Tiling a Plane in a Dynamical Process and its Applications to Arrays of Quantum Dots, Drums, and Heat Transfer

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(Received 18 February 2005; published 19 August 2005)

We present a reaction-diffusion system consisting of N components. The evolution of the system leads to the partition of the plane into cells, each occupied by only one component. For large N, the stationary state becomes a periodic array of hexagonal cells. We present a functional of the densities of the components, which decreases monotonically during the evolution and attains its minimal value in the stationary state. This value is equal to the sum of the first Laplacian eigenvalues for all cells. Thus, the resulting partition of the plane is determined by minimization of the sum of the eigenvalues, and not by the minimization of the total perimeter of the cells as in the famous honeycomb problem.

DOI: 10.1103/PhysRevLett.95.088304 PACS numbers: 82.40.Ck, 05.70.Ln, 47.54.+r

One of the most famous problems related to space division is the theorem that the regular honeycomb has the smallest perimeter among all partitions of the plane into regions of equal area. Interestingly, the theorem was proven only recently [1], despite the fact that it was conjectured almost 2000 years ago by Pappus of Alexandria. Division of space into the cells of a hexagonal shape emerges in many problems of physics. As an example, one can give the ideal, infinite 2D foam structure [2,3]. For a fixed area of foam bubbles, the minimization of the line energy leads naturally to the hexagonal structure of the foam. In the 2D electron liquid kept in a weak magnetic field, with partially filled upper Landau levels, the charge density waves assume the hexagonal structure for a small filling parameter (called a super Wigner crystal) [4]. The 2D Wigner crystal made of charges of the same sign also forms a hexagonal periodic structure. The hexagonal array is often used to start the optimization processes, for example, in the photonic band gap materials [5,6]. Most of its optimization properties are directly related to the original honeycomb problem through the minimization of various quantities associated with the total perimeter of the honeycomb structure, or the total energy of the structure. In mentioned cases the variational principle selecting the hexagonal pattern is known.

Far from equilibrium, hexagonal patterns are observed in reaction-diffusion systems, such as chloride-iodine-malonic acid in gel media [7–9], or in Rayleigh-Bénard convection (e.g., [10]). However, in these cases it is not clear at all what is optimized or what is the variational principle that leads to the appearance of the hexagonal structures. In this Letter we present a stochastic process of the reaction-diffusion type [11–13], which in the stationary state divides space into regular hexagonal cells. We present a selection criterion (for the appearance of different patterns or tilings), which corresponds to the minimization of the sum of the first Laplacian eigenvalues for the cells; i.e., we show that in the stationary states the division of space into cells is such as to minimize that sum. Starting from the set of nonlinear equations, we construct a functional of the densities that decreases monotonically during the evolution and becomes equal to the sum of the Laplacian eigenvalues in the stationary state. Since the Laplacian operator is common in many physical phenomena, we believe that the scheme of space partitioning under consideration can be used in many different situations: from heat exchange in 2D systems, to the coverage of a plane with a regular array of quantum wells, or to the escape of particles in open diffusion systems.

We consider a system of many Brownian particles confined in a rectangular box of size $L_x \times L_y$, with periodic or absorbing boundary conditions. There are N types of particles (each type consists of the same number of particles). When two particles of different types (say i and j) meet, both disappear from the system. At the same time, two particles, one of type i and one of j, are chosen at random and duplicated. Similarly, when any particle approaches a boundary, it is removed, and another particle of the same type is duplicated. Thus, the number of particles for each type is conserved. Diffusion, together with annihilation of particles of different types, lead to their spatial segregation and eventual tiling of the plane. The process can be considered as reaction diffusion. In the continuous limit, it can be described by the following system of integro-differential equations, with i and $j = 1, \ldots, N$:

$$\frac{\partial}{\partial t} p_i = D\Delta p_i + \Lambda_i(t) p_i, \tag{1}$$

$$\int_V p_i dV = 1, \tag{2}$$

$$p_i p_j = 0 \qquad (\text{for } i \neq j), \tag{3}$$

where D is the diffusion constant (the same for each component), $p_i(\mathbf{r}, t)$ is the density of component i, and the time dependent Lagrangian multipliers, $\Lambda_i(t)$, are unambiguously determined to reconcile the evolution, Eq. (1), with the normalization, Eq. (2), and the free boundary condition, Eq. (3). Physically, the last term in Eq. (1) describes how many particles are duplicated at a given point and time. In the stationary state of the process, the system is divided into N subsystems separated by sharp boundaries. On the basis of analysis of the single component subsystem [11], we conjectured that the stationary state follows from the minimization of the functional:

