Adaptation of Autocatalytic Fluctuations to Diffusive Noise

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Evolution of a system of diffusing and proliferating mortal reactants is analyzed in the presence of randomly moving catalysts. While the continuum description of the problem predicts reactant extinction as the average growth rate becomes negative, growth rate fluctuations induced by the discrete nature of the agents are shown to allow for an active phase, where reactants proliferate as their spatial configuration adapts to the fluctuations of the catalysts density. The model is explored by employing field theoretical techniques, numerical simulations and strong coupling analysis. For $d \leq 2$, the system is shown to exhibits an active phase at any growth rate, while for $d > 2$ a kinetic phase transition is predicted. The applicability of this model as a prototype for a host of phenomena which exhibit self organization is discussed.

I. INTRODUCTION

There is a growing interest in the dynamics of catalytic systems with diffusing reactants [1]. These models has been considered in the theory of population biology [2], chemical kinetics [3] and physics of contact process [4], as well as magnetic systems [8]. In the most simple case, where agents undergo only birth (autocatalytic reproduction) and death (spontaneous annihilation), the total growth rate, i.e., the difference between the typical rates for these two processes, is the critical parameter for the system. While negative growth rate implies exponential decrease in the number of particles toward extinction of the “colony”, positive rate gives exponential growth. Usually, the number of reactants saturates to some constant value which reflects the finite holding capacity of the environment. The most simplified mathematical description of this process is given by the continuum Fisher equation [4]:

$$\frac{\partial b(x, t)}{\partial t} = D \nabla^2 b(x, t) + \sigma b(x, t) - \lambda b^2(x, t)$$

(1)

where $b(x, t)$ stands for the density of reactants, $\sigma$ is the total growth rate, and $-\lambda b^2$ is introduced phenomenologically as the “minimal” nonlinear term which leads to saturation at positive growth rate. Since the density $b$ is positive semi-definite, at negative growth rate ($\sigma < 0$) there is only one steady state, the absorbing state, where $b(x, t) = 0$ everywhere. At positive $\sigma$, this state becomes unstable, and the system flows into the uniform state $\tilde{b} = \sigma/\lambda$. In this simplified framework the diffusion is irrelevant to the steady state, and only governs the dynamical approach to it, an effect which has been considered at [2]. It turns out that the typical invasion of the unstable phase by the stable one is in the form of Fisher fronts (of width $\sqrt{\Delta D/\sigma}$) which propagate with velocity $v \geq 2\sqrt{\Delta D/\sigma}$. At the stable state, any small fluctuation with wavelength $k$ decays as $\exp[-(\sigma + \Delta k^2)t]$. The phase transition from the inactive to the active state takes place at $\sigma = 0$.

Equation (1) describes the continuum limit of many underlying discrete processes. A typical example is a system with particles diffusing (random walk), annihilating ($B + B \rightarrow \emptyset$) and reproducing autocatalytically ($B \rightarrow 2B$). The discrete nature of individual reactants and their stochastic motion introduce a (multiplicative) noise, which may dominate the evolution of the system and violate the predictions of (1). For the above mentioned and similar processes, it turns out that, at low dimensionality ($d \leq 2$), the extinction phase is stable even at small, positive growth rate, and the transition from active to inactive state falls into the equivalence class of directed percolation [6] (Reggeon field theory). Moreover, it has been conjectured that any transition with single absorbing state falls into the same equivalence class, unless some special symmetry or conservation laws are introduced, as the even offspring case considered by Grassberger [9], and Cardy and Tauber [4].

Recently, a new type of active-inactive phase transition has been introduced, for the process (1) in the presence of quenched disorder in the relevant term, $\sigma(x)$. It has been shown by Janssen [10], that the renormalization group (RG) flow of that process has only a runaway solutions in the physical domain (due to the “ladder” diagrams which changes the effective mass of the free propagator), hence the phase transition is not of directed percolation type. Nelson and Shnerb [11], using the continuum approximation, showed that the local growth is related only to $\sigma(x)$ at the vicinity of the domain, i.e., localization of Anderson type [4] takes place and the extinction transition is given by the effective growth rate of small, localized islands. Although the effect of intrinsic noise due to discreteness fluctuations has not been considered in [1], it seems reasonable that the actual transition takes place when the time scale for tunneling between two positive growth islands is smaller than the time scale for absorbing state decay of a single “oasis”.

