Unbounded autocatalytic growth on diffusive substrate: the extinction transition

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The effect of diffusively correlated spatial fluctuations on the proliferation-extinction transition of autocatalytic agents is investigated numerically. Reactants adaptation to spatio-temporal active regions is shown to lead to proliferation even if the mean field rate equations predict extinction, in agreement with previous theoretical predictions. While in the proliferation phase the system admits a typical time scale that dictates the exponential growth, the extinction times distribution obeys a power law at the parameter region considered.

PACS numbers: 05.40.-a, 64.60.Ak, 64.60.Ht

I. INTRODUCTION

Catalyst induced proliferation systems are very common in a variety of fields in nature such as biology, chemistry, physics, and even in finance and social sciences. Technically, there is one type of agents that catalyze a reaction among other species, like enzymes in living animals, catalysts in chemical reactions or traders in social networks. In many cases the catalyst is not influenced by the reaction it facilitates. The spatio temporal dynamics of the catalysts agents dictates the dynamics of the reactive system. The theoretical understanding of such processes is usually based on partial differential equations for population densities, like the rate equations or (if the system is not well mixed) reaction-diffusion equations. Although very useful, these equations neglect the intrinsic noise build up in any realistic system due to the stochastic motion of individual reactants. Intuitively, the approximation involved in the study of deterministic processes for continuum variables rather then the noisy wandering of discrete agents is valid at high densities, fast diffusion limit. Unfortunately, no general systematic methodology for consistent perturbative expansion around this "mean field" limit is available, and the corrections are calculated on the basis of an ad-hoc methods for spacial cases or by numerical simulations.

In a model presented recently the disagreement between the deterministic rate equations and the realistic stochastic process is emphasized for a very simple and generic system. The model includes two species: an immortal catalyst A that only diffuses randomly in space, and a reactant agent B which decays at rate $\mu$ and proliferate in the presence of A-s at rate $\lambda N_A$, where $N_A$ is the number of A agents (local density of A) at the reactant spatial location. Both A and B undergo diffusion with rates $D_A$ and $D_B$ respectively. Schematically, the local reactions considered are:

$$B \rightarrow \odot$$

$$B + A \rightarrow B + B + A.$$ (1)

The continuum description for this process is given by the mean-field rate equations for the densities of A and B, $a(x,t)$ and $b(x,t)$, respectively. The corresponding reaction diffusion equations,

$$\frac{\partial a(x,t)}{\partial t} = D_A \nabla^2 a(x,t)$$

$$\frac{\partial b(x,t)}{\partial t} = D_B \nabla^2 b(x,t) - [\mu - \lambda a(x,t)] b(x,t),$$ (2)

admit a simple solution: since A only diffuses, catalyst density becomes a constant $n_A$ (where $n_A$ is the average A density) after long time, and the second rate equation becomes linear:

$$\frac{\partial b(x,t)}{\partial t} = D_B \nabla^2 b(x,t) - mb(x,t),$$ (3)

where $m \equiv \mu - \lambda n_A$ is the decay/growth rate of the system, depending on its sign. This mean field theory predicts a phase transition at $m = 0$. For positive $m$ the reactant concentration decays exponentially, while negative $m$ yields exponential growth (proliferation). In realistic systems, of course, one expects some saturation mechanism that prevents explosion, perhaps in the form of B agents competition for resources. If this work this process is neglected and the system admits two fixed points, $b = 0$ and $b = \infty$. The significance and limitations of this approximation are discussed in the last section.

In previous work the effects of stochasticity due to the discrete character of the reactants was considered for this "AB model". The main observation is that diffusion never kills spatial fluctuations for discrete A agents: instead,
one gets at any time Poissonian fluctuations of the A density, entailing that at any time there will be a finite chance for a site to be "active" (with local \( m(x) = \mu - \lambda N_A(x) \) smaller than zero) even if the average \( m \) is positive. At each of these "oases" the B population grows exponentially and a colony of B agents is developed. This leads to a shift of the transition from \( m = 0 \) to finite, positive \( m \).

Let us present the main results of [3, 4]. The technical tool used is a general approach for the consideration of the effect of stochastic noise in reactive systems on spatial domains, suggested and applied by various authors [5, 6, 7]. This theoretical framework is based on the exact Master equation of the full stochastic process. Translating the Master equation to the form of Schrödinger-like equation for second quantized fields one may find the effective action and integrate fast modes to get the same effective action with reaction parameters that depend on time and length scale (renormalization group flows).

