Scaling and Selection in Cellular Structures and Living Polymers

David Mukamel

Department of Physics of Complex Systems, The Weizmann Institute of Science
Rehovot 76100, Israel

ABSTRACT

The dynamical behavior of two types of non-equilibrium systems is discussed: (a) two-dimensional cellular structures, and (b) living polymers. Simple models governing their evolution are introduced and steady state distributions (cell side in the case of cellular structures and length in the case of living polymers) are calculated. In both cases the models possess a one parameter family of steady state distributions. Selection mechanism by which a particular distribution is dynamically selected is discussed.

PACS No: 05.70.Ln 47.20.Ky 82.70.Rr
Pattern selection is well known to take place in systems far from thermal equilibrium such as growing crystals, reaction diffusion problems and in many others. In these systems a particular pattern, or structure, is dynamically selected out of a family of possible structures. The canonical problem for which selection has been studied and explicitly demonstrated is that of a front propagation, where the velocity with which a stable state propagates into an unstable one is selected [1, 2]. This mechanism was then applied to study the pattern selection occurring in systems quenched beyond their limit of stability [3–8].

In the present paper we briefly review two interesting classes of systems which have recently been suggested to display dynamics governed by selection. The first class includes systems with cellular structures [9, 10] and the second is living polymers [11]. Here the selected quantity is not a spatial structure but rather the steady state distributions of certain quantities like that of the cell side in the case of cellular structures and the polymer length distribution in the case of living polymers. This review summarizes results obtained in Refs. [9–11].

A. Two Dimensional Cellular Structures

Cellular structures are rather common in nature [12]. Examples include polycrystal [13–15], foams, soap froths [16, 17], magnetic bubbles [18–21], and many others. In many cases these structures are metastable and they keep changing in time, evolving towards equilibrium. For example in the case of polycrystals, the cells are composed of single crystallites which are randomly oriented. Neighboring cells are separated by grain boundaries which cost some energy. In an attempt to reduce this energy the cells coarsen, thus reducing their area and the energy of the grain boundaries. Similarly, foams are made up of liquid film membranes separating gas filled cells. The energy of the system is given by the surface energy of the membranes. Here too the energy is reduced via the coarsening process. The main difference between the two systems is that while the surface free energy of liquid membranes is isotropic, the grain boundary energy strongly depends on the relative orientation of the neighboring crystallites and on the direction of the boundary. This certainly affects the details of the dynamics, but not the general tendency of coarsening. The evolution of these systems leads to a scale invariant state, with steady state distributions of some of their properties. Most studies so far have concentrated on two dimensional (2D) systems which are much simpler to investigate both theoretically and experimentally than in 3D [22–29]. Here we discuss the evolution of 2D soap froth.

Consider a two dimensional array of soap bubbles made up of liquid film membranes separating gas filled cells. The edges of the cells meet at vertices with coordination number \( q = 3 \). The reason is that any vertex with higher coordination number tends to split into several vertices, generically reducing the energy, or the total edge length, of the configuration. If the gas cannot diffuse through the membranes, the system reaches a mechanical
equilibrium in which the angle between any pair of edges meeting at a vertex is 120°. However, due to the permeability of the membranes, the gas diffuse from one cell to another and the system slowly evolves in a way such that its total edge length is reduced. In 1952 von Neumann considered the evolution of 2D soap froth under the assumption that the diffusion process is sufficiently slow so that the system is at a mechanical equilibrium at any given time. He showed that in this limit, the area of an $l$ sided cell, $A_l$, satisfies the following equation [22]

