Mean-Field Analysis of a Dynamical Phase Transition in a Cellular Automaton Model for Collective Motion

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When in the course of evolutionary events it became possible for cells to actively crawl and move towards more favorable habitats, this led to an acceleration of evolutionary change. Another important step was the development of social behavior, manifested in cooperative motion of individual cells or organisms. In particular, a change from independent crawling to cooperative motion is typical of life cycles in many microorganisms.

Moving cells can orient themselves by means of indirect physico-chemical signals like electrical fluxes or molecular concentration gradients; the response of individual cells to such environmental information may result in collective streaming behavior and swarm patterns. Many models have been formulated along these lines of argument, all focusing on similar aspects of physico-chemical communication (see examples in Ref. ¹).

Here we are interested in the implications of direct communication between biological units (e.g. cells or birds). Based on the assumption that the units have an inherent direction of motion, and try to locally align with other units, several microscopic models for swarming behavior have recently been proposed ², ³. These models can be viewed as itinerant XY-models that can be analyzed using renormalization group methods, starting from a postulated equation of motion ³.

In this Letter we take a different approach. We define a cellular automaton model ⁴ that has the necessary features to produce swarming behavior, while the discreteness in time and space allows for relatively easy analysis. We analyze our model directly, using an approximate mean-field kinetic equation, and identify and derive dispersion relations for the various collective modes. An important question is how alignment is achieved, starting from a random spatial distribution. We show that swarming formation is associated with a continuous dynamical phase transition, occurring when a sensitivity parameter reaches a critical value. Spontaneous symmetry breaking leads to states with a global particle drift. The initial formation of patches is related to the fact that only at sufficiently large wavenumbers the density and longitudinal momentum modes merge to form a pair of propagating sound modes. We calculate the critical exponents governing the behavior of the average drift velocity close to criticality.

The model we use is a lattice gas cellular automaton ⁴ defined on a two-dimensional $L \times L$ square lattice with periodic boundary conditions. Each node $r$ can contain up to four particles in different velocity channels corresponding to nearest neighbor vectors $c_i = (\cos \phi_i, \sin \phi_i)$ with $\phi_i = \pi(i - 1)/2$ and $1 \leq i \leq 4$. The state of the entire lattice at time $t$ is specified by the occupation numbers $s_i(r, t) = 0, 1$ denoting the absence resp. presence of a particle in the channel $(r, c_i)$. The state of node $r$ is denoted by $s(r, t) = \{s_i(r, t)\}_{1 \leq i \leq 4}$.

The evolution from time $t$ to time $t + 1$ proceeds in two stages: first an interaction step is performed during which the preinteraction state $\{s_i(r, t)\}$ is replaced by a postinteraction state $\{\sigma_i(r, t)\}$ according to stochastic rules that are applied to each node independently; the interaction step is followed by a propagation step during which particles move to nearest neighbor sites in the direction of their velocity, i.e., $s_i(r + c_i, t + 1) = \sigma_i(r, t)$.

To implement the local alignment interaction we define

$$D(r, t) = \sum_{p=1}^{4} \sum_{i=1}^{4} c_i s_i(r + c_p, t),$$

specifying the average flux of particles at the nearest neighbors of node $r$. We require that the number of particles at each node, $\rho(r, t) = \rho[s(r, t)] = \sum_{i=1}^{4} s_i(r, t)$, is conserved during interaction; this implies that the spatially averaged density of particles per node $\bar{\rho}$ is constant in time. Let $J(\sigma) = \sum_{i=1}^{4} c_i \sigma_i$ be the particle flux immediately after interaction. The transition probability from $s(r, t)$ to $\sigma(r, t)$ in the presence of $D(r, t)$ is given by

$$A[s \to \sigma|D] = \frac{1}{Z} \delta[\rho(\sigma), \rho(s)] \exp \left[ \beta D \cdot J(\sigma) \right],$$

where the normalization factor $Z(\rho(s), D)$ is chosen such
that \( \sum_{x} A[s \rightarrow \sigma][D] = 1 \) for all \( s \). The interaction rules are designed to minimize the angle between the director field \( D \) and the postinteraction flux \( J(\sigma) \).

The sensitivity parameter \( \beta \), playing the role of an inverse temperature, controls the degree of local alignment: for \( \beta = 0 \) there is no alignment at all; for \( \beta \rightarrow \infty \) the two-dimensional inner product \( D \cdot J(\sigma) \) — and therefore the local alignment — is maximized. It will turn out that a dynamical phase transition occurs at a critical value \( \beta_c \) of the sensitivity. Figure 1 shows the time evolution of an initially random distribution for \( \beta > \beta_c \). The formation of locally aligned patches can clearly be observed. There is some anisotropy due to the square lattice; it is however straightforward to extend the model to the triangular lattice. It is an interesting question whether the phase ordering kinetics shown in Fig. 1 can be described in terms of dynamical scaling theory 8.