Here, the RG transformation involves the rescaling:

\[
\begin{align*}
  x & \to sx, \\
  t & \to s^2 t, \\
  a & \to s^{-d} a, \\
  b & \to s^{-d} b, \\
  \Lambda & \to \Lambda/s,
\end{align*}
\]

where \( s \) is the scaling factor \((s > 1)\), \( d \) is the dimension and \( \Lambda \) is the upper momentum cutoff. This rescaling yields the flow equations for the model parameters:

\[
\begin{align*}
  \frac{d\lambda}{d\ln s} &= (2 - d)\lambda + \frac{\lambda^2 \Lambda^{d-2}}{2\pi D 1 + \frac{m}{D\Lambda^2}}, \\
  \frac{dm}{d\ln s} &= 2m - \frac{n_A \lambda^2 \Lambda^{d-2}}{2\pi D 1 + \frac{m}{D\Lambda^2}}, \\
  \frac{dn_A}{d\ln s} &= dn_A,
\end{align*}
\]

where the average diffusion rate is \( D = (D_a + D_b)/2 \). These flow equations were obtained by one loop perturbative expansion of the effective action around its mean field limit, where \( \lambda/D \) and \( m/D \) are the small parameters. One can see that there is a negative correction to \( m \) and this implies that the effective "mass" \( m \) may flow to the proliferation phase \( m < 0 \) as the system size increased, even if the bare mass is larger than zero. A sketch of the flow lines according to Eqs. (5) is presented in Figure (1).

The aim of this work is twofold: first, to compare the theoretical predictions about the location of the extinction transition with numerical simulations; second, to study the nature of that phase transition. Clearly, the existence of proliferation phase with diverging number of reactants compels a simulation that involves with large number of agents, and is possible only when \( D \) is comparable with the reaction parameters. Accordingly, the RG results should be taken only as a qualitative guides, as the "small parameter" of the expansion is \( O(1) \) in the numerical experiments. In Figure (1) these theoretical predictions for the extinction-proliferation phase transition, along with few RG flow lines are shown for \( d = 1, n_A = 1, D = 2 \) and \( \Lambda = 2\pi/a_0 \) where \( a_0 = 1 \) is the lattice constant.

The intuition gathered from the RG approach is that there are two parameter regions. In the proliferation phase the effective coupling constant \( \lambda \) grows with the basic length scale of the system and for infinite sample this process leads to negative \( m \). In the extinction phase, on the other hand, the growth of \( m \) dictates the system and the flow is toward extinction.

In order to implement this intuition to finite samples, one should bear in mind that positive mass corresponds to extinction. Thus, the crossover to proliferation depends on the ability of the system to support more and more rescaling transformations: even if the bare mass is in the proliferation region of Figure (1) system of finite size may be in the extinction phase, depending on the bare parameters \( \lambda, m \) and \( n_A \).

In the next section the numerical technique is presented, the location of the transition is identified for finite samples and the results are compared with the theoretical predictions. The third section deals with the statistical properties of the results in different regimes where the essential difference between the phases is emphasized. In the last section we discuss the results and compare our study with known facts about extinction transition for bounded growth like the contact process in homogenous and heterogenous environments.
FIG. 1: RG results for AB model phase transition, $D_A = D_B = 2$, $d = 1$, $n_A = 1$ and $\Lambda = 2\pi/a_0$ where $a_0 = 1$ is the lattice constant. Above the dashed line is the extinction phase for infinite system while below is the proliferation region where the death rate $m$ flows to negative values. One can see that catalyst fluctuation induce proliferation in area where the mean-field predicts extinction ($m > 0$). Finite system size implies truncation of the RG flow lines, so the final effective $m$ value may be positive even if the bare mass is in the proliferation region.