$$\sigma[p_1, p_2, \dots p_N] = \sum_{i=1}^{N} \sigma_i[p_i], \quad (4)$$

where

$$\sigma_i[p_i] = -\frac{\int_{V_i(t)} p_i \Delta p_i dV}{\int_{V_i(t)} p_i^2 dV}. \quad (5)$$

Here $V_i(t)$ is the area where p_i is nonzero. As all $p_i(\mathbf{r})$ are continuous functions of $\mathbf{r}$, the integration area can be extended to the whole volume of the box. In the stationary state, p_i becomes an eigenfunction of the Laplacian. It satisfies the equation $\Delta p_i + \lambda_i^1 p_i = 0$, where λ_i^1 is the first (smallest) eigenvalue of Laplacian on the domain of nonzero p_i. In the stationary state, $\sigma_i[p_i] = \lambda_i^1$. Beyond the stationary state both sides of the latter equation are functions of time, and the left-hand side is always larger than the right-hand one. Despite the fact that σ_i may decrease as well as increase during the evolution, we find that their sum, $\sigma[p_1, p_2, \dots, p_n]$, decreases monotonically in time and attains a minimum in the stationary state. It means that, in the stationary state, the boundary lines between domains adopt such a location, which minimizes the sum of the first eigenvalues of the Laplacian on the domains separated by these boundary lines:

$$\lambda_i^1 + \lambda_2^1 + \cdots + \lambda_N^1 = \sigma_{\mathrm{stat}} = \text{minimum}. \quad (6)$$

It does not have to be a global minimum—there may exist several stationary states with different σ and with separated basins of attraction. Since any permutation of the components leads to the equivalent stationary state, the optimization covers only the shape of partition lines—assigning components to domains does not matter.

In order to be able to compare systems varying in sizes and even in N, we define the partition cost functional:

$$\tilde{\sigma} = \frac{L_x L_y}{N^2} \sigma[p_1, p_2, \dots, p_n] = \bar{A}\bar{\lambda}^1, \quad (7)$$

where $\bar{A} = L_x L_y / N$ is the average area of a single domain, and $\bar{\lambda}^1 = \sigma/N$ is the average first eigenvalue. Both $\bar{A}$ and $\bar{\lambda}^1$, and $\tilde{\sigma}$ as well, describe the "average shape" of a single domain in the tiling. L_x and L_y describe the periodic box (if the periodic boundary conditions are used) or the rectangle which encapsulates the boundaries (otherwise). Values of $\tilde{\sigma}$ for several shapes of domain are shown in Table I. As long as we take into account only the shapes that form regular tiling, $\tilde{\sigma}$ is smallest for the regular hexagons.

TABLE I. Values of partition cost functional, $\tilde{\sigma}$, defined in Eq. (7), for selected tiling cells, and for a circle.

	Shape of tile	Exact	Approx.
$\tilde{\sigma}_{\mathrm{eqt}}$	Equilateral triangle	$\frac{4\sqrt{3}}{3}\pi^2$	22.792 875
$\tilde{\sigma}_{\mathrm{rect}}$	Rectangle, $N_y/N_x = \sqrt{3}/2$	$\frac{7\sqrt{3}}{6}\pi^2$	19.943 766
$\tilde{\sigma}_{\mathrm{sqr}}$	Square	$2\pi^2$	19.739 209
$\tilde{\sigma}_{\mathrm{hex}}$	Regular hexagon	unknown	18.5901
$\tilde{\sigma}_{\mathrm{circ}}$	Circle	Bessel $Z_{10}^2\pi$	18.168 415

In relation to the partition cost functional, $\tilde{\sigma}$, we formulate two conjectures: (1) Partition of the rectangular area of size $L_x \times L_y$ (both periodic, and bounded by constant, absorbing frame) into N subregions, gives $\tilde{\sigma}$ which is not smaller than $\tilde{\sigma}_{\mathrm{hex}}$. Moreover, in the limit $N \to \infty$, the infimum of the set of possible values of $\tilde{\sigma}$ approaches $\tilde{\sigma}_{\mathrm{hex}}$. (2) Among all possible partitions of infinite plane, none has $\tilde{\sigma}$ smaller than $\tilde{\sigma}_{\mathrm{hex}}$.

