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Configurational transition in a Fleming–Viot-type model and probabilistic interpretation of Laplacian eigenfunctions

Krzysztof Burdzy[†], Robert Hołyst[‡], David Ingerman[†] and Peter March[§]

† Department of Mathematics, University of Washington, Seattle, WA 98195, USA
‡ Institute of Physical Chemistry of the Polish Academy of Sciences and College of Sciences, Department III, Kasprzaka 44/52, 01224 Warsaw, Poland
§ Department of Mathematics, Ohio State University, Columbus, OH 43210, USA

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Abstract. We analyse and simulate a two-dimensional Brownian multi-type particle system with death and branching (birth) depending on the position of particles of different types. The system is confined in a two-dimensional box, whose boundaries act as the sink of Brownian particles. The branching rate matches the death rate so that the total number of particles is kept constant. In the case of *m* types of particle in a rectangular box of size $a \times b$ and elongated shape $a \gg b$ we observe that the stationary distribution of particles corresponds to the *m*th Laplacian eigenfunction. For smaller elongations a > b we find a configurational transition to a new limiting distribution. The ratio a/b for which the transition occurs is related to the value of the *m*th eigenvalue of the Laplacian with rectangular boundaries.

1. Introduction

It is remarkable how simple systems with just a few deterministic rules (such as Life [1] or cellular automata [2]) can generate complex structures. When considering population dynamics, however, one often uses stochastic models, as the following examples illustrate. The addition of stochastic factors into the Life game [3] favours diversity of structures, in contrast to the original model in which diversity is a decreasing function of time. Introduction of a probabilistic factor in the cellular automata description of the dynamics of social impact in a population [4] leads to the complex spatial and time intermittent behaviour. In genome population dynamics [5, 6] one uses stochastic processes such as super-Brownian motion or Fleming–Viot processes. The model presented in this paper is a stochastic population dynamics model related to Fleming–Viot processes.

The dynamics of systems with two competing species has been studied with an emphasis on the influence of spatial heterogeneity on temporal evolution and spatial organization [7-9]. In the case of strong competition it is typical that only one of the two species survives, which means, in particular, that average lifetimes of the two species can be different. In contrast to this situation, we are interested in the spatial distribution of several species when their average lifetimes are comparable and species coexist in equilibrium.

In our model we consider the long-time behaviour of a population of m different species of Brownian particle confined in a two-dimensional box. We choose very simple interactions among species which guarantee confinement in the box, spatial segregation of species and long time coexistence. Specifically, we assume that the walls of the box act as sinks for the particles and we assume that if two particles of different type occupy the same lattice point, then both are killed. The birth rules are chosen in such a way as to keep the number of



Figure 1. Nodal lines for stationary distribution of particles of three particle types. Each region, separated by full lines, is occupied by only one type of particle. (*a*) The side ratio $r_3 = a/b = 1.64$; elementary configuration corresponding to the third Laplacian eigenfunction, (*b*) $r_3 = 1.63$; configuration close to the transition point (non-elementary configuration), (*c*) $r_3 = 1$; configuration far from the transition point (non-elementary configuration).

particles constant at each time step and to ensure that the average lifetime of each species of particle is the same in the long-time limit. As will be seen, our model corresponds to a Fleming–Viot-type process in which particle interactions are position dependent. We point out here, and justify below, that our model leads to a deterministic limiting distribution, whereas the limiting distributions for super-Brownian motion and Fleming–Viot processes have a random, fractal nature.

By way of illustration, figure 1 shows the stationary configuration for m = 3 types of particle in a rectangular box D of size $a \times b$. The side ratio a/b is a critical parameter in our study. We find that for a/b > 1.63 the particles of different types occupy domains of rectangular shapes (figure 1(*a*)). We call this an elementary configuration and show (in section 5) that it is related to the third Laplacian eigenfunction in D. When the side ratio decreases below 1.63 the configuration changes its character as shown in figure 1(*b*) and (*c*). Here the domains occupied by distinct species have shapes which are not related to Laplacian eigenfunctions in D. We call this a configurational transition.

In section 7 we show that the side ratio a/b at the transition can be obtained from a simple condition involving the third Laplacian eigenvalue of D. In a natural way our model provides, in some circumstances, a probabilistic interpretation of the higher Laplacian eigenfunctions.