$$\frac{dA_l}{dt} = K(l - 6) \quad (1)$$

where $K$ is a constant which is proportional to the surface tension and to the permeability of the membranes. This is a very important and surprising result, since it shows that the evolution of the area of a cell is independent of the details of its neighborhood (such as the area, the shape and the number of edges of the adjacent cells), but only on the number of edges of the cell itself. Eq. (1) suggests that $l < 6$ sided cells shrink and eventually disappear while cells with $l > 6$ sides grow in time. The area of hexagonal cells remains unchanged. As a result of the disappearance of an $l < 6$ cell, the number of sides of its neighboring cells change (see Fig.1a). When the disappearing cell is a triangle, each of its adjacent cells lose a side. For a disappearing square, two of its neighbors lose a side and two remain with the same number of sides. In the case of a pentagon, two neighbors lose a side, one gain a side and two remain unchanged. These events are known as $T2$ processes. As a result of these processes, $l < 6$ sided cells do not disappear from the system altogether. This is consistent with Euler’s law which states that $V - E + F = 2$ where $V$ is the number of vertices, $E$ is the number of edges and $F$ is the number of faces of a closed two-dimensional graph in a plane. Using the fact that in our case three edges meet at each vertex, it is easy to show that the the average number of sides per cell is 6. Therefore, any configuration in which $l > 6$ sided cells are present, must include $l < 6$ sided cell too. In addition to the $T2$ processes, one also finds $T1$ processes corresponding to edge switching events (see Fig.1b). In soap froth these are rather rare events and therefore we will not consider them here. Also, two sided cells are metastable and they are not generated during the evolution. We therefore assume that the system is composed of $l \geq 3$ sided cells only.
Figure 1: (a) T2 processes, describing the disappearance of 3, 4 and 5 sided cells, respectively. (b) side switching T1 process.

To study the evolution of soap froth we consider $N_l(t)$, the number of $l$- cells (i.e. $l$-sided cells) at time $t$. Let $N = \sum_{l=3}^{\infty} N_l$ be the total number of cells in the system, and define

$$x_l = N_l/N$$  \hfill (2)

Clearly, the concentration $x_l$ of $l$- cells satisfy

$$\sum_{l=3}^{\infty} x_l = 1$$  \hfill (3a)

Moreover, due to Euler’s law one also has

$$\sum_{l=3}^{\infty} lx_l = 6$$  \hfill (3b)
To proceed, we introduce three parameters \( w_3, w_4 \) and \( w_5 \) which yield the vanishing rates of triangles, squares and pentagons, respectively. These rates together with the \( T2 \) processes determine the evolution equations of \( N_l \). For example the resulting equation for \( N_3 \) takes the form

\[
\frac{dN_3}{dt} = -w_3N_3 + [3P_R(4, 3)w_3N_3 + 2P_R(4, 4)w_4N_4 + 2P_R(4, 5)w_5N_5] - P_A(3, 5)w_5N_5 \quad (4)
\]

where \( P_R(l, m) \) is the probability that an edge of a disappearing \( m \leq 5 \)-cell is shared by an adjacent \( l \)-cell which undergoes a side removal process. Similarly, \( P_A(l, 5) \) is the probability that an edge of a disappearing pentagon is shared by an adjacent \( l \)-cell which undergoes a side addition process. In this equation the first term represents the rate at which triangles disappear due to the von-Neumann evolution. The next three terms yield the rate at which squares turn into triangles due to the disappearance of a neighboring 3, 4 and 5 cells, respectively. The last term gives the rate at which triangles gain a side and become squares due to the disappearance of a neighboring pentagon.

We now introduce the mean field approximation for \( P_R(l, m) \) and \( P_A(l, 5) \). In considering \( P_A(l, 5) \) we neglect all correlations between neighboring cells and take

\[
P_A(l, 5) = \frac{lN_l}{6N} = \frac{lx_l}{6} \quad (5)
\]

In \( P_R(l, m) \) some correlations have to be retained. In particular, in order not to generate 2-cells a side removal process should not take place in a triangle. We therefore take

\[
P_R(l, m) = \begin{cases} 0, & l = 3 \\ \frac{lx_l}{(6 - 3x_3)}, & l > 3 \end{cases} \quad (6)
\]

where the denominator \( (6 - 3x_3) \) is taken to ensure that the normalization condition \( \sum_{l=3}^\infty P_R(l, m) = 1 \) is satisfied. One can easily write down similar equations for \( N_l, l > 3 \). Summing these equations one obtains an equation for the decreasing rate of the total number of cells

\[
\frac{dN}{dt} = -(w_3N_3 + w_4N_4 + w_5N_5) \quad (7)
\]

Combining this equation with the equations for \( N_l \) one obtains the following equations for \( x_l, l \geq 3 \)

\[
\frac{dx_l}{dt} = -wx_l + K_0x_l + K_1[(l + 1)x_{l+1} - \alpha_llx_l] - K_2[\alpha_l(l - 1)x_{l-1}] \quad (8)
\]

where

\[
K_0 = w_3x_3 + w_4x_4 + w_5x_5
\]

\[
K_1 = (3w_3x_3 + 2w_4x_4 + 2w_5x_5)/(6 - 3x_3)
\]

\[
K_2 = w_5x_5/6
\]
and
\[ \alpha_l = \begin{cases} 
0, & l = 3 \\
1, & l > 3
\end{cases} \]

Also \( w_l = 0 \) for \( l > 5 \).