Although we cannot prove these statements rigorously, we give some convincing illustrations for the first of the above conjectures, both in the case of absorbing and periodic boundary conditions. In Fig. 1 we show the stationary states for 4, 6, 16, and 320 components in a square frame with absorbing boundaries. For large N, there may exist several stationary states for different local minima of $\tilde{\sigma}$. Therefore, some of the dislocations visible for $N = 320$ are dependent on the initial condition (here, the simulation was started from random mixture). Most of the cells, however, are hexagonal and their deformations are mainly due to the shape of the box. In Fig. 2 we show the stationary values of $\tilde{\sigma}$ as a function of N in a square with absorbing boundaries. For the cases with many stationary states, we show those with the smallest $\tilde{\sigma}$. As a function of increasing N, minimal $\tilde{\sigma}$ varies nonmonotonically, but, in general, it seems to decrease towards $\tilde{\sigma}_{\mathrm{hex}}$.

The dynamics of the process is shown in Figs. 3 and 4 for 4 components in the rectangle with $L_y/L_x = \sqrt{3}/2$, with

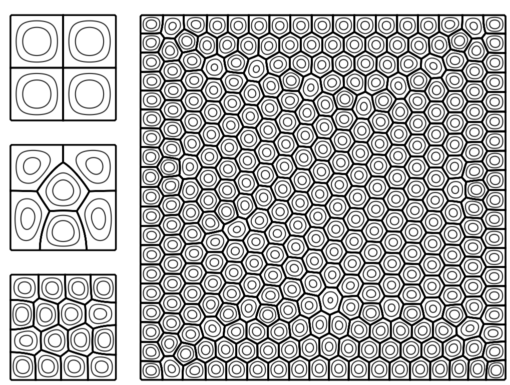

FIG. 1. The stationary states of N components in the square with absorbing sides, for $N = 4$, 6, 16, and 320.

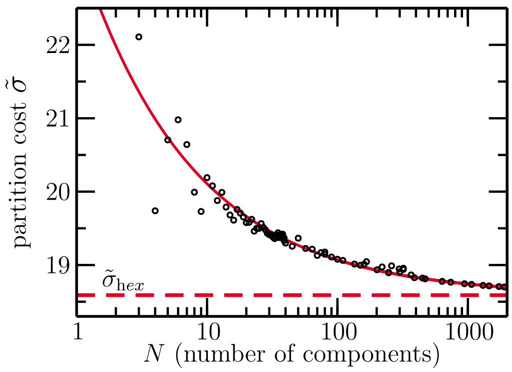

FIG. 2 (color online). The lowest $\tilde{\sigma}$ [see Eq. (7)] among stationary states found for N components in absorbing square frame, as a function of N. The solid line shows the algebraic function: $\tilde{\sigma}_{\text{hex}} + \alpha/\sqrt{N}$, with $\alpha = 4.8$. This power-law behavior corresponds to the fact that the deviation from $\tilde{\sigma}_{\text{hex}}$ is mainly due to the components that stay in contact with the frame. Their relative number is of the order of $1/\sqrt{N}$.

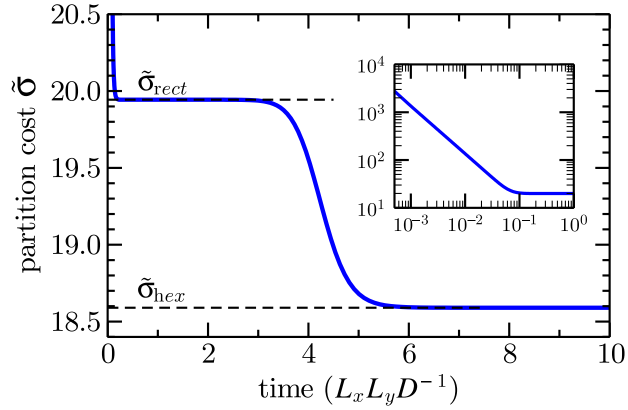

FIG. 4 (color online). Time dependence of the partition cost functional, $\tilde{\sigma}$, during the evolution of the system shown in Fig. 3. The inset shows the rapid, algebraic decay of $\tilde{\sigma}$ for small time. The values of $\tilde{\sigma}_{\text{rect}}$ and $\tilde{\sigma}_{\text{hex}}$ are given in Table I.