The paper is organized as follows. In section 2 we briefly discuss discrete analogues of super-Brownian motion and Fleming–Viot processes and their relationship to our model. In sections 3 and 4 we describe our model in detail. The connection between the stationary state of the model and the Laplacian eigenfunctions is given in section 5 and computer simulations are described in section 6. The analysis of the configurational transition and concluding remarks are contained in section 7.

2. Super-Brownian and Fleming-Viot processes: particle systems with death rates independent of position

Super-Brownian motion and Fleming–Viot processes are usually discussed in the continuous time and space state setting. We will present their discrete analogues for the purpose of

comparison with our own model introduced in sections 3 and 4 below. Full details of these constructions, and much else, are presented in [6] and [11], so we will be brief.

In the first model we consider particles on the two-dimensional square lattice. At every time step t = 1, 2, 3, ..., each particle either dies or branches into two offspring, each with probability $\frac{1}{2}$. If the particle branches, both offspring occupy the same lattice site as the parent particle and then each offspring chooses one of the four neighbour lattice sites with probability $\frac{1}{4}$ and goes there. These events are independent for all the particles in the population.

Suppose that at time t = 1 the particle system consists of j particles and every particle is located at (0, 0). Let X_s^j be a measure-valued process whose value at time s is defined as follows. The measure $X_s^j(A)$ of an open subset A of \mathbb{R}^2 is equal to the number of particles at time t = [s] which lie in $\sqrt{j}A$. Here [s] is the integer part of s. Consider the sequence of processes $\{X_{ju}^j/j, u \ge 0\}_{j\ge 1}$ where s = ju and u plays the role of the rescaled time. This sequence converges as $j \to \infty$ to a measure-valued diffusion called super-Brownian motion with the initial state $\delta_{(0,0)}$ (mass 1 concentrated at (0,0)).

There are several existing results showing that this process has a fractal nature in dimensions $d \ge 2$. For example, at any fixed time, the state of super-Brownian motion is a random singular measure whose support has Hausdorff dimension 2 [10], for dimensions $d \ge 2$. In other words, the volume occupied by particles in a box of linear size L scales as L^2 when $L \rightarrow 0$, irrespective of dimension $d \ge 2$. For d = 1, the limiting distribution of the process at a fixed time has a continuous density.

The second model differs from the first in that the population size is fixed and equal to *j*. The dynamics are now the following. First suppose that k = 1, 2, ..., j - 1 and $n \ge 1$. In order to obtain the state of the process at time t = nj + k + 1 from that at t = nj + k, we choose randomly one particle and kill it. Next, another particle is chosen from the surviving ones and it branches into two offspring which occupy the same lattice site as the parent particle. If t = nj then we obtain the new configuration at time t = nj + 1 by letting each of the particles move to one of the four nearest sites on the lattice, with probability $\frac{1}{4}$, independent of all other particles.

We renormalize the system in order to obtain a continuum limit. Suppose that at time t = 1 the system consists of j particles located at (0, 0). Let Y_s^j be a measure defined as in the first model, i.e. the measure $Y_s^j(A)$ of an open subset A of \mathbb{R}^2 is equal to the number of particles at time t = [s] which lie in $\sqrt{j}A$. Setting $s = j^2 u$, the sequence of processes $\{Y_{j^2u}^j/j, u \ge 0\}_{j\ge 1}$ converges as $j \to \infty$ to a measure-valued diffusion called the Fleming–Viot process with the initial state $\delta_{(0,0)}$. This process has a similar fractal nature as super-Brownian motion. Indeed, it is known that the Fleming–Viot process Y_t is just super-Brownian motion X_t when the latter is conditioned on the event $X_t(\mathbb{R}^d) = 1$; that is, conditioned to have a constant total mass [16].

Recently there has been growing interest in models incorporating dependence of the motion of individual particles on the current configuration [11, 12]. We propose to study a model with a constant population size in which particles can die and branch at rates which depend on location. It will be seen that the simplest case is when a particle dies if and only if it moves to a set of designated sites on the lattice. In this way our model differs from the two described above.