We are interested in the steady state solutions of Eqs. (8,9) for which \( dx_l/dt = 0 \). It is easy to demonstrate that these equations have a one parameter family of steady state solutions. To see that this indeed is the case we notice that for any given \( 0 < x_3 < 1 \) the first two equations (corresponding to \( l = 3, 4 \)) could be solved to yield \( x_4 \) and \( x_5 \). One can then solve iteratively for the rest of the distribution, finding \( x_l \) from the \((l-1)\)-th equation. The family of distributions obtained in this way may thus be parametrized by \( x_3 \).

We now consider the steady state distributions in more detail. Let
\[ y_l = lx_l \tag{10} \]
The steady state equations for \( l > 5 \) take the form
\[ K_1 y_{l+1} - (K_1 + K_2 - \frac{K_0}{l}) y_l + K_2 y_{l-1} = 0 \tag{11} \]
These equations have solutions of the form
\[ y_l = \lambda^l \kappa^l (1 + O\left(\frac{1}{l}\right)) \tag{12} \]
Inserting this form into Eq. (11) the parameters \( \lambda \) and \( \kappa \) may be obtained. Two solutions are found. One with
\[ \lambda_1 = \frac{K_2}{K_1}, \quad \kappa_1 = \frac{K_0}{K_1 - K_2} \tag{13a} \]
and the other with
\[ \lambda_2 = 1, \quad \kappa_2 = \frac{-K_0}{K_1 - K_2} \tag{13b} \]
The general solution, therefore, takes the form
\[ x_l = A \left( \frac{K_2}{K_1} \right)^l l^{\kappa_1 - 1} + B l^{\kappa_2 - 1} \tag{14} \]
The full distribution (including the \( l \leq 5 \) concentrations) is found by first choosing a particular value for \( x_3 \) and solving the \( l = 3, 4 \) equations to obtain \( x_4 \) and \( x_5 \). One then uses the form (14) for the \( l > 5 \) cell concentrations and determine the parameters \( A \) and \( B \) by demanding that the two sum rules (3a and 3b) are satisfied. The tail of the distribution is thus given as a sum of two terms: an \( A \) term which decays exponentially with \( l \) and a \( B \)
term which decays algebraically. By varying $x_3$ the whole family of possible steady state distributions is obtained.

In calculating these distributions it is found that $B$ is positive for sufficiently small $x_3$, and it changes sign at some point $x_3 = x_3^*$. The distributions with $B < 0$ are unphysical since $x_l$ become negative for large $l$. Moreover, linear stability analysis shows that those solutions with $B < 0$ are unstable while those with $B > 0$ are stable. As in other problems where selection takes place it is expected that the physical solution which exhibits the fastest decay of $x_l$ with $l$ is the one which is selected. Here it is the $B = 0$ solution, which is the only one exhibiting exponential decay. All other physically relevant distributions (with $B > 0$) display algebraic decay for large $l$. Numerical studies of the dynamical equations indicate that indeed this is the case and that the system evolves towards the $B = 0$ steady state distribution. The resulting distribution agrees well with experimental results obtained in soap froth [9, 10].

In order to check how good is the mean field approximation applied in this work, we consider now the case in which only $T_1$ processes take place. Here it is assumed that the gas does not diffuse from one cell to another, hence $T_2$ processes do not take place and cells do not disappear. Thus, the number of cells in the system is conserved throughout the evolution. This problem has been solved exactly [30], yielding a distribution which for large $l$ takes the form

$$x_l \sim \frac{\lambda^l}{\sqrt{l}}$$

with $\lambda = 3/4$.