periodic boundary conditions. The initial configuration corresponds to four delta peaks, placed regularly in the periodic box. As we can see from the snapshots of evolution given in Fig. 3, and from the corresponding changes of $\tilde{\sigma}$ shown in Fig. 4, the first plateau in the evolution corresponds to the regular array of rectangles. This long-living, unstable configuration corresponds to $\tilde{\sigma} = \tilde{\sigma}_{\text{rect}}$, and it eventually collapses to the final stationary state, which is regular hexagonal tiling, where $\tilde{\sigma} = \tilde{\sigma}_{\text{hex}}$. Please note that for $N = 4$ the hexagons may be regular only if the aspect ratio is $\sqrt{3}/2$.

Similarly, Fig. 5 and, respectively, Fig. 6, show the evolution of the system with $N = 8$. Evolution starts from delta peaks placed at the vertices of regular hexagonal mesh. The first plateau at $\tilde{\sigma} = \tilde{\sigma}_{\text{eqt}}$ corresponds to the tiling by equilateral triangles, and the next one to the tiling by pentagons and heptagons. The final, stationary state consists of identical hexagonal domains, which are, however, not regular hexagons (the aspect ratio L_y/L_x is again $\sqrt{3}/2$, but now the number of components $N = 8$ does not allow tiling by regular hexagons). The time intervals, during which the evolution is stuck at the long-living, unstable states, depend on infinitesimally small asymmetries of the initial configuration. Perfect symmetry of the initial state cannot be spontaneously broken by the deterministic model of evolution.

Finally, in Fig. 7 we show the stationary values of $\tilde{\sigma}$ for $N = 4$, 5, and 6 components in the periodic box, as functions of $\ln(L_y/L_x)$. These functions are symmetric, because there is no difference between aspect ratio L_y/L_x and L_x/L_y. For some shapes of the box the hexagonal tiling is possible with perfect hexagons. From the figure it is clear that $\tilde{\sigma}$ attains a minimum for the regular hexagonal tiling.

Finally, we comment on the dynamical process itself. We called it reaction diffusion, but Eqs. (1)–(3) do not resemble chemical kinetics equations. In fact, Eqs. (1)–(3) can be obtained from the reaction-diffusion kinetics using the assumption that the annihilation rate constant approaches infinity. Moreover, we assumed that each instance of annihilation is accompanied by a single instance of creation. These complementary processes occur at the same time, but not at the same point of space. This kind of "teleportation" is not physical. In order to give them a

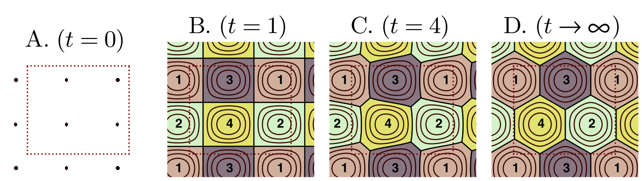

FIG. 3 (color online). Snapshots of the evolution of the system of $N = 4$ components in the periodic rectangle with the aspect ratio $L_y/L_x = \sqrt{3}/2$.

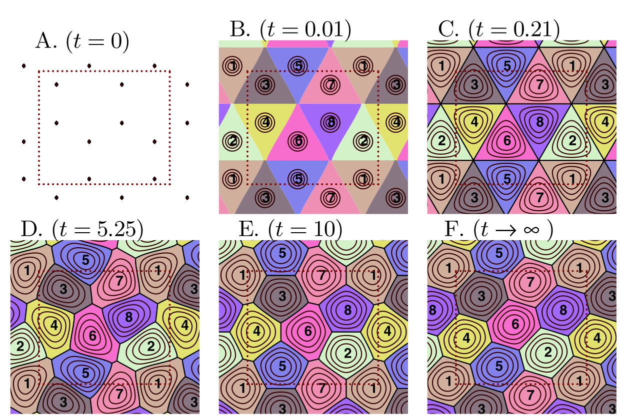

FIG. 5 (color online). Snapshots of the evolution of the system of $N = 8$ components in the periodic rectangle with the aspect ratio $L_y/L_x = \sqrt{3}/2$.