II. NUMERICAL STUDY OF THE EXTINCTION TRANSITION

A. Simulation technique

In order to simulate the AB model, a one dimensional array of $L$ lattice points with periodic boundary conditions is used. Each site $i$ is associated with an integer ($N^A_i$) number of catalysts and another integer ($N^B_i$) stands for the number of reactants. The hopping rates of the catalyst and the reactants are $D_A$ and $D_B$ respectively. The death rate of a reactant is $\mu$, while the proliferation rate at each site is given by $\lambda N^A_i$. The initial densities of the catalyst and the reactant are $n_A$ and $n_B$ correspondingly. For each system realization the catalysts are initially randomly distributed. The mean-field effective mortal rate (also defined as the reactant "mass" in the corresponding effective field theory) is therefore $m = \mu - \lambda n_A$.

The main technical obstacle for a single agent based simulation of that system is the large number of reactants in the proliferation phase. It turns out that an event driven algorithm based on individual agents leads to diverging simulation times way before any conclusive statement about the actual phase of the system is extracted. In particular, even a case of very large reactant "colony" may be recognized as a transient that ends up with complete extinction of the colony. Accordingly, a site based simulation has been used. For heavy populated sites ($N^B_i > 10^6$) the mean-field equations are solved with gaussian noise proportional to the square root of the reactant density, while if $N^B_i < 10^6$ a "global" Monte Carlo method is used. For example, the number of particles that decay ("died") at certain site per small unit time $dt$ is determined by generating a random number taken from a binomial distribution with probability $\mu dt$ and $N^B_i$ Bernoulli trials (instead of checking $N^B_i$ times whether a reactant died during this time step). This combination of two methods allow us to reach a huge number of reactants, up to $N_B = 10^{300}$, without neglecting the effect of discretization at low densities.

The simulation is initiated with reactant density $n_B = 100$ and catalyst density $n_A = 1$. All the results presented here correspond to reactant and catalyst diffusion rates $D_B = D_A = 2$. The "mass" is therefore $m = \mu - \lambda n_A = \mu - \lambda$.

The simulation of an individual process ends when the system reaches either extinction or proliferation.

An extinction of the process is declared if there are no reactants in the system. The definition of proliferation phase, on the other hand, is more subtle as there is no upper bound for the reactant density. We thus set an upper threshold of $N_B = 10^{300}$; above this number the simulation stops and the phase of the system is identified as proliferation phase. This criterion was justified by increasing the upper bound to be so large that transient effects are avoided. In fact, setting the threshold to be $N_B = 10^{300}$ no significant differences were identified.
FIG. 2: Survival probability (average over 1,000 realizations) $P_\infty$ vs $m$, $\lambda = 1$, $n_A = 1$, $n_B = 100$. According to the reaction diffusion equations the extinction phase is above $m = 0$. Here one finds a region of almost sure proliferation and a region of almost sure extinction, separated by an uncertain region. The proliferation region grows with the system size $L$ and saturates at a critical value, $m_c$, that correspond to the extinction transition for an infinite system.

B. The transition: theory vs. simulations

As the system is stochastic in nature, the flow to the extinction or proliferation phase is non-deterministic, and for the same set of parameters one may find microscopic realizations that leads to different states. In Figure (2), for example, the probability $P_\infty$ for the system to reach the proliferation phase is plotted against $m$ for $L = 128$ and $\lambda = 1$, where each point reflects the fraction of systems (out of 1000 runs) that reach proliferation. According to the mean field theory (3) above $m = 0$ the system should flow to the extinction phase. In contrary, here one finds a region of almost sure proliferation and a region of almost sure extinction, separated by an uncertain region. In what follows (for the sake of comparison between the numerics and the analytic prediction for the location of the phase transition) the definition of the extinction transition is taken at $m$ for which $P_\infty = 0.5$, in order avoid the stronger effects of noise as $P_\infty$ approaches zero or one.

Using that analysis it is possible to continue our quest of finding the critical mass $m_c$ for the (infinite size system) extinction-proliferation phase transition. As a first step, the system size $L$ is multiplied by 2 while the reaction rates and agents densities are kept constant. Next the survival probability $P_\infty$ is plotted vs $m$ for each system size (in order to change $m$ only $\mu$ is modified while $\lambda$ and $n_A$ are kept constants). As mentioned, the phase transition for a finite size system is defined where $P_\infty = 0.5$. The critical $m$ of the finite size system is plotted versus $\ln L$ in Figure (3.a). One can see that for small system sizes, the critical "mass" increases as the system size $L$ increases, since the probability for larger catalyst fluctuation grows with size. There is, however, an intrinsic limit (independent of the system size) on these spatial fluctuations, and according to the RG analysis one expects that for large enough bare mass there will be no further increase in the critical mass as a function of the system size [see Figure (3.b)]. Indeed, the simulation indicates that for larger system sizes the critical mass begins to saturate while it approaches the "real" phase transition. Since the "real" phase transition at the thermodynamic limit is beyond our computational abilities, the critical mass $m_c$ for certain $\lambda$ is evaluated by fitting the results to the function