To analyze the behavior of the model we consider the time evolution of a statistical ensemble of systems. For technical details we refer to Ref. 3, where a model with only slightly different interaction rules 11 yet entirely different behavior was analyzed. In a mean-field description a central role is played by the average occupation numbers \( f_i(\mathbf{r}, t) \equiv \langle s_i(\mathbf{r}, t) \rangle \). It is assumed that at each time step just before interaction the probability distribution is completely factorized over channels \( \{ \mathbf{r}, \mathbf{c}_i \} \), so that the probability to find a microstate \( \{ s_i(\mathbf{r}) \} \) at time \( t \) is given by \( \prod_{\mathbf{r}} \prod_{i=1}^{4} f_i(\mathbf{r}, t) \alpha(\mathbf{r})[1 - f_i(\mathbf{r}, t)]^{1 - \alpha(\mathbf{r})} \).

We denote the factorized average by \( \langle \cdot \cdot \cdot \rangle_{\text{MF}} \). Replacing \( \langle \cdot \cdot \cdot \rangle \) by \( \langle \cdot \cdot \cdot \rangle_{\text{MF}} \), i.e., neglecting all correlations between occupation numbers, we obtain a closed evolution equation for \( f_i(\mathbf{r}, t) \): the nonlinear Boltzmann equation,

\[
f_i(\mathbf{r} + \mathbf{c}_i, t + 1) = f_i(\mathbf{r}, t) + I_i(\mathbf{r}, t).
\]

Here the term \( I_i(\mathbf{r}, t) \equiv \langle s_i(\mathbf{r}, t) - s_i(\mathbf{r}, t) \rangle_{\text{MF}} \), taking values between \(-1\) and \(1\), equals the average change in the occupation number of channel \( \{ \mathbf{r}, \mathbf{c}_i \} \) during interaction.

It follows from the conservation of particle number, \( \sum_i I_i = 0 \), combined with the invariance of the interaction rules under discrete rotations and translations that a possible solution to Eq. (3) is \( f_i(\mathbf{r}, t) = f = \bar{\rho}/4 \). To assess the stability of this spatially homogeneous and stationary solution with respect to fluctuations \( \delta f_i(\mathbf{r}, t) = f_i(\mathbf{r}, t) - f \) we linearize Eq. (3), perform a Fourier transformation, \( \delta f_i(k, t) = \sum_{\mathbf{r}} e^{-i k \cdot \mathbf{r}} \delta f_i(\mathbf{r}, t) \), and obtain

\[
\delta f_i(k, t + 1) \approx \sum_{j=1}^{4} \Gamma_{ij}(k) \delta f_j(k, t).
\]

The mean-field or Boltzmann propagator \( \Gamma(k) \) describes how a small perturbation around a spatially uniform state evolves in time. It is given by

\[
\Gamma_{ij}(k) = e^{-i k \cdot c_i} \left[ \delta_{ij} + \sum_{p=0}^{4} e^{i k \cdot c_p} \Omega_{ij}^p \right],
\]

with \( c_0 \equiv 0 \) and \( \Omega_{ij}^p = \partial I_i(\mathbf{r}, t)/\partial f_j(\mathbf{r} + \mathbf{c}_p, t) \). It can be shown that \( \delta_{ij} + \Omega_{ij}^p = 1/4 \) for all \( i, j \); this is a consequence of the fact that the outcome \( \sigma(\mathbf{r}) \) of an interaction step only depends on \( s(\mathbf{r}) \) through \( \rho(\mathbf{r}) \) (see Eq. (3) and Ref. 3).

For \( 1 \leq p \leq 4 \) the elements \( \Omega_{ij}^p \equiv \omega_{ij} \) do not depend on \( p \), as can be seen from the definition of \( D \) in Eq. (4). We note that \( \omega_{ij} \) is a cyclic matrix whose first row has the structure \( (\alpha + \gamma, -\gamma, -\alpha + \gamma, -\gamma) \). To determine \( \alpha(\beta, \bar{\rho}) \) and \( \gamma(\beta, \bar{\rho}) \) for given values of the sensitivity \( \beta \) and the average density \( \bar{\rho} \) we evaluate the expression (this is done numerically because of the highly nonlinear dependence on \( f_i \) and \( \beta D \), combined with the large number of terms)

\[
\omega_{ij} = \sum_{s} A[s \rightarrow D(\{s(\mathbf{r} + \mathbf{c}_p)\})] \prod_{p' = 0}^{4} F(s(\mathbf{r} + \mathbf{c}_{p'})),
\]

where \( F(s) = \prod_{i=1}^{4} \bar{f}^s(1 - \bar{f})^{1-s} \) is the factorized distribution. Note that the expression for \( \omega_{ij} \) does not depend on \( \mathbf{r} \) since it represents a derivative evaluated in a spatially uniform state.

