

PHASE TRANSITIONS IN AUTOCATALYTIC CYCLES (TRANZICIONET FAZORE NË QARQET AUTOKATALITIKE)

Margarita IFTI^a and Birger BERGERSEN^b

^a) Department of Physics, Faculty of Natural Sciences, University of Tirana,
ALBANIA

^b) Department of Physics and Astronomy, University of British Columbia,
CANADA

ABSTRACT

We discuss an autocatalytic reaction system: the cyclic competition model $A_1+A_2 \rightarrow 2A_2$, $A_2+A_3 \rightarrow 2A_3$, $A_3+A_4 \rightarrow 2A_4$, $A_4+A_1 \rightarrow 2A_1$, as well as its neutral counterpart. Migrations are introduced into the model. When stochastic phenomena are taken into account, a phase transition between a "fixation" and a "neutral" regime is observed. In the "fixation" regime, species A_1 and A_3 form an alliance against species A_2 and A_4 , and the final state is one in which one of the symbiotic pairs has won. The odd-even "coarse-grained" system is mapped onto the two-species neutral (Kimura) model. In the "neutral" regime, all four species survive for long (evolutionary) times. The analytical results are checked against computer simulations of the model. The model is generalized for n species.

Keywords: cyclic competition, autocatalytic system, nonequilibrium phase transition, system size dependence

PËRMBLEDHJE

Sistemi në shqyrtim është një reaksion vetëkatalizues: modeli i konkurrencës ciklike $A_1+A_2 \rightarrow 2A_2$, $A_2+A_3 \rightarrow 2A_3$, $A_3+A_4 \rightarrow 2A_4$, $A_4+A_1 \rightarrow 2A_1$, si edhe analogu i tij neutral. Në

model lejohen migracione të pjesëzave. Kur merren parasysh dukuritë stokastike, vërehet një kalim fazor ndërmjet një regjimi të "fiksimit" dhe atij "neutral". Në regjimin e "fiksimit", speciet A_1 dhe A_3 formojnë një aleancë kundër specieve A_2 and A_4 , dhe në gjendjen përfundimtare fiton njëri nga çiftet simbiotike. Sistemi "i bluar trashë" i specieve tek e çift është ekuivalent me modelin neutral të Kimurës. Në regjimin "neutral" të katër speciet mbijetojnë për një kohë shumë të gjatë. Rezultatet analitike verifikohen me simulime kompjuterike të modelit. Modeli përgjithësohet për n specie.

INTRODUCTION

There is a class of processes in which the competition plays a very important role. Examples are ecological, political, epidemiological, economic, chemical, reaction-diffusion, biological systems. An important sub-class of those is the cyclic competition systems. In ecology, cases when variants of a species compete with one-another in a cyclic fashion have been observed [13, 7, 15]. Another system of interest are cyclic food webs. In politics, different political parties compete and replace one-another in the helm of power. In the epidemiological context, examples are diseases which do

not leave permanent immunity, known otherwise as *SIRS* (Susceptible-Immune-Recovered-Susceptible) models [1, 4]. Goodwin [3] introduced a system of interacting biochemical metabolic oscillators, which has an autocatalytic feedback mechanism. Biochemical reactions in a cell support its activities, hence assuring its very existence. Autocatalytic reactions are an important class of reactions within a cell. They are reputed to have made possible the birth and existence of life itself.

The simplest example of an autocatalytic reaction is the loop of the type $A_i + A_{i+1} \rightarrow 2A_{i+1}$, where $i = 1, \dots, k$; $A_{k+1} = A_1$. The molecules are in a well-stirred container (the cell), which is in contact with a reservoir (the outside environment). They can migrate into and out of the container, to and from the reservoir, according to the following rules: a molecule (individual) of species i leaves the container at a rate $D \cdot a_i$, and enters it at a rate $D \cdot s_i$, where a_i and s_i are its concentrations in the cell and the reservoir, respectively. In another (ecological) context, the $\{A_i\}$'s are versions of a biological species, and in the epidemiological one, states of an individual (e.g. susceptible, infected, etc.)

In ecological systems it makes sense to also study the neutral version of this model, in which $A_i + A_{i+1} \rightarrow 2A_{i+1}$, or $2A_i$ with equal probability, corresponding to the Kimura model of neutral genetic drift [8, 9, 10]. The behaviour of the two allele almost neutral drift model with mutations is well studied [11, 2]. For small mutation probabilities, smaller than $1/N$, there is extinction of one species and fixation. Otherwise, both species coexist forever in the high mutation ("neutral") regime. The transition is second-order, and critical behaviour is observed.