If the disorder is uncorrelated, $\sigma(x, t)$ with $\langle \sigma(x, t)\sigma(x' t') \rangle = \Delta \delta(x-x')\delta(t-t')$, the linear part of Eq. (1) also governs the statistics of a directed poly-
mer on a heterogeneous substance, where the time in (1) is identified with the polymer’s preferred direction [13]. With the Cole-Hopf transformation, this problem is mapped to the noisy Burger’s process [14] (KPZ surface growth [15]). In contrast with the “localization” in the case of static disorder, uncorrelated environment induces superdiffusion of the reactants, where the “center of mass” of the population wanders in space as \( r \sim t^2 \), with \( \zeta > 0.5 \). The effect of intrinsic stochasticity due to discretization is, again, limited, and the statistical properties of the eigenenergies of the directed polymer problem determines the extinction transition. This is also the case when the system under quenched disorder is subject to strong convection, as has been shown by [11].

In this paper, we consider the case of diffusive disorder.

\[
B \xrightarrow{\mu} \emptyset
\]

\[
B + A \xrightarrow{\lambda} 2B + A
\]

when both \( B \) and \( A \) undergo diffusion with rates \( D_B \) and \( D_A \), respectively. The mortal agent, \( B \), dies at rate \( \mu \), and proliferates in the presence of the (eternal) catalyst \( A \). The continuum description for this process is given by the “mean-field” (rate) equations for the densities \( a(x, t) \) and \( b(x, t) \):

\[
\frac{\partial b(x, t)}{\partial t} = D_b \nabla^2 b(x, t) - \mu b + \lambda ab
\]

\[
\frac{\partial a(x, t)}{\partial t} = D_a \nabla^2 a(x, t).
\]

As \( t \to \infty \), \( a \) flows into its average \( \bar{a} \), thus the effective mortality rate for \( b \) is given by \( m = \mu - \lambda \bar{a} \) (the mortality rate turns out to be the “mass” of the effective field theory, hence denoted by \( m \)). For positive “mass” the \( b \) population decays exponentially while negative mass implies exponential growth. The active-inactive phase transition takes place at \( m = 0 \). One observes that equation (2) is obtained from (1) by dropping the non-linear term and replacing \( \sigma \) by \( \lambda \bar{a} - \mu \), accordingly, at long times the process introduced in (3) is the linearized form of (1) with the proliferation rate, \( \sigma \), fluctuates “diffusively” around its mean \( \lambda \bar{a} - \mu \). As for this system the disorder is not static but is correlated, it somehow interpolates between the above mentioned models and one may wonder weather it leads to localization of the reactants or to superdiffusion [16]. It turns out that the reactants may adapt themselves to the environment and the colonies are localized on the diffusing islands. Moreover, these correlated fluctuations due to the stochastic motion of individual reactants will change the character of the transition; the transition point is pushed to negative values of \( m \) and the \( b \) reactants survive below the “classical” threshold. Some of our results, along with a numerical study of the transition, are summarized in previous publication [17].

II. STRONG COUPLING ANALYSIS

The basic intuition beneath the phenomenon we describe is in the concept of adaptive fluctuations. Let us take a look, first, at the case of frozen \( A \)'s, where we have random, quenched, growth rate as in [11]. The linearized continuum equation then takes the form

\[
\frac{\partial b}{\partial t} = D\nabla^2 b - m(x)b
\]

where \( m(x) = \mu - \lambda n_A(x) \), and \( n_A(x) \) is the random concentration of the catalyst \( A \). The system is in its active phase if the linearized evolution operator

\[
L = D\nabla^2 - m(x)
\]

admits at least one positive eigenvalue, and its localization properties are almost determined by the corresponding eigenfunctions. Since the same operator governs the physics of quantum particles in random potential, one may use the known results [13] of this field, i.e., that in low dimensionality or strong disorder all the wavefunctions are exponentially localized and the diffusion becomes irrelevant on large length scales [19]. Accordingly, the system may be in its active phase at localized islands even if the average \( m \) is positive.