$$m(x) = m_c - \frac{m_c}{1 + (x/x_0)^p}$$

where $x \equiv \ln(L)$. As indicated in Figure (3b), this function yields an almost perfect fit to the RG based theory, and seems also to fit the numerical experiment quite well [Figure (3a)]. After the critical mass for a specific $\lambda$ is determined, using the above procedure, one proceeds to plot the infinite system size phase transition line $m_c$ vs $\lambda$, Figure (4). Above the transition line is the extinction phase for the infinite size system, while below is the proliferation phase. The theoretical phase transition line, based on the RG analysis, is plotted together with the line obtained from the numerical experiment on a logarithmic scale. Both theoretical and numerical results suggests that $m_c \sim \lambda^\alpha$, where the values of $\alpha \approx 1.4$ (for the RG phase transition curve) and $\alpha \approx 1.45$ (for the numerics) are close and the curves are almost parallel. This, again, implies a qualitative similarity between the numerical simulations and the picture emerges from the theory.
FIG. 3: $m$ Vs $\ln(L)$: (a) Simulation results (squares) for $\lambda = 1$, $n_A = 1$, $n_B = 100$. One can see that the system robustness is increasing (proliferation for larger death rates) as the system size grows. The critical "mass" $m_c$ (the mass for which there is no proliferation even in the limit $L \to \infty$) is determined using the best fit to the logistic function (6) (full line). (b) RG results (squares) for $\lambda = 1$, $n_A = 1$ and $\Lambda = 2\pi/a_0$ where $a_0 = 1$ is the lattice constant. There is a region where the phase transition depends on the system size, but above a critical mass $m_c$ there is no growth independent of $L$, in agreement with Figure (1). The full line is the best fit to (6). The qualitative resemblance between the RG predictions to the simulation results is clear.

FIG. 4: Phase transition lines in the $m$ - $\lambda$ plane. The full line is the theoretical prediction based on the RG perturbative analysis while the squares are the results of the numerical experiment (see text).

III. SAMPLE TO SAMPLE FLUCTUATIONS AND THE PHASE TRANSITION

Let us take a deeper look at the dynamics of the system, trying to describe the different regions of Figure (2). For a point in the distinguished proliferation region ($m < 0.6$, $P_\infty \sim 1$), all the samples proliferate. The growth of the B population is exponential, and both the average over the logarithm of the population and the logarithm of the average grow linearly in time [Figure (5)]. (If most of the realization decay and only few show exponential growth, $\langle N_B \rangle$ is dominated by rare events and grow, while $\langle \ln(N_B) \rangle$ decays to zero since the logarithm kills the influence of rare events on the average.) If we further plot a histogram of the "end times" for various realization (i.e., the time needed to the system to reach the proliferation upper bound) one can see that there is a typical end time and the histogram corresponds to Gaussian distribution around its value [Figure (6)]. The lines of Figure (5) do not coincide.
FIG. 5: \(\ln\langle N_B \rangle\) and \(\langle \ln(N_B) \rangle\) vs time (average over 1,000 realizations), \(\lambda = 1, m = 0.6, n_A = 1, n_B = 100\). The typical case is shown to be similar to the average over all realizations. The lines do not collapse since \(\langle \ln(N_B) \rangle\) is dominated by the peak of the gaussian of Figure (6), while \(\ln\langle N_B \rangle\) is dominated the tail of this histogram.

FIG. 6: End times histogram (1,000 realizations), \(\lambda = 1, m = 0.6, n_A = 1, n_B = 100\). One can see that there is a typical time for the system to reach the proliferation upper bound.

since \(\ln\langle N_B \rangle\) is dominated by the peak of the gaussian, while \(\ln\langle N_B \rangle\) is dominated by its tail.