We first investigate the stability of the spatially uniform state, i.e. \( \bar{\rho} = 0 \). It can be seen that the propagator
\(\Gamma_{ij}(k = 0)\) has an eigenvalue \(\lambda_1 = 1\) with corresponding eigenvector \(e_1 = (1, 1, 1, 1)\), reflecting the fact that the total density is conserved. Furthermore there is a twofold degenerate eigenvalue \(\lambda_{x,y} = 8\) so with an eigenspace spanned by \(e_x = (1, 0, -1, 0)\) and \(e_y = (0, 1, 0, -1)\), corresponding to the \(x\)- and \(y\)-components of the total particle flux. The remaining eigenvector \(e_{x^2-y^2} = (1, -1, 1, -1)\) has eigenvalue \(\lambda_{x^2-y^2} = 16\gamma\), corresponding to the difference between the number of horizontally and vertically moving particles. Numerically \(\gamma\) is found to be about two orders of magnitude smaller than \(\alpha\), so that the onset of instability of the homogeneous state is determined by the condition \(\lambda_{x,y} = 1\). The location of the critical line in the \((\beta, \bar{\rho})\) parameter plane is shown in Fig. 3, which was obtained by numerically solving the equation \(\alpha(\beta, \bar{\rho}) = 1/8\).

To see if in addition to the emergence of a global drift we can explain the formation of spatial structure in terms of the eigenvalue spectrum, we study the case \(k \neq 0\). It is convenient to work with \(z(k) = \ln \lambda(k)\) so that excitations behave as \(\delta f(r, t) \propto \exp[z(k) t + ik \cdot r]\). Unstable modes have \(\text{Re} z(k) > 0\) while stable modes have \(\text{Re} z(k) < 0\). An imaginary part of \(z(k)\) indicates that the mode has a nonzero propagation velocity \(v(k) = \text{Im} z(k)/|k|\). Figure 3 shows that the fastest growth occurs at \(k = 0\). For \(k \neq 0\) the degeneracy of \(\lambda_{x,y}\) is lifted, and it is then the transverse velocity (i.e., perpendicular to \(k\)) that grows fastest. At \(|k| = k_p\), with \(k_p = k_p(\bar{\rho}, \beta)\), where \(k\) is the unit vector in the direction of \(k\), the density and longitudinal velocity modes merge to form a pair of propagating sound-like modes, with \(\text{Im} z(k) \neq 0\), and traveling in the directions \(\pm k\). Thus, traveling waves cannot occur on spatial scales larger than \(2\pi/k_p\), which may explain the length scale for short times of the spatial structure shown in Fig. 3.

Our mean-field stability analysis illuminates the nature of the observed phase transition. An appropriate order parameter is the spatially averaged velocity,

\[
\bar{\mu}(t) = \frac{1}{L^2} \sum_r \sum_{i=1}^4 c_i(r, t),
\]

which takes values between 0 and 1. For \(\beta < \beta_c\), we have \(\bar{\mu} = 0\). When the sensitivity parameter \(\beta\) reaches its critical value, this “rest” state becomes unstable, leading to a breaking of rotational symmetry, and a stationary state where \(\bar{\mu} \neq 0\).

We have compared the results of our stability analysis with computer simulations. Fig. 4 shows \(\bar{\mu}\) versus \(\beta\) for averaged density \(\bar{\rho} = 0.4\). There is an abrupt change in \(\bar{\mu}\) at \(\beta \simeq 0.7\), which agrees well with the prediction \(\beta_c = 0.67\) obtained from our stability analysis.

