 35 (1978), and references therein.

[6] M. A. Peshkin, K. J. Strandburg, and N. Rivier, Phys. Rev. Lett. **67**, 1803 (1991).