3. Particle system with death rates depending on position

We fix a connected subset D_{ε} of the square lattice with the mesh size ε , denoted by $(\varepsilon \mathbb{Z})^2$. The particles in our model die if they move outside D_{ε} , so D_{ε} plays the role of the state space. The number of particles is fixed and equal to j. Transitions from the state of the system at time t = k to that at time t = k + 1 may be described as follows. First, each particle goes to one of the four nearest neighbours on the lattice $(\varepsilon \mathbb{Z})^2$, with probability $\frac{1}{4}$, independent of all other particles. Then all particles which are outside D_{ε} die. An equal number of particles is chosen uniformly from among the surviving particles. Each of the chosen particles splits into two offspring which occupy the same site as the parent particle. Hence, the number of particles in our model is constant between generations.

Fix some open connected set $D \subset \mathbb{R}^2$ and let $D_{\varepsilon} = D \cap (\varepsilon \mathbb{Z})^2$. Suppose that at time t = 1 each of the *j* particles occupies a site in D_{ε} . Let $X_s^{j,\varepsilon}$ be the measure-valued process whose value at time *s* is defined as follows. The measure $X_s^{j,\varepsilon}(A)$ of an open subset *A* of \mathbb{R}^2 is equal to the number of particles which are in *A* at time [*s*].

Below we offer a heuristic argument to show that as $j \to \infty$ with $\varepsilon = 1/\sqrt{j}$ and $s = s/\varepsilon^2$ then $X_s^{j,\varepsilon}$ converges to a non-random measure X_s having a density and relate the density, in the limit $s \to \infty$, to the first Laplacian eigenfunction in D with zero boundary values, normalized to have unit integral over D. More precisely, let f(x, y) denote the first eigenfunction of the Laplacian with zero boundary values in D. Then for every open subset $A \subset \mathbb{R}^2$, we have $\lim X_{s/\varepsilon^2}^{j,\varepsilon}(A)/j = \int_A cf(x, y) dx dy$, where $1/c = \int_D f(x, y) dx dy$. Thus it appears that the qualitative long-time behaviour of our system is very different

Thus it appears that the qualitative long-time behaviour of our system is very different from that of super-Brownian motion or the Fleming–Viot process. A typical configuration of particles in these models has a fractal nature. Strictly speaking, the limiting continuous models are measure-valued diffusions whose states are measures supported on fractal sets [11]. In our model, increasing the number of particles j and decreasing the mesh ε of the lattice so that $\varepsilon = 1/\sqrt{j}$ results, in the long run, in a non-random distribution equal to a suitably normalized first eigenfunction of the Laplacian on D with zero boundary values. One physical interpretation of the corresponding first eigenvalue λ_1 is as the exponential rate of decay of the probability that a free Brownian particle remains in D for long times. The corresponding interpretation of the normalized first eigenfunction is that it represents the probability distribution, after a long time delay, for a Brownian particle conditioned to stay within the domain [13]. The asymptotic behaviour of our model gives another, related, interpretation.

Here is a heuristic argument showing the convergence of distributions in our model. These remarks are not meant to be a rigorous proof—this does not seem to be trivial and will be the subject of a forthcoming paper [14].

Notice first that because of the diffusive scaling $x \to \varepsilon x$ and $s \to \varepsilon^{-2}s$, each particle, in the limit $\varepsilon \to 0$, executes a Brownian motion in *D* with a jump, upon exiting *D*, to a point occupied by a fellow particle chosen uniformly at random. Second, since particles interact only through the boundary of *D* by a random choice from the remaining particles, the equal time pair correlations are inversely proportional to the total particle number *j*, and therefore the particles are uncorrelated in the limit $j \to \infty$. Thus the limiting measure $X_s = \lim_{\varepsilon,j} X_{s/\varepsilon^2}^{\varepsilon,j}/j$ exists and is deterministic, by a variant of the law of large numbers. Let us express this limit via its density $X_s(A) = \int_A \xi(s; x, y) dx dy$. Since all particles reside in *D* it follows that $\xi(s; x, y) \ge 0$ and it vanishes for points on the boundary of *D*.