In two previous studies [5, 6] we have considered an *ABC* model with cyclic competition/neutral drift and mutations (migrations) at a constant probability. The system exhibits a critical transition from a "fixation" regime to a "neutral" one. The survival probability decays exponentially below the transition point, but the exponent decreases as the mutation (migration) probability per particle increases, until it becomes zero at the critical point. The critical mutation (migration) probability depends on system size as $1/N$, and

the models have the same power-law exponent: -1. There is no qualitative difference between the system with mutations and that with migrations.

In the present paper we study the system with four species, and show that the above-described picture still holds. Next we generalize for the n -species system.

2. SYSTEM-SIZE EXPANSION OF THE MASTER EQUATION

The rate equations of our model read:

$$\frac{da_i}{dt} = a_{i-1}a_i - a_i a_{i+1} + D(s_i - a_i) \quad (1)$$

In the rate equations approximation, the system size is conserved. The rate equations (1) have a fixed point, and it is a stable solution. Hence in this approximation, the system will approach the centre (all a_i 's are equal), and remain there. However, the rate equations only describe the behaviour of the average values of the individual populations. In the real world, the system is subject to stochastic noise due to birth and death processes (intrinsic noise), which we take to be Poisson-distributed. The random nature of these processes need be taken into consideration, if we want to obtain the correct and complete behaviour of the system. For that we ought to write the master equation, and then solve it. Unfortunately, very few master equations are simple enough to accept analytical solutions. We deal with this situation by expanding them into a Fokker-Planck equation, which then helps us draw the necessary information about the behaviour of the system.

We use the "shift" operators notation:

$$\varepsilon_i f(A_1, A_2, A_3, A_4) = f(A_1 + 1, A_2, A_3, A_4) \quad (2)$$

$$\varepsilon_i^{-1} f(A_1, A_2, A_3, A_4) = f(A_1 - 1, A_2, A_3, A_4)$$

and similarly for the other concentrations.

Using the "shift" operators notation (2), the master equation for the cyclic competition system with migrations reads:

$$\begin{aligned} \frac{\partial P(\{A_i\}, t)}{\partial t} = & \int \frac{1}{N} \left[(\varepsilon_4 \varepsilon_1^{-1} - 1) A_1 A_4 + (\varepsilon_1 \varepsilon_2^{-1} - 1) A_1 A_2 + \right. \\ & + (\varepsilon_2 \varepsilon_3^{-1} - 1) A_2 A_3 + (\varepsilon_3 \varepsilon_4^{-1} - 1) A_3 A_4 \left. \right] P \left[(\varepsilon_1 - 1) A_1 + (\varepsilon_2 - 1) A_2 + \right. \\ & \left. + (\varepsilon_3 - 1) A_3 + (\varepsilon_4 - 1) A_4 + \frac{N}{4} (\varepsilon_1^{-1} + \varepsilon_2^{-1} + \varepsilon_3^{-1} + \varepsilon_4^{-1} - 4) \right] P(\{A_i\}, t) \end{aligned} \quad (3)$$

For systems like the one above, whose rate equations have a stable solution, the Ω -expansion of van Kampen [17] works exceptionally well. Its idea is to split the variables of the problem into a non-fluctuating part, and a fluctuating one, i.e. deal separately with the mean-field solutions and the fluctuations (which are taken to be of the order \sqrt{N}). In this approach, the numbers of the individual populations are written:

$$A_i = N\phi_i + \sqrt{N}x_i \tag{4}$$

Here the ϕ_i are the steady-state (non-fluctuating) concentrations of the i -th species respectively (which only depend on time), and the x_i are the fluctuations. Then the probability distribution $P(A_i, t)$ is transformed into $P(\{x_i\}, t)$ and:

$$\begin{aligned} \Pi &= N^2 P(N\{\phi_i + \sqrt{N}x_i\}, t) \\ \frac{\partial P}{\partial t} &= \frac{1}{N^2} \frac{\partial \Pi}{\partial t} - \frac{1}{N} \sum \frac{d\phi_i}{dt} \frac{\partial \Pi}{\partial x_i} \\ \varepsilon_i &= 1 + \frac{1}{\sqrt{N}} \frac{\partial}{\partial x_i} + \frac{1}{2N} \frac{\partial^2}{\partial x_i^2} + K \\ \varepsilon_i^{-1} &= 1 - \frac{1}{\sqrt{N}} \frac{\partial}{\partial x_i} + \frac{1}{2N} \frac{\partial^2}{\partial x_i^2} + K \end{aligned} \tag{5}$$

Next we substitute everything into the master equation, leave only the term $\partial \Pi / \partial t$ on the left hand side, and group the right hand side terms according to powers of \sqrt{N} . The first term is of order $N^{1/2}$, and it must be equal to zero, for an expansion in terms of $N^{1/2}$ to make sense. That term reproduces the rate equations in terms of the concentrations ϕ_i , with steady state solution $\phi_i = 1/4$.