To model this process within the mean field approximation, we define the rate $w$ as the probability that a $T_1$ process takes place per time unit per edge. Each such event results in a removal of a side from two cells and addition of a side to two others. The process cannot take place if either of the two neighboring cells which lose an edge in this process is a three-cell. This ensures that no two-cells are generated in this dynamics. The evolution equations of $x_l$ are given by

$$\frac{dx_l}{dt} = w \frac{6 - 3x_3}{6} [(l+1)x_{l+1} - lx_l] + w \left(\frac{6 - 3x_3}{6}\right)^2 [(l-1)x_{l-1} - lx_l]$$

These equations process a single fixed point distribution

$$x_l \sim \frac{\lambda^l}{l}$$

with $\lambda \approx 0.85$. This qualitatively agree with te exact answer.

B. Living Polymers

Another example of a dynamical system whose steady state distribution is uniquely selected out of a family of distributions is given by living polymers. Here we consider a
system of aggregates (say, polymers or micells), each composed of \( n \) units. Let \( c_n \) be the number of \( n \)-mers in the system. Under equilibrium condition the system reaches a well defined length distribution \( c_n \). We consider the case in which the system is driven out of equilibrium by pulling out monomers (or small size aggregates) at some rate. Clearly, \( c_n \) decrease with time and the system eventually vanishes. The question is how does the length distribution \( c_n \) look like in the long time limit. To study this problem we consider the concentrations \( x_n = c_n/c \) where

\[
c = \sum_{n=1}^{\infty} n c_n
\]  

and ask whether these quantities reach a well defined limit for large time.

As in the case of cellular structures, one finds that the dynamical equations which govern the evolution of \( x_n \) possess not just a single fixed point but rather a one parameter family of steady state distributions. Again a dynamical selection takes place by which a particular distribution is selected. To study this behavior we introduce a model describing the evolution of living polymers. For simplicity we assume that the interaction between the various \( n \)-mers take place via association-dissociation process in which an \( n \)-mer absorbs or emits a single monomer and becomes \((n+1)\) or \((n-1)\)-mer, respectively. The equations governing this process take the form:

\[
\frac{dc_1}{dt} = -k x_1 \sum_{n=1}^{\infty} c_n + \bar{k} \sum_{n=2}^{\infty} c_n - ac_1,
\]

\[
\frac{dc_2}{dt} = k x_1 (c_1/2 - c_2) + \bar{k} (c_3 - c_2/2),
\]

\[
\frac{dc_n}{dt} = k x_1 (c_{n-1} - c_n) + \bar{k} (c_{n+1} - c_n) \quad \text{for } n \geq 3.
\]  

(19)

where \( \bar{k} \) is the dissociation rate, \( k x_1 \) is the association rate of an \( n \)-mer with a monomer and \( a \) is the rate at which monomers are pulled out of the system, \( x_1 \). The association rate is taken to be proportional to the concentration of the monomers in the system. For simplicity it is assumed that \( k \) and \( \bar{k} \) are independent of \( n \). This assumption does not change the qualitative results derived here. The equation for \( c_2 \) is somewhat different from equations for \( c_n \) with \( n > 2 \). First, the rate at which two monomers combine to yield a dimer is \( k x_1/2 \) and not \( k x_1 \). In addition, while a dissociation of \( n \)-mer with \( n > 2 \) can take place near either of its two ends, in the case of a dimer the dissociation can take place only at one point. Hence the factor of a \( 1/2 \) in its dissociation rate. Summing Eqs.(19) one finds

\[
\frac{dc}{dt} = -ac_1,
\]  

(20)
This equation yields the rate at which the number of units in the system decreases with time.

Combining Eqs. (20) with (19) one obtains the following equations for \( x_n \).

\[
\begin{align*}
\frac{dx_1}{dt} &= -kx_1 \sum_{n=1}^{\infty} x_n + k \sum_{n=2}^{\infty} x_n - ax_1 + ax_1^2, \\
\frac{dx_2}{dt} &= kx_1(x_1/2 - x_2) + \bar{k}(x_3 - x_2/2) + ax_1x_2, \\
\frac{dx_n}{dt} &= kx_1(x_{n-1} - x_n) + \bar{k}(x_{n+1} - x_n) + ax_1x_n \quad \text{for } n \geq 3.
\end{align*}
\]

(21)

This is a set of non-linear equations with non-local interactions of the type found in the equations describing the evolution of cellular structures. Here the "head" of the distribution, \( x_1 \), directly interacts with its "tail", \( x_n \), for arbitrarily large \( n \). The fixed point distribution of these equations yield the long time behavior of \( c_n \). Note that the normalization

\[
\sum_{n=1}^{\infty} nx_n = 1.
\]

(22)

is preserved by Eqs. (21).