Let $1/\lambda(s)$ be the expected exit time from *D* of a Brownian particle with initial distribution equal to $\xi(s; x, y) dx dy$. Then the per particle rate at which jumps take place is exactly $\lambda(s)$. Thus the density $\xi(s; x, y)$ is the solution of a heat flow problem in *D* with a heat source of strength $\lambda(s)\xi(s; x, y)$ and absorption at the boundary, i.e.

$$\frac{\partial \xi}{\partial s} + \Delta \xi = \lambda(s)\xi \,. \tag{3.1}$$

Here, $\Delta = -1/2(\partial^2/\partial x^2 + \partial^2/\partial y^2)$ is the Laplacian. As $s \to \infty$, the density converges to a solution of the stationary problem, which is the eigenvalue problem for the Laplacian in *D*.

Thus ξ is a non-negative eigenfunction of the Laplacian in *D*. Because the Laplacian is self-adjoint, its eigenfunctions are mutually orthogonal. Since ξ is non-negative, it cannot be orthogonal to the first eigenfunction *f* and therefore must be a scalar multiple $\xi = cf$. It follows that $1/c = \int_D f(x, y) dx dy$, since ξ has total integral 1, and that in equilibrium the expected exit time from *D* is $1/\lambda_1$, the reciprocal of the first eigenvalue.

4. Multi-type particle system

The first eigenfunction of the Laplacian with zero boundary values already has a natural probabilistic interpretation [13] and the model described in the previous section provides a new one. It seems that so far the higher eigenfunctions do not have a natural probabilistic interpretation. A model described in this section may be a first step towards such an interpretation.

Fix a connected subset D_{ε} of the square lattice $(\varepsilon \mathbb{Z})^2$ with the mesh size ε . In this model, each particle will reside in D_{ε} and have one of *m* possible types \mathcal{L}_k , k = 1, 2, ..., m. Typically, at each time t = l some particles will be chosen to split into two offspring. In such a case we will say that a new offspring was born at time t = l and if this particle is killed at some later time t = n then we will say that the lifetime of this particle was T = n - l. The transition mechanism of the system, which depends on the positions, types and lifetimes of the particles, is the following one. First each of the particles goes to one of the four nearest sites on the lattice $(\varepsilon \mathbb{Z})^2$, with probability $\frac{1}{4}$, independent of all other particles. Then all particles which moved outside D_{ε} are killed. If a site in D_{ε} is occupied by particles of several types, then two particles of different types are chosen randomly and are also killed. We repeat the procedure, killing pairs of particles of different type occupying the same site until there are no sites in D_{ε} with more than one type of particle. Killed particles will be replaced with new offspring as follows. For every k, we choose n_k (to be defined below) particles of type \mathcal{L}_k randomly from among the surviving ones and each of these particles splits into two offspring of the same type which then occupy the same site as the parent particle. Now we define n_k . Let n_k^1 be the number of particles of type \mathcal{L}_k which died because they moved outside D_{ε} . Let n_k^2 be the number of the pairs of particles which were killed inside D_{ε} such that the types and lifetimes of the particles involved were (\mathcal{L}_i, T_1) and (\mathcal{L}_k, T_2) and $T_1 > T_2$ (i.e. the particle with type \mathcal{L}_k had a shorter lifetime). Let n_k^3 be defined just as n_k^2 except that we replace the condition $T_1 > T_2$ with the condition $T_1 = T_2$. Then we set $n_k = n_k^1 + 2n_k^2 + n_k^3$. Note that the total number of particles in our model is constant between generations but the number of particles of type \mathcal{L}_k can vary, for each k.

Again, we consider the high-density limit distribution for the system. Fix some open connected set $D \subset \mathbb{R}^2$, let $D_{\varepsilon} = D \cap (\varepsilon \mathbb{Z})^2$ and assume that at time t = 1 all particles occupy sites in D_{ε} . Recall that we have a total of j particles which belong to m different types \mathcal{L}_k . Let the measure $X_s^{k,j,\varepsilon}$ of an open subset A of \mathbb{R}^2 be equal to the number of particles of type \mathcal{L}_k which are in A at time [s].

