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Damage Spreading in a Single-Component Irreversible Reaction Process: Dependence of the System's Immunity on the Euclidean Dimension

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The spreading of a globally distributed damage, created in the stationary regime, is studied in a single-component irreversible reaction process, i.e., the BK model [Browne and Kleban, *Phys. Rev. A* **40**, 1615 (1989)]. The BK model describes one variant of the $A + A \rightarrow A_2$ reaction process on a lattice in contact with a reservoir of A species. The BK model has a single parameter, namely the rate of arrival of A species to the lattice (Y). The model exhibits an irreversible phase transition between a stationary reactive state with production of A_2 species and a poisoned state with the lattice fully covered by A species. The transition takes place at critical points (Y_C) which solely depend on the Euclidean dimension d. It is found that the system is immune for $d = 1$ and $d = 2$, in the sense that even 100% of initial damage is healed within a finite healing period (T_H). Within the reactive regime, T_H diverges when approaching Y_C according to $T_H \propto (Y_C - Y)^{-\alpha}$, with $\alpha \cong 1.62$ and $\alpha \cong 1.08$ for $d = 1$ and $d = 2$, respectively. For $d = 3$ a frozen–chaotic transition is found close to $Y_S \cong 0.4125$, i.e., well inside the reactive regime $0 \leqslant Y \leqslant Y_C \cong 0.4985$. Just at Y_S the damage $D(t)$ heals according to $D(t) \propto t^{-\delta}$, with $\delta \cong 0.71$. For the frozen–chaotic transition at $d = 3$ the order parameter critical exponent $\beta \cong 0.997$ is determined.

KEY WORDS: Irreversible reaction processes; damage spreading; irreversible phase transitions.

1. INTRODUCTION

Damage spreading (DS) is being studied with growing attention in the field of reversible phase transitions,[1-5] such as the Ising model,[1,2] the XY

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model,[2] spin glasses,[3, 5] etc. The DS problem consists, first, in taking a steady-state configuration of the system $\{\sigma^A\}$ and creating at $t=0$ an initial damage $D(0)$ in that configuration (this procedure gives a second configuration $\{\sigma^B\}$). Then, one investigates the time evolution of both configurations using the same dynamics calculating their Hamming distance, defined by

$$D(t)=(1/N)\sum_{i=1}^{N}|\sigma_i^A(t)-\sigma_i^B(t)| \tag{1}$$

where N is the number of sites of the system. Physically $D(t)$ just measures the fraction of sites for which the configurations are different. Starting with a small $D(0)$ value, $D(t)$ will go asymptotically to zero in the so-called frozen phase, whereas it will tend to a finite value different from zero in the so-called chaotic phase.[5] While the study of DS in systems exhibiting reversible phase transitions has received much attention,[1-5] similar studies in systems undergoing irreversible transitions are still in their infancy.[6, 7] Irreversible reaction processes often appear in many fields of science, such as solid-state physics, astrophysics, biophysics, ecology, catalysis, etc., and consequently they are a subject of current interest. Particular attention has been devoted to the study of irreversible phase transitions occurring between a stationary reactive state and a configuration from which the system cannot escape.[8-18]

Very recently, I have shown that DS introduces a new kind of dynamic critical behavior in some irreversible reaction processes such as the monomer–monomer reaction process[6] and the ZGB model.[6, 7] So far, all these models have involved multicomponent reaction processes. However, irreversible phase transitions also occur in single-component reaction models (see, e.g., refs. 8, 11, 12, 17, and 18). The aim of the present work is to investigate the spreading of damage in an irreversible single-component reaction model as proposed by Browne and Kleban (the BK model).[11, 12] This reaction system has been selected considering that its critical behavior is very well known in dimensions $d=1$, 2, and 3.

2. SIMULATION DETAILS AND THEORETICAL BACKGROUND

2.1. The Model

The BK model describes one variant of the irreversible reaction $A+A \rightarrow A_2$ in a lattice. Each lattice site can be either occupied by an atom (state A) or vacant (state V). The simulation algorithm is as follows: at a given time step a site is selected at random. If the chosen site is in the state

A, it remains unchanged. If the site is vacant, then the update depends on the number of nearest-neighbor (NN) sites that are in state A. If none are occupied, the chosen site is changed to A. If at least one NN is in state A, then with probability Y the chosen site is converted to A and the NNs are unchanged. Otherwise, one of the occupied NNs is chosen at random and vacated, with the central site remaining V (this step corresponds to the reaction $A + A \rightarrow A_2$). In $d = 1$ the model exhibits a continuous irreversible phase transition, just at $Y_C \cong 0.2762$, such that for $Y \geqslant Y_C$ the lattice becomes irreversibly covered by A species while for $Y < Y_C$ a stationary reactive state with A_2 production is observed.[12] In higher dimensions the critical points are $Y_C \cong 0.4730$ ($d = 2$) and $Y_C \cong 0.4985$ ($d = 3$), respectively.[12]

The model is simulated in d dimensions and using lattices of side $L = 10^4$ ($d = 1$), $L = 100$ ($d = 2$), and $L = 30$ ($d = 3$). One time unit corresponds to a number of trials equal to L^d.

2.2. Damage Spreading

A steady-state configuration is obtained after $t = 2 \times 10^3$, then the damage is created in a second configuration and its spreading is monitored following the dynamics of both configurations simultaneously. For this purpose, the crucial idea is to apply, on the configurations $\{\sigma^\gamma\}$, the same sequence of random numbers in the algorithm in order to produce the same dynamics. In Eq. (1) all contributions to D given by V–A terms are taken to be equal to unity. Furthermore, we study the spreading of an initial damage globally distributed through the system, in contrast with another approach, which only considers the spreading of a local initial damage.

3. RESULTS AND DISCUSSIONS

3.1. Results for $d = 1$ and $d = 2$

In both one and two dimensions we have observed that any small initial damage $[D(t = 0) \ll 1]$ becomes quickly healed within both the poisoned and the reactive phases. Increasing the initial damage, we found that, surprisingly, even for $D(0) = 1$ the damage becomes healed, as shown in Fig. 1 ($d = 2$). These results are in contrast to standard damage studies, where one works in the limit $D(0) \rightarrow 0$, e.g. taking $D(0) = 1/L^d$. Furthermore, one concludes that in one and two dimensions this irreversible reaction system is immune in the sense that even the largest damage becomes