Eqs. (21) possess a one parameter family of fixed point distributions. To see that this is the case one first makes an arbitrary choice for \( x_1 \) and \( x_2 \). The second equation of (21) determines \( x_3 \). One can then successively solve the remaining equations, obtaining \( x_n \) for \( n > 3 \). The two free parameters \( x_1 \) and \( x_2 \) may now be varied so as to satisfy the equation for \( x_1 \) (or equivalently, the normalization condition (22)), leaving one free parameter, say, \( x_1 \).

The fixed point distributions may easily be obtained by noting that for a given \( x_1 \), Eqs. (21) are linear in \( x_n, n \geq 2 \). Setting \( dx_n/dt = 0 \) one finds that the fixed point distributions are of the form

\[
x_n = A\lambda_{-n-2} + B\lambda_{+n-2}, \quad n \geq 2,
\]

(23)

where \( \lambda_{\pm} \) are the roots of the characteristic equation

\[
\bar{k}\lambda^2 - (\bar{k} + kx_1 - ax_1)\lambda + kx_1 = 0.
\]

(24)

Here \( A \) and \( B \) are parameters which are determined by the first two equations in (22)

\[
\begin{align*}
\frac{A}{1 - \lambda_-} + \frac{B}{1 - \lambda_+} &= \frac{(k - a)x_1^2 + ax_1}{k - kx_1}, \\
A[\bar{k}\lambda_- - (\bar{k}/2 + kx_1 - ax_1)] + B[\bar{k}\lambda_+ - (\bar{k}/2 + kx_1 - ax_1)] &= -kx_1^2/2.
\end{align*}
\]

(25)
Eqs. (25) yield the two parameters $A$ and $B$, thus determining the length distribution. Clearly, all $x_n$’s obtained in this way must be non-negative for the distribution to be physically meaningful. For this to be the case one has to require that (a) the roots $\lambda_{\pm}$ are real with $0 < \lambda_- < \lambda_+ < 1$, (b) $x_2 = A + B > 0$ and (c) $B > 0$. These requirements ensure that $x_n$ decays with $n$ purely exponentially without oscillations. When the decay is oscillatory some of the $x_n$’s become negative and thus unphysical. The $B > 0$ requirement is needed since $B$ corresponds to the slower decay rate of $x_n$. A negative $B$ yields negative $x_n$’s for large $n$.

We now consider the question of selection of a unique steady state distribution out of this family. By examining Eq. (24) one can verify that for any set of parameters $k, \bar{k}$ and $a$ there exists an $x_M$ such that as long as $0 < x_1 < x_M$, condition (a) is satisfied. It is also easy to verify by solving Eq. (25) that condition (b) is satisfied as long as $0 < x_1 < x_M$. As for condition (c), one can show that the parameter $B$ is positive for small $x_1$ and changes sign at $x_1 = x_S$, where $x_S$ depends on the parameters $k, \bar{k}$ and $a$. For $x_S > x_M$ all fixed points with $0 < x_1 < x_M$ are physically relevant. On the other hand for $x_S < x_M$ only those with $0 < x_1 < x_S$ correspond to physical distributions. These two cases yield two different selection mechanisms. Following the work of Aronson and Weinberger [1], and Dee et al [3] one may conjecture that in the first case the marginal fixed point corresponding to $x_1 = x_M$ is selected, in the sense that as long as the initial length distribution decays sufficiently fast with $n$, the system evolves towards the $x_1 = x_M$ fixed-point. On the other hand, in the second case (the non-linear marginal stability, or case II) the selected fixed-point is the one corresponding to $x_1 = x_S$. In both cases the selected distribution corresponds to the physically accessible fixed-point with the fastest decay rate of $x_n$ with $n$.

This model has been studied numerically, and it was shown that indeed the long time behavior of the system is governed by either the $x_1 = x_M$ or the $x_1 = x_S$ fixed points depending the parameters $k, \bar{k}$ and $a$. One of the parameters, say $\bar{k}$, may be taken as 1. It determines the time scale in the problem and does not affect the steady state distribution. The resulting $(k, a)$ phase diagram is given in Fig. 2.
Figure 2: The \((k, a)\) phase diagram of the model (21) for \(\bar{k} = 1\). Two regions are found. One \((M)\) in which the marginal fixed point \(x_1 = x_M\) is selected, and the other, \((S)\), in which \(x_1 = x_S\) is selected.