Fix $m \ge 2$ and $D \subset \mathbb{R}^2$ and let $j \to \infty$, $\varepsilon \to 0$ and $s \to \infty$. In the limit, for every k, the measure $X_{s/\varepsilon^2}^{k,j,\varepsilon}(dx, dy)/j$ will converge to $c_k f_k(x, y) dx dy$ (in other words, $X_{s/\varepsilon^2}^{k,j,\varepsilon}(A)/j \to \int_A c_k f_k(x, y) dx dy$ for every open set $A \subset \mathbb{R}^2$) where $0 < c_k < \infty$ and f_k is the first eigenfunction of the Laplacian with zero boundary values on a subdomain D_k of D. Because of the dynamics, particles of different types become segregated so the subdomains D_k are disjoint and their union is D. Our transformation rules have been chosen so that the average lifetimes of particles of different types are equal in the limit. If at a certain time the average lifetime of particles of type \mathcal{L}_k is smaller than that for type \mathcal{L}_n , the collisions of the particles of these two types will result in an increase of the number of particles of type \mathcal{L}_k . This will imply the growth of the subregion D_k occupied by particles of type \mathcal{L}_k and hence their average lifetime will increase. The opposite will be true for the particles of type \mathcal{L}_n and so in the limit the average lifetimes of all types of particle will be the same.

The average lifetime of a particle of type \mathcal{L}_k is equal to the inverse of the first eigenvalue in D_k . Hence, the first eigenvalue for the Laplacian with zero boundary conditions in D_k is the same for every k, in the limit.

Let (x, y) be a point on the boundary between two subregions D_k and D_n and let N be the normal unit vector to the boundary at (x, y) pointing inside D_k . Note that the normal unit vector \hat{N} at (x, y) pointing inside D_n is the same as -N. Then we must have $\partial c_k f_k / \partial N = -\partial c_n f_n / \partial(\hat{N})$ because the particles of both types are killed on the boundary at the same rate.

5. Limit distribution and Laplacian eigenfunctions

Let $F(x, y) dx dy = F_m(x, y) dx dy$ be equal to the limit of $X_{s/\epsilon^2}^{k,j,\epsilon}(dx, dy)/j$ on D_k . In other words, $F(x, y) = c_k f_k(x, y)$ on D_k and the constants c_k are such that $\partial c_k f_k/\partial N = -\partial c_n f_n/\partial(\hat{N})$ on the boundary between D_k and D_n , where N is the inward normal vector on the boundary of D_k and $\hat{N} = -N$. Hence, $\partial F/\partial N = -\partial F/\partial(\hat{N})$ on the boundary between D_k and D_n .

Suppose that g is an eigenfunction for the Laplacian in D with zero boundary values. The lines where g is equal to zero are called 'nodal lines' and they divide D into a number of subregions \widetilde{D}_k . The function g is differentiable, so we must have $\partial |g|/\partial N = -\partial |g|/\partial(\hat{N})$ on the boundary between \widetilde{D}_k and \widetilde{D}_n . Moreover, |g| is the first eigenfunction for the Laplacian on every subregion \widetilde{D}_k . This suggests that F_m may be equal to |g| for some eigenfunction g of the Laplacian in D.

A simple example shows that for some D and m, the limit distribution F_m cannot be equal to |g| for any eigenfunction g in D. This is the case when an odd number of 'nodal lines' for F_m meet at a single point. The number of nodal lines meeting at one point must be even for an eigenfunction since the sign of the eigenfunction in adjacent regions defined by its nodal lines must alternate. There would be no consistent way of assigning signs to adjacent regions if an odd number of them met at an intersection point of nodal lines. Figure 1(*b*) illustrates a limit distribution for a system with three particle types. In this case, there are three nodal lines for F_m which meet at one point and consequently F_m cannot be equal to |g| in this case.

One may ask, then, when the limit distribution F_m for a multi-type particle system corresponds to a higher eigenfunction. We concentrated our efforts on one particular class of domains, namely rectangles D, because in this case, the eigenvalues and the corresponding eigenfunctions can be calculated explicitly.