A discussion of the question whether the transition is first order or continuous is only meaningful if we consider the limit \(t \to \infty\), the analogue of the thermodynamic limit \(L \to \infty\). For \(\beta < \beta_c\) all modes are stable and we have \(\bar{\mu}(t \to \infty) = 0\). To determine the behavior of \(\bar{\mu}\) for \(\beta > \beta_c\), we consider spatially homogeneous and stationary solutions to the nonlinear Boltzmann equation (3), i.e. \(\delta f_i(r) = \delta f_i\) and \(I_i = 0\). Knowing that the “rest” solution, \(f_i = \bar{f}_i = \bar{\rho}/4\), is stable for \(\beta < \beta_c(\bar{\rho})\), we expand around the critical point \((\bar{\rho}, \beta_c)\):

\[
I_i(\bar{\rho} + \Delta \rho , \beta_c + \Delta \beta) = \sum_k \left( \bar{\Omega}_{ik} + \frac{\partial \bar{\Omega}_{ik}}{\partial \beta} \Delta \beta \right) \delta f_k + \frac{1}{2} \sum_{k_1 \leq k_2} \bar{\Omega}_{ik_1,k_2} \delta f_{k_1} \delta f_{k_2} + \ldots
\]

where \(\bar{\Omega}_{ik_1 \ldots k_n} = (\partial/\partial f_{k_1}) \cdots (\partial/\partial f_{k_n}) I_i\).

We use a particular parametrization for “drift” solutions along the \(x\)-axis: \(\delta f_1 - \delta f_3 = \bar{\mu}, \delta f_2 = \delta f_4 = 0\). Utilizing \(I_1 = I_2 = 0\), together with the symmetry properties of the expansion coefficients \(\bar{\Omega}_{ik_1 \ldots k_n}\) and the fact that at the critical point all three vectors, \(c_x\), and \(c_y\) are zero eigenvectors of \(\bar{\Omega}_{ik}\), we can eliminate \(\delta f_i\) and for small \(\Delta \rho\) and \(\Delta \beta\) obtain the following equation of state:

\[
(c_3 \Delta \beta + c_\rho \Delta \rho) \bar{\mu} - \bar{\mu}^3 \simeq 0.
\]

Here \(c_3\) and \(c_\rho\) are positive constants that depend on the expansion coefficients \(\bar{\Omega}_{ik_1 \ldots k_n}\).

Consider now the case \(\Delta \beta \neq 0, \Delta \rho = 0\). The solution \(\bar{\mu} = 0\) is stable only for \(\beta < \beta_c\), or \(\Delta \beta < 0\). From Eq. 4 we see that for \(\Delta \beta > 0\) there is an additional, stable solution \(\bar{\mu} \sim \sqrt{\beta}\). Thus for the critical exponent \(\beta'\) defined by \(\bar{\mu} \sim (\beta - \beta_c)^{\beta'}\) in Ref. 3 we find \(\beta' = \frac{1}{2}\). A different exponent \(\delta\), defined by \(\bar{\mu} \sim (\rho - \rho_c)^{\delta}\), governs the behavior for \(\Delta \rho \neq 0, \Delta \beta = 0\). From Eq. (4) we obtain \(\delta = \frac{1}{2}\).
The essential elements of our analysis are the “hydrodynamic” variables density and velocity. Therefore we expect that many of our predictions — including the value of the critical exponents — should also apply to the continuum swarming model of Ref. [3]. From a coarse-grained point of view our model and that of Ref. [3] are equivalent. In particular the noise parameter \(\eta\) in Ref. [3] plays a role analogous to \(1/\beta\) in our model.

Our analysis confirms the numerical finding of Ref. [3] that the phase transition is continuous, but is in conflict with the results of Ref. [2]. The exponents \(\beta'\) and \(\gamma\) have been measured in computer simulations [5]. From a coarse-grained point of view our model and that of Ref. [3] are equivalent. In particular the noise parameter \(\eta\) in Ref. [3] plays a role analogous to \(1/\beta\) in our model.

Our model has an interesting biological interpretation since the dynamical phase transition suggests two possible scenarios for a change from non-cooperative to cooperative behavior. On one hand, genetically caused minor microscopic effects on receptor properties of interacting cells influencing their sensitivity can have severe macroscopic implications with respect to swarming if they occur close to criticality (cf. Fig. 2). On the other hand, a transition from the stable into the unstable region can also be achieved by simply increasing cell density (cf. Fig. 2). This result provides a possible clue to explain the behavioral change between non-cooperative and cooperative stages in individual life cycles of some bacteria and amoebae in which a reproductive feeding phase of individually moving cells is followed by social (coordinated) aggregation. Other models for complex bacterial pattern formation, including vortex and colony organization, have also been proposed (see Refs. [4][5] and references therein).

Finally, we want to stress that the methods employed here can easily be adapted to gain theoretical insight in the behavior of a wide range of biologically motivated cellular automaton models, that so far have mainly been analyzed by observation of simulation outcomes [10].

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