Acknowledgements

I thank E. Domany, O. Krichevsky, A. C. Maggs, C. A. Pillet, D. Segel, and J. Stavans with whom I collaborated on the studies described in this brief review.
References

1. D.G. Aronson, H.F. Weinberger Adv. Math. 30, 33 (1978).
2. Pierre Collet and Jean-Pierre Eckmann Instabilities and Fronts in Extended Systems, Princeton University Press, New Jersey (1990).
3. G. Dee and J.S. Langer Phys. Rev. Lett. 50, 383 (1983). J.S. Langer and H. Muller-Krumbhaar Phys. Rev. A 27, 499 (1983).
4. E. Ben-Jacob, H. Brand, G. Dee, L. Kramer and J.S. Langer Physica 14D, 384 (1985).
5. Wim van Saarloos Phys. Rev. Lett. 58, 2571 (1987).
6. G.T. Dee and Wim van Saarloos, Phys. Rev. Lett. 60, 2641 (1988).
7. Wim van Saarloos Phys. Rev. A37, 211 (1988); Phys. Rev. A 39, 6367 (1989).
8. Wim van Saarloos and P.C. Hohenberg, Physica D56, 303 (1992).
9. J. Stavans, E. Domany and D. Mukamel, Europhys. Lett. 15, 479 (1991).
10. D. Segel, D. Mukamel, O. Krivevsky and J. Stavans, Phys. Rev. E 47, 812, (1993).
11. A.C. Maggs, D. Mukamel and C.A. Pillet, Phys. Rev. E 50, 774 (1994).
12. For a recent review see J. Stavans, Rep. Prog. Phys. 56, 733 (1993).
13. R.W. Armstrong, Adv. Mater. Res. 4, 101 (1970).
14. C.J. Simpson, C.J. Beingessner and W.C. Winegard, Trans. Metall. Soc. AIME 239, 587 (1967).
15. S.K. Kurtz and F.M.A. Carpay, J. Appl. Phys. 51, 5725 (1981).
16. J.A. Glazier, S.P. Gross and J. Stavans, Phys. Rev. A 36, 306 (1987); J. Stavans and J.A. Glazier, Phys. Rev. Lett. 62, 1318 (1989).
17. J. Stavans, Phys. Rev. A 42, 5049 (1990).
18. K.L. Babcock and R.M. Westervelt, Phys. Rev. A 40, 2022 (1989).
19. K.L. Babcock and R.M. Westervelt, Phys. Rev. Lett. 64, 2168 (1990).
20. K.L. Babcock, R. Seshardri and R.M. Westervelt, Phys. Rev. A 41, 1952 (1990).
21. D. Weaire, F. Bolton, P. Molho and J.A. Glazier, J. Phys. Condens. Matter 3, 2101 (1991).
22. J. von Neumann, in Metal Interfaces, edited by C. Herring (American Society of Metals, Cleveland, 1952), p. 108.
23. D. Weaire and N. Rivier, Contemp. Phys. 25, 59 (1984); N. Rivier, Philos. Mag. B 52, 795 (1985).
24. M.P. Marder, Phys. Rev. A 36, 438 (1987).
25. J.R. Iglesias and R.M.C. de Almeida, Phys. Rev. A 43, 2763 (1991).
26. V.E. Fradkov, D.G. Udler and R.E. Kris, Philos. Mag. Lett. 58, 277 (1988).
27. C. Beenakker, Physica A 147, 256 (1987).
28. C. Godrèche, I. Kostov and I. Yekutieli, Phys. Rev. Lett. 69, 2674 (1992).
29. B. Levitan, E. Slepyan, O. Krichevsky, J. Stavans and E. Domany, Phys. Rev. Lett. 73, 756 (1994).
30. E. Brézin, C. Itzykson, G. Parisi and J.-B. Zuber, Comm. Math. Phys. 59, 35 (1978); D.V. Boulavot, V.A. Kazakov, I.A. Kostov and A.A. Migdal, Nucl. Phys. B275, 641 (1986).