Deep in the extinction region (e.g., \(m = 2, P_\infty = 0\)) the situation is different. In this region all the samples end up in extinction, but the corresponding time scale (the effective decay rate, or the effective mass) shows strong sample to sample fluctuations. In Figure (7) a histogram of death times (the inverse mass) is shown. If one assumes that, at long times, the reactant concentration decays like \(\exp(-t/\tau)\), this figure implies that \(P(\tau) \sim \tau^{-\theta}\) where for the results of figure (7) \(\theta \approx 5\). The strong decay of \(P(t)\) manifest itself in the similarity between the typical and the average cases, Figure (8).

Close to the edge of proliferation (e.g., \(m = 1.1, P_\infty << 1\)) the power law for the decay is much smaller. In Figure (9) the histogram of death times indicates \(\theta \approx 2\). Accordingly, there is a lot of difference between the average (\(\ln\langle N_B \rangle\), Figure (10a)) and the typical (\(\langle \ln(N_B) \rangle\), Figure (10b)) time evolution of the total B population. While the typical case decays smoothly to zero, on average the system grows, saturates, and decays after much larger time. The samples for which \(\tau\) is large are samples where the reactant population grows rapidly on time scales smaller than \(\tau\) and then decays. Accordingly, these samples dominate the average population while the typical population is determined by the large number of samples that admits small \(\tau\).

In the middle region, say, \(0.6 < m < 1.1\), the survival probability is between zero and one, and accordingly two peaks of death and proliferation times are seen in Figure (11), corresponding to the proliferating and to the extinction events. Again there is a Gaussian like distribution around a typical time scale associated with the proliferation samples, and power law distribution of time scales in the extinction samples.

Our numerical experiment suggest, thus, that the extinction transition of the saturation free AB model takes place
FIG. 7: Death times histogram (log-log scale, 200,000 realizations) for $\lambda = 1$, $m = 2$, $n_A = 1$, $n_B = 100$. The death times histogram seems to maintain its power-law tail even above the "real" extinction phase transition. However, it decay much faster with exponent $\theta \sim 5$. The rare events in that case are "too rare" and the average is dominated by the typical events, as emphasized in Figure 8.

FIG. 8: $\ln\langle N_B \rangle$ and $\langle \ln(N_B) \rangle$ vs time (average over 1,000 realizations), $\lambda = 1$, $m = 2$, $n_A = 1$, $n_B = 100$. One can see that the average case is similar to the average over the realizations. There are no significant fluctuation (within our finite realization number) since finding exponentially rare events is almost impossible.

in the following way: deep inside the extinction phase there is a power law distribution of decay times with $\theta > 2$, and $\theta$ becomes smaller and smaller while decreasing $m$. Close to the proliferation threshold $\theta \sim 2$, and from now on there is finite fraction of the samples that proliferate to infinity. The sample to sample fluctuations decrease as the transition is approached, and in the "living" phase Gaussian statistics is observed.

IV. CONCLUSIONS AND DISCUSSION

This paper presents a numerical experiment that confirms, qualitatively, some of the theoretical predictions about the extinction transition in system of autocatalytic agents with diffusively correlated fluctuations. The extensive simulations used render a phase diagram similar to the predictions of the exact Master equation based renormalization group technique, even in the parameter region where the "small parameters" of the perturbative technique are $O(1)$. As expected, resources fluctuations increase the ability of species to survive, but in order to extract the potential of these fluctuation via the adaptation mechanism that associate reactant colonies with catalysts islands, the size of the system must be large enough. This finite size effect has been demonstrated, and the system is taken to the large scale limit in order to approach the "real" phase transition.
FIG. 9: Log-log scale death times histogram (200,000 realizations), $\lambda = 1$, $m = 1.1$, $n_A = 1$, $n_B = 100$. The probability of realization to decay ($N_B = 0$) between $t$ to $t + \Delta t$ is shown. The data correspond to a power law distribution of decay times with $P(\tau) \sim \tau^{-\theta}$ with $\theta \approx 2$. This implies that, to the accuracy of our numerical experiment, the average time associated with the decay of the system in the extinction phase diverges.

FIG. 10: Typical (a) versus average (b) decay patterns. In the upper panel $\langle \ln(N_B) \rangle$ is plotted against time and shows a smooth decay, while in the lower panel $\ln(\langle N_B \rangle)$ shows completely different pattern with different time scales. The average is taken from 200,000 different realizations, for $\lambda = 1$, $m = 1.1$, $n_A = 1$, $n_B = 100$. Most of the samples decay to extinction very fast, but the average (b) is dominated by rare events, due to strong sample to sample fluctuations.