In our case, however, the catalysts diffuse, and these colonies survives only if the reactants cluster is able to “trace” a specific catalyst or to find some other wandering island. This implies the significance of the system dimensionality: while two typical random walkers (such as the catalyst and the reactant) encounter each other in finite time for \( d < 2 \), they will (typically) never collide for \( d > 2 \). One may expect, accordingly, that below \( 2d \) quantization induced fluctuations are much more dominant than above two dimensions.

Consider one “frozen” catalyst at the origin. The effective growth rate in the vicinity of the origin is positive, i.e., \( m(r < R) = m_{\text{in}} < 0 \) in a region of typical catalyst size \( R \) around it. In the “desert”, out of this island, the “mass”, \( m_{\text{out}} \), is positive. The colony is then localized at \( r = 0 \), with growth rate \( |m_{\text{in}}| \) and an exponentially decreasing tail into the desert [11]. In the continuum approximation, the time dependent profile of the tail is given by [20]:

\[
b(r) \sim e^{m_{\text{in}}|t-r|^{1-m_{\text{out}}/D}},
\]

and the tail front, which is the size of the reactants colony, moves away from the origin with typical velocity \( v \sim m_{\text{in}} \sqrt{D/m_{\text{out}}} \). If the catalyst is moving, the colony will die only when the \( A \) molecule detaches from the \( B \) colony. This, however is almost impossible for a diffusively moving \( A \) since the colony’s front moves ballistically. As this argument involves only one catalyst it is independent of system dimensionality. Thus, at strong
coupling some localized islands are active in any dimension, in contradiction with the mean field prediction of extinction at positive average mass. This mechanism is illustrated in figure 1, which manifests the ability of the B colony to adapt to the location of the moving catalyst. We stress that this adaptive skill is solely due to the “dumb” diffusion and multiplication of the reactants, and thus is an emergent self-organized feature.

There is, however, a possibility for a different scenario, the weak coupling limit, where the local properties of the system do not support the formation of colonies in the inactive phase. For a B molecule having a spatial overlap with an A catalyst, the multiplication time is proportional to $\lambda$. If this time is much larger than the relevant hopping rate, the typical birth event is singular and no colony is formed. If, furthermore, the decay time for a B particle in the absence of A is much smaller than the typical time to find a new catalyst one may expect that the system is in its inactive phase, unless some global, collective effect turns this local analysis void.

Before looking for global effects, let us try to consider the strong coupling limit more carefully. Consider a single A agent located at the point $r_0$, and the “island” of B reactants which surrounds it. Keeping the A stationary and working on a $d$-dimensional lattice (with lattice constant $l$), the growth rate is $\frac{l^d}{2}$ and the hopping rate is $2D_B l^d$. The following equation holds for the concentration of B’s:

$$n_B \sim e\left(\frac{l^d}{2} - \frac{2D_B}{l^2} - \mu \right) t e^{\log \left(\frac{2D_B}{l^2} l^{d-2} \frac{\rho + a}{\lambda} \right)},$$

where we assume $D_B l^{d-2} \ll \lambda$ (thus the very steep slope suppresses the effect of diffusion returning inwards). Consequently,

$$\frac{\partial \log [n_B (r_0, t)]}{\partial t} \sim \left(\frac{\lambda - 2dD_B}{l^2} - \mu \right).$$

Now consider a hopping event of the A, by a single lattice spacing. Measuring $n_B (r_0 (t), t)$, at the new A site, it reduces by a factor of

$$e^{-\log \left(\frac{2D_A}{l^2} l^{d-2} \frac{\rho + a}{\lambda} \right)}.$$  

The rate at which the hopping events occur is $2dD_A$, accordingly the rate equation (5) is modified to:

$$\frac{\partial \log [n_B (r_0 (t), t)]}{\partial t} \sim \lambda - 2dD_B - \mu - 2dD_A \log \left(l^{d-2} \frac{D_B}{\lambda} \right),$$

where we have assumed that there is enough time between hopping events so that the island shape stabilizes to the long time behavior [1], namely $D_A l^{d-2} \ll \lambda$. Equation (8) has the solution:

$$n_B (r_0 (t), t) \sim e^{\left(\frac{\lambda - 2dD_B}{l^2} - \frac{2D_A}{l^2} \log \left(l^{d-2} \frac{D_B}{\lambda} \right) \right) t}.$$  