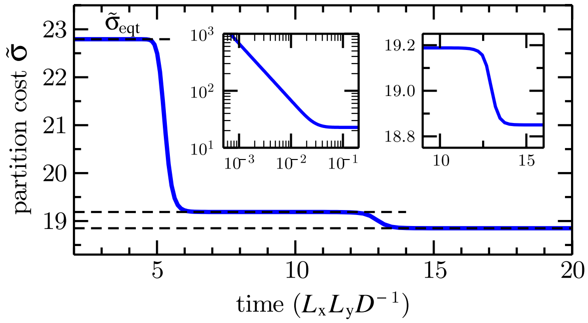

FIG. 6 (color online). Time dependence of $\tilde{\sigma}$ during the evolution of the system shown in Fig. 5. The insets show the same graph in the region of small time, and near the transition to the stationary state.

physical meaning, we should introduce N new species, each corresponding to one of the basic components. Instead of annihilation, the particles of two different components, say A and B, must change into the transient forms A^* and B^*. Then the transient forms have to be regenerated in a catalytic reaction $A + A^* \rightarrow 2A$ (same for B). When the rate constant of this reaction is relatively low, but the diffusion speed for the transient forms is much higher than for the basic forms, then the spatial distributions of transient forms become uniform, and for the basic forms the kinetics can be described by Eqs. (1)–(3). Hence, one can make an analogy with the chemistry of Turing patterns, where the emerging of patterns from the reaction-diffusion process is connected with two conditions: there must be an autocatalytic step of reaction, and the diffusion constants for reactant and autocatalyst must be considerably different [14,15]. In our case the ratio of these diffusion constants approaches infinity. So far we assumed that all N species have the same number of particles, and the same diffusivity. Without these assumptions we would obtain a wide family of patterns, which can be compared to different mutations of honeycomb conjecture described in [16].

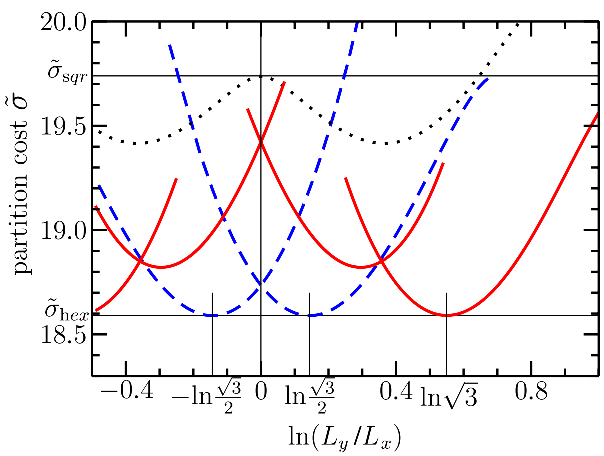

FIG. 7 (color online). The partition cost functional $\tilde{\sigma}$ as a function of $\ln(L_y/L_x)$ for stationary states of N components in the periodic box of size $L_y \times L_x$. Solid, dotted, and dashed lines are for $N = 4$, 5, and 6, respectively.

Our conjecture states that, among all possible tilings of a plane by tiles of a given average area, the sum of the first Laplacian eigenvalues for all tiles is minimized by the periodic array of regular hexagons. The analogous problem in quantum mechanics is as follows: cover the plane with the infinitely deep quantum wells in such a way as to minimize the total energy of the lowest energy levels of the wells. Whether this result will find applications in the periodic array of quantum dots for information processing [17–19] is an open question. In 1966 Kac [20] posed a question "Can you hear the shape of a drum?" The answer is negative [21]—we may have differently shaped drums with the same spectrum of modes. Our results give an answer to a different question concerning drums: Can you tile the plane with the drums in such a way that the total sum of their lowest frequencies attains minimum? Another question is "What should be the arrangement and shape of the cells such that the cooling of all the cells is the slowest?" Finally, let us consider the periodic array of traps for particles. The question is "What is the shape of a trap such that the mean escape rate is the slowest for all the traps?" Hexagonal tiling is the most likely answer to all these questions.

This work was supported by KBN Grant No. 2P03B00923.

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