FIG. 11: Histogram of death times (a) and of proliferation times (b) in the intermediate parameter region. One sees that the death times distribution admits a long tail corresponds to power-low [see the inset of panel (a)], while proliferation times distribution is sharply peaked around its typical value.
Another result, not predicted by the theory, is the appearance of a scale free fluctuations in the extinction phase, in contrary with the Gaussian distribution associated with the characteristic time in the growth phase.

Let us compare, now, these findings with some known results about extinction transitions. A common conjecture, first suggested by Grassberger and Janssen \[9, 10\] is that, in the absence of conservation laws, all the extinction transitions belong to the directed percolation (DP) equivalence class \[11\]. This proposal is based on the following intuition: close to the transition point the average density of the reactants is zero. In a single time step reactant may decay, survive or yield an offspring. These processes are the basic rules of DP, hence all transitions are at the same equivalence class.

In the presence of spatial heterogeneity, on the other hand, the situation is more complicated as quenched randomness appears to be a relevant operator. It was shown by Janssen \[12\] that the corresponding field theory admits only runaway solutions and no stable fixed point is reached in the physical domain, so the transition in that case is not in the DP equivalence class. This analysis supports the numerical work of Moreira and Dickman \[13\], who used Monte Carlo simulations to analyze the 2d contact process with various fractions of randomly distributed inactive sites. In the extinction region these authors identify the Griffith phase, with nonuniversal power laws. In that regime the local dynamics, associated with rare events, dictates the system’s evolution. While the chance to find a "good" region (with no inactive sites) of linear size \(R\) decays exponentially with \(R\), its typical lifetime \(grows\) exponentially with size, yielding a non universal power law below the transition.

One may a-priori suggest that, for the AB model considered here, the diffusive dynamics of the catalysts simply average out their effect, thus the resulting transition should be in the directed percolation equivalence class, like the transition on homogenous substrate. This assumption is wrong, since a diffusive heterogeneity is a relevant operator at the transition. One may either apply the Harris criterion or consider the naive scaling for the action associated with the Reggeon field theory with diffusive disorder:

\[
S = \int dt dx \, \psi^* \frac{d\psi}{dt} + D\psi (\nabla \psi^*) (\nabla \psi) + u(\psi^* \psi - \psi^* \psi^*) + \phi^* \frac{d\phi}{dt} + D\phi (\nabla \phi^*) (\nabla \phi) - \nu(\phi \psi^* \psi + \phi^* \psi^* \psi) \tag{7}
\]

to see that it supports only runaway solutions, and that \(D\phi\) flows to zero upon rescaling transformation.

Since the system seems to flows into the quenched disorder phase one may suggest that, for an unbounded growth, the colonies on the rare cases grow without limit, so there is no phase transition in the thermodynamic limit (unless the catalyst distribution and dynamical rules are such that they never allows for \(m < 0\) at any finite region). However, Kesten and Sidorov several \[14\] proofed that, even without saturation term, there is a parameter regime that corresponds to the extinction phase, where all processes decay with probability one for an infinite sample. The stochastic wandering of the catalysts, thus, seems to control the system and to yield a possibility of extinction even in the infinite capacity limit.

The emerging picture, supported by the numerical simulations presented here, is that the phase transition exists, with a wide (power law) distribution of extinction times (Griffith phase) below that transition. The diffusive wandering of the catalysts is not strong enough in order to replace the fluctuating concentration by its average and the adaptation of the reactant colonies to the Poissonian noise is of crucial importance. On the other hand, even if the carrying capacity is unbounded this wandering is strong enough to yield a finite range of parameters where the process ends up at extinction with probability one.

V. ACKNOWLEDGEMENTS

We thank Prof. David Kessler and Prof. Sorin Solomon for very helpful discussions about both theory and simulation techniques. This work was supported by the Israeli Science Foundation (grant no. 281/03) and by Yeshaya Horowitz Fellowship.

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It was already proofed by Kesten \cite{14} that the average number of reactants approaches infinity (in one and two dimensions) due to rare events, even if the typical system decays. This phenomena, however, depends on exponentially rare events that yields super exponential population growth and apparently not related to the power law extiction times presented here.

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