Let $D = \{(x, y) \in \mathbb{R}^2 : 0 < x < a, 0 < y < b\}$. Then all eigenvalues of the Laplacian in D with zero boundary values are given by $\lambda_{j,k} = \pi^2[(j/a)^2 + (k/b)^2]$, where j and k are arbitrary integers greater than 0 [15]. The eigenfunction corresponding to $\lambda_{j,k}$ has the form $f_{j,k}(x, y) = \sin((j\pi/a)x)\sin((k\pi/b)y)$. It may happen that $\lambda_{j_1,k_1} = \lambda_{j_2,k_2}$ even though $j_1 \neq j_2$ and $k_1 \neq k_2$ but this is possible for only a countable number of side ratios r = b/a. We can also write $\lambda_{j,k}$ as $(\pi/a)^2(j^2 + (k/r)^2)$. It is clear intuitively that when the number of types of particle *m* is constant but the side ratio of *D* is very large then particles of different types will occupy *m* rectangles arranged in a linear order (see, for example, figure 1(*a*)). We will call this arrangement 'elementary'. It corresponds to an eigenfunction $f_{j,k}$ of the Laplacian with either j = 1 or k = 1. This effect is due to the tendency of different populations to segregate and an elementary configuration seems to be a natural way to achieve maximum segregation. It is not so clear what happens when the side ratio is moderate. When *m* is fixed, say m = 3, and the side ratio is close to 1, we obtain in computer simulations a configuration illustrated in figure 1(*b*) which does not correspond to any eigenfunction. We determined by simulation the critical side ratio at which we observe the transition between the elementary configuration and a configuration which does not correspond to any eigenfunction.

6. Computer simulations

Further discussion of the limiting distributions and eigenvalues will be illustrated by computer simulations so we make a digression to explain our figures. In all simulations we took D to be a rectangle. The figures show the regions D and the boundaries between the subregions occupied by different particle types. All simulations were done for rectangles D with sides b = 100 and 100 < a < 300. Because of memory constraints, the results of the simulations were compressed in the following way. Every region D was divided into a number of small identical rectangles, usually with side lengths between 5 and 10. The numbers of particles of different type were found in every small rectangle and the rectangle was declared of type \mathcal{L}_k if the number of particles of this type was the greatest of all particle types. Only rectangles close to the boundaries between D_k 's contained different particle.

We simulated the long-time behaviour of a system with 100 000 particles in rectangles of different side ratios. Most simulations ran for 150 000 or 200 000 time steps. The starting configurations included 'elementary configurations', other configurations with polygonal separating lines and totally random configurations. We used various initial proportions of different particle types. We did simulations with m = 3, 4 and 5 particle types. In each case we determined the critical side ratio $r_m = a/b$ at which we observed a transformation of the stationary configuration. The simulations were performed in 20 different rectangles. Due to the time-consuming nature of the simulations, the number of independent samples varied from one to five per rectangle. The final configurations for the segregation phases were unique and did not depend on the initial configuration except when the side ratios were close to the critical values discussed below.

When the number of particle types is m = 3, the critical side ratio is 1.64 ± 0.01 (figure 1). The simulations starting from various initial distributions show that the limit distribution is elementary for the ratio 1.65 and it is not for the ratio 1.62. In the case of side length ratios 1.63 and 1.64, the particle configuration had a tendency to preserve its initial shape if the initial shape was as in figure 1(*a*) and (*b*).

The results of the simulations are most clear in the case of four particle types. Each of the simulations was started from an asymmetric configuration. The critical ratio is 2.26 ± 0.01 . The particle distributions are given in figure 2.

Simulations with five particle types (figure 3) were also started from asymmetric distributions. In this case, the critical side ratio is 2.85 ± 0.01 .

An 'asymmetric' initial configuration is illustrated in figure 4.



Figure 2. Nodal lines for stationary distribution of particles of four particle types. Each region, separated by full lines, is occupied by only one type of particle. (*a*) The side ratio $r_4 = a/b = 2.27$; elementary configuration corresponding to the fourth Laplacian eigenfunction, (*b*) $r_4 = 2.24$; configuration close to the transition point (non-elementary configuration), (*c*) $r_4 = 1$; configuration far from the transition point (non-elementary configuration).



Figure 3. Nodal lines for stationary distribution of particles of five particle types. Each region, separated by full lines, is occupied by only one type of particle. (*a*) The side ratio $r_5 = a/b = 2.88$; elementary configuration corresponding to the fifth Laplacian eigenfunction, (*b*) $r_5 = 2.84$; configuration close to the transition point (non-elementary configuration), (*c*) $r_5 = 1$; configuration far from the transition point (non-elementary configuration).