The terms of order N^0 give a linear Fokker-Planck equation of the form:

$$\frac{\partial \Pi}{\partial t} = \sum [-A_k \frac{\partial}{\partial x_k} (x_k \Pi) + \frac{1}{2} B_{ik} \frac{\partial^2 \Pi}{\partial x_i \partial x_k}] \tag{6}$$

where the A-matrix for the cyclic system is:

$$\begin{pmatrix} \phi_4 - \phi_2 - D & -\phi_1 & 0 & \phi_1 \\ \phi_2 & \phi_1 - \phi_3 - D & -\phi_2 & 0 \\ 0 & -\phi_3 & \phi_2 - \phi_4 - D & -\phi_3 \\ -\phi_4 & 0 & \phi_4 & \phi_3 - \phi_1 - D \end{pmatrix}$$

The B-matrix is has diagonal elements of the form $B_{ii} = D(s_i + \phi_i) + \phi_i(\phi_{i-1} + \phi_{i+1})$, and off-diagonal ones: $B_{ij} = -\phi_i \phi_j$. The Fokker-Planck equation obtained this way is linear. We are interested in fluctuations around the steady state, otherwise known

as ‘‘linear noise approximation’’. The solution is known to be a Gaussian; the problem represents itself as an Ornstein-Uhlenbeck process. For our purposes, it suffices to determine the first and second moments of the fluctuations. Following van Kampen [17], we can multiply the Fokker-Planck equation by x_i and integrate by parts to get:

$$\frac{d\langle x_i \rangle}{dt} = \sum_j A_{ij} \langle x_j \rangle \tag{7}$$

For simplicity we can assume that all the concentrations in the reservoir are equal: $s_i = s = 1/4$. The eigenvalues of the A matrix are $-D$ (doubly-degenerate), and $-D \pm i\phi\sqrt{2}$ where ϕ is the steady state value of the concentrations. The negativity of the eigenvalues guarantees the stability of the zero solutions to the first moments equations. Hence, the average of the fluctuations decays to zero and remains zero.

The equations for the second moments can be obtained similarly:

$$\frac{d\langle x_i x_j \rangle}{dt} = \sum_k A_{ik} \langle x_k x_j \rangle + \sum_k A_{jk} \langle x_i x_k \rangle + B_{ij} \tag{8}$$

By symmetry, all the diagonal terms $\langle x_i^2 \rangle$ are equal, as well as off-diagonal terms (correlations) $\langle x_i x_j \rangle$. They depend on the migration probability D alone. The steady state solutions for the diagonal terms (and also for the variances, since the mean values are zero), are as follows:

$$\langle x_i^2 \rangle = \frac{(2\phi^2 + D(\phi + s))}{2D} \tag{9}$$

where s is the concentration of any of the species in the reservoir. The number of individual species will fluctuate around $N \cdot \phi_s$ where ϕ_s is the steady-state concentration. All the species survive forever. This way, (sufficient) migrations into and out of the container maintain diversity in the system.

It is worth noting that the only difference between the three [5, 6] and four species systems expansion is the appearance of an ‘‘off-diagonal’’ of zeroes, in positions (i, j) for which the species A_i and A_j do not react. This means that the above algebra will remain exactly valid when there are more than four species in the system. Hence, our results will hold for any number of species, and any reasonable system size.

If there is only migrations into and out of the container (i.e. no cyclic reactions), the system remains near the centre point, and the product of the

concentrations remains considerably above zero; in other words, all species are present in the system at (almost) all times. When both the cyclic/neutral mechanism and migrations are present, one can occasionally observe temporary extinctions. Since the boundary is not absorbing, occasional migrations will return the system to the state with maximal symmetry (diversity) where all species coexist. The migrations then manage to keep the system maximally disordered, since they are stronger than the fluctuations (which try to drive the system toward the boundary, i.e. fixation, and keep it there). The migration rate acts then as some sort of “temperature”, and decreasing the migration rate would be analogous to annealing the system.

However, by looking at the expression for the variance of the fluctuations above (9), one can observe that when the migration probabilities per particle (migration rate) approach zero, the variance of the concentrations of individual populations is of the order, and

$$\frac{(2\phi^2 + D(\phi + s))}{2D}$$

it becomes of order 1 (i.e. the order of macroscopic concentrations,) when $D \propto 1/N$. This gives us the critical value for the migration probability.