This shows that in the strong coupling regime the exponent is positive and the number of reactants grows exponentially, independent of the dimension and of the catalyst density. The inset of Fig. 1 shows the fit of the expression (8) to the numerical results on a lattice.

III. WEAK COUPLING

In order to consider global effects of spatial fluctuations, let us write the Master equation for the probability $P_{nm}$ to find $m$ reactants and $n$ catalysts at a single point (with no diffusion)

$$\frac{dP_{nm}}{dt} = -\mu \left[mP_{nm} - (m + 1)P_{n,m+1} \right] - \lambda \left[\sum P_{nm} - n(m - 1)P_{n,m-1} \right].$$

Following [21] we define a set of creation-annihilation operators,

$$a^+ |n, m\rangle = |n + 1, m\rangle \quad b^+ |n, m\rangle = |n, m + 1\rangle$$

and a wavefunction

$$\Psi = \sum_{n,m} P_{n,m} |n, m\rangle.$$  

The Master equation then takes the Hamiltonian form:

$$\frac{\partial \Psi}{\partial t} = -H\Psi$$

with
\[ H = \sum_i \left[ D^a_i \sum_{<e-i>} a_i^+ (a_i - a_e) + \frac{D^b}{t^2} \sum_{<e-i>} b_i^+ (b_i - b_e) \right. \\
+ \mu [b_i^+ b_i - b_i] + \frac{\lambda}{\sqrt{t^2}} [a_i^+ a_i b_i^+ b_i - a_i^+ a_i a_i^+ b_i^+ b_i] \right] \] (10)

Where \( i \) runs over all lattice points, and the sum, \( \langle i - e \rangle \), is over nearest neighbors.

Shifting the creation operators to their vacuum expectation value \( a^+ \rightarrow \overline{a} + 1 \) and \( b^+ \rightarrow \overline{b} + 1 \), the value of the catalyst density to its average, \( \frac{1}{a} a \rightarrow a + n_a \), and finally, \( \frac{1}{b} b \rightarrow b \) the evolution operator takes the following form in the continuum limit:

\[ H = \int d^d x \left[ -D^a_i \nabla^2 b - D^a_i \pi \nabla^2 a + \mu \overline{b} \right. \\
- \lambda \overline{b} (\overline{a} + 1) (\overline{b} + 1) (a + n_a) \left. \right] (11) \]

The action is simply:

\[ S = \int dt \left[ \int d^d x \left( \overline{a} \frac{\partial}{\partial t} a + \overline{b} \frac{\partial}{\partial t} b \right) + H \right]. \] (12)

Note that the coefficient of \( \overline{b} b \), which plays the role of mass, is given by \( m = \mu - \lambda n_a \).

Now this system may be analyzed using the standard renormalization group (RG) technique. We impose a change of scale

\[ x \rightarrow sx \]
\[ t \rightarrow s^2 t \]
\[ a \rightarrow s^{-d-n_a} a \]
\[ \Lambda \rightarrow \Lambda/s \] (13)

where \( s \) is the renormalization group scale factor. The renormalization flows of the parameters of the action (12) are given by their naive dimensionality and the corrections from the diagrams shown in Fig. (4), using the basic vertices as in Fig. (2). The flow equations for the mass and the coupling constant are given by

\[ \frac{d \lambda}{d \ln(s)} = \epsilon \lambda + \frac{\lambda^2}{2 \pi D} \Lambda^{d-2} \]
\[ \frac{dm}{d \ln(s)} = \frac{\lambda^2 n_a}{2 \pi D} \Lambda^{d-2} \] (14)