7. Configurational transition and Laplacian eigenvalues

We will argue that the critical side ratios obtained from the computer simulations match exceptionally well the critical rectangle side ratios for the following problem. *When is it true that the elementary configuration with m subregions corresponds to the mth eigenfunction?* Here we order the eigenfunctions according to their eigenvalues, i.e. the *m*th eigenfunction corresponds to the *m*th smallest eigenvalue.

Recall the formulae for the eigenvalues of the Laplacian given in section 3. We have $\lambda_{j,k} = (\pi/a)^2 (j^2 + (k/r)^2)$ for a rectangle with sides equal to *a* and *b* and side ratio r = b/a. The elementary configuration is defined by the eigenfunction corresponding to $\lambda_{1,m}$. Whether $\lambda_{1,m}$ is the *m*th eigenvalue depends only on *r* and does not otherwise depend on the values of *a* and *b*. Note that $\lambda_{1,k} < \lambda_{1,m}$ for k < m so $\lambda_{1,m}$ is the *m*th eigenvalue if and only if



Figure 4. An 'asymmetric' initial configuration with four particle types. Configurations of this type were used as initial configurations for many simulations.

$$\lambda_{1,m} < \lambda_{2,1} \,. \tag{7.1}$$

This is equivalent to (section 5)

$$1^{2} + (m/r)^{2} < 2^{2} + (1/r)^{2}.$$
(7.2)

We take m = 3, 4, 5 and solve this equation for r to obtain the following critical side ratios r_m : $r_3 = \sqrt{8/3} \approx 1.63$, $r_4 = \sqrt{5} \approx 2.24$, $r_5 = 2^{3/2} \approx 2.83$.

Since our simulations were done on a discrete lattice, the critical side ratios calculated for the rectangle D in \mathbb{R}^2 are only approximate. Eigenfunctions for the discrete Laplacian on a rectangle $D = \{(x, y) \in \mathbb{Z}^2 : 1 \le x \le a, 1 \le y \le b\}$ are given by $\tilde{f}(x, y) = g(x)h(y)$ where g and h satisfy g(0) = g(a + 1) = 0, h(0) = h(b + 1) = 0, and

$$g(x-1) - 2g(x) + g(x+1) = -\lambda^x g(x) \qquad 1 \le x \le a$$

$$h(y-1) - 2h(y) + h(y+1) = -\lambda^y h(y) \qquad 1 \le y \le b.$$

Then $\tilde{\lambda} = \tilde{\lambda}^x + \tilde{\lambda}^y$ is the eigenvalue corresponding to the eigenfunction $\tilde{f}(x, y) = g(x)h(y)$. If g changes sign j - 1 times and h changes sign k - 1 times then $\tilde{\lambda} = \tilde{\lambda}_{j,k}$ is a discrete analogue of $\lambda_{j,k}$. We have the following explicit formulae for the eigenfunctions and the corresponding eigenvalues.

$$g_j(x) = \sin(j\pi x/(a+1)) h_k(y) = \sin(k\pi y/(b+1)) \tilde{\lambda}_j^x = 2(1 - \cos(j\pi/(a+1))) \tilde{\lambda}_k^y = 2(1 - \cos(k\pi/(b+1)))$$

The discrete analogues of inequalities (7.1) and (7.2) are

$$\widetilde{\lambda}_{m,1} < \widetilde{\lambda}_{1,2}$$

and

$$\cos(m\pi/(a+1)) + \cos(\pi/(b+1)) > \cos(\pi/(a+1)) + \cos(2\pi/(b+1)).$$

In the case where b = 100, the critical values for a in the last inequality are in the following intervals,

$$\begin{array}{ll} 163 < a < 164 & m = 3\\ 224 < a < 225 & m = 4\\ 284 < a < 285 & m = 5 \end{array}$$

These values match very well the critical side lengths discussed in the previous section.

It is quite intriguing that the configurational transition takes place for side ratio related to the eigenvalue of the Laplacian (equations (7.1) and (7.2)). It would be interesting to find an explanation for this phenomenon. We hope that our results will be useful in the future studies of population dynamics.

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