Our analytical results agree very well with those of Togashi and Kaneko [16], who simulated the four-species autocatalytic system with a very small number of molecules. They keep the diffusion rate D constant, and vary the system size. As the system size decreases and goes through a certain value (which coincides with $1/D$, the inverse of migration rate), they observe the above-described transition into the broken-symmetry state.

As a final remark regarding the even-number cyclic system, it is useful to try and “coarse-grain” its dynamics into two species: odd- and even-numbered. For simplicity, let us consider the four-species system. In this case:

$$A_{\text{odd}} = A_1 + A_3 \quad A_{\text{even}} = A_2 + A_4 \quad (10)$$

and the master equation will transform as follows:

$$\frac{\partial P(A_{\text{odd}}, A_{\text{even}}, t)}{\partial t} = \left\{ \frac{2}{N} \left[(\epsilon_{\text{even}} \epsilon_{\text{odd}}^{-1} - 1) + (\epsilon_{\text{odd}} \epsilon_{\text{even}}^{-1} - 1) \right] A_{\text{odd}} A_{\text{even}} + D \left[(\epsilon_{\text{odd}} - 1) A_{\text{odd}} + (\epsilon_{\text{even}} - 1) A_{\text{even}} + \frac{N}{4} (\epsilon_{\text{odd}} \epsilon_{\text{even}}^{-1} - 2) \right] \right\} P(A_{\text{odd}}, A_{\text{even}}, t)$$

This is exactly the master equation for Kimura’s two-species neutral drift system [8, 9, 10], if we recall that the odd-even system size is $N' = N/2$. Duty [2] has shown that this system is equivalent to a branching process [14] with selection coefficient $s = 0$. It is critical, and the probability of survival decays with time as t^{-1} , as verified from simulations (Figure 1).

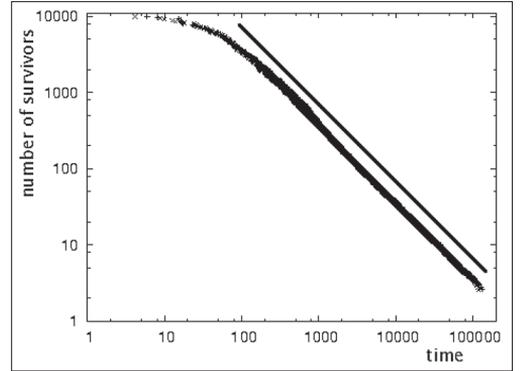


Figure 1. Number of survivors vs. time in log-log axes, for the “coarse-grained” odd-even species, system sizes $N=4000$ and $N=20.000$ (they can not be distinguished). The slope of the line is -1.03 ± 0.05 for $N=4000$, and -1.006 ± 0.009 for $N=20.000$ (a line of slope -1 is shown for comparison)

It is easy to see that for systems with more species (but always an even number of them) we will obtain the same “coarse-grained” master equation.

CONCLUSIONS

The transition observed by Togashi and Kaneko [16] in the four-species autocatalytic loops is the same critical transition we have previously [6] observed for three-species systems. It corresponds to a crossover from a fully symmetric state in the high-migration regime, to a “fixation” state for low-migration rates, in which the symmetry is broken in favour of one or more species. The “fixation” regime in the four-species system consists in species A_1 and A_3 joining their efforts against species A_2 and A_4 , and the final state of the system is one in which one of the pairs has completely “eaten up” the other. This situation is reminiscent of symbiosis, being yet another example of a system in which competition leads to cooperation.

Since the system size is always finite (no matter how large), there is a value of the migration probability per particle, for which the fluctuations of the concentrations become of order one, and the system undergoes a critical transition. The critical diffusion rate varies with system size as $1/N$, and the product $DN \propto 1$, i.e. the number of migrants per unit time, necessary for the symmetry to be preserved in the system (all species to survive) is of order 1. This result is a bit counterintuitive, since it does not depend on system size. But let us recall that it takes only one bad apple... This manifests itself in epidemics situations, when it poses serious problems.

The analytical calculations are in excellent agreement with the simulation results, obtained for three- and four-species systems [6, 16]. The form of the equations for the moments of the fluctuations suggests that systems with n species will exhibit a similar transition. This situation, known as diffusion-limited reaction, has been observed in physical systems in low dimensions, when diffusion is not efficient in mixing the reactants, such as the Ovchinnikov-Zeldovich segregation phenomenon [12].

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