where \( \epsilon = 2 - d, D = \frac{D^a + D^b}{2} \) and \( \Lambda(s) \) is the upper momentum cutoff. Note that, as indicated by naive dimensional analysis, the Gaussian fixed point \( \{ \lambda = 0, m = 0 \} \) is stable at \( d > 2 \), hence there is no perturbative corrections to \( \eta \) and \( \varepsilon \) in this regime. If the momentum cutoff is much larger than any other quantity of the problem one has,

\[ \frac{d \lambda}{d \ln(s)} = \Lambda \left( \epsilon + \frac{\lambda}{2 \pi D} \right) \]

and the flow lines are shown in Figs. (1) and (3) for \( d \leq 2 \) and \( d > 2 \), respectively. Below two dimensions, the Gaussian fixed point is always unstable and the system flows to the strong coupling limit, where adaptive B colonies grow indefinitely, as indicated by the negative values of the effective mass. At higher dimensionality, on the other hand, there is a finite region in the parameter space where the trivial fixed point is stable and \( \lambda \) flows into zero, while higher values of initial coupling constant flow to infinity. For a system of finite size \( L^d \), the flows should be truncated at \( s = \frac{L}{\Lambda} \), and the phase is determined by the end point of the flow lines at this \( s \). For finite \( \Lambda \), equations (14) take the form:

\[ \frac{d \gamma}{d \ln(s)} = \epsilon \gamma + \frac{\gamma^2}{1 + M} \]
\[ \frac{d M}{d \ln(s)} = 2 M - \frac{\alpha \gamma^2}{1 + M} \]

where the dimensionless quantities are \( \gamma = \frac{\lambda \Lambda^{d-2}}{2 \pi D}, M = \frac{m}{\partial^4 \Lambda^{d-2}}, \) and \( \alpha = 2 \pi n_a \). The flow lines for \( d = 2 \) are shown in figure (3) and exhibit a transition due to the finite lattice spacing.
FIG. 4. The RG flow lines at the continuum limit for $d \leq 2$. While at short times $m$ grows, the system flows into its active phase $m < 0$ on large time scales.

FIG. 5. Renormalization flows for $d > 2$. The shaded region flows into active phase while at the unshaded region the system flows to the inactive phase ($m \to \infty$).

FIG. 6. Renormalization flows for $d = 2$ at finite lattice spacing. Unlike [1], here there is a region in parameter space (unshaded) where the extinction phase is stable.

IV. DISCUSSION

Since the classical works of Malthus and Verhulst [2], it has been recognized that most of the processes in living systems are autocatalytic and thus are characterized by exponential growth. In fact, the appearance of an autocatalytic molecule may be considered as the origin of life. In this paper, these autocatalytic system are shown to admit self organization in the presence of fluctuating environment. The exponential amplification of “good” fluctuations in the catalysis parameters prevails, in the situations discussed above, the globally hostile environment and is robust against the random motion of both the reactants and the catalysts. Our result may be interpreted as an indication that “life” (in the above sense) is resilient and is able to adapt itself to the changing environment. The applicability of this model ranges from biological evolution (where the environment is the genome space) to the role of enzymes in chemical reactions and even in social or financial settings.

More realistic models, however, should take into account the depletion of resources by the catalytic process and the finite carrying capacity of the substrate. Although the model discussed above is relevant at time scales which are small in comparison with the mean time for consumption or saturation, the stable fixed point of the system may be different. In particular, on a uniform, inexhaustible, autocatalytic substrate with finite carrying capacity the discreteness induced fluctuations have been shown [3] to decrease the effective growth rate, and to give a directed percolation type transition at $d < 2$. The competition between this effect and the effect of adaptive fluctuations will be considered elsewhere.

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[19] Actually, all the states in the tail are localized for any dimensionality or disorder strength, and the first state to become “active”, with positive eigenvalue, is always localized. However, as we have noted before, taking into account the discrete nature of the reactants implies the extinction of any finite colony due to rare fluctuations, and the activation of the system takes place only as the time scale for this extinction of single colony is comparable with the “tunneling rate” to neighboring oases. For the sake of simplicity, we assume that all the relevant eigenstates of $L$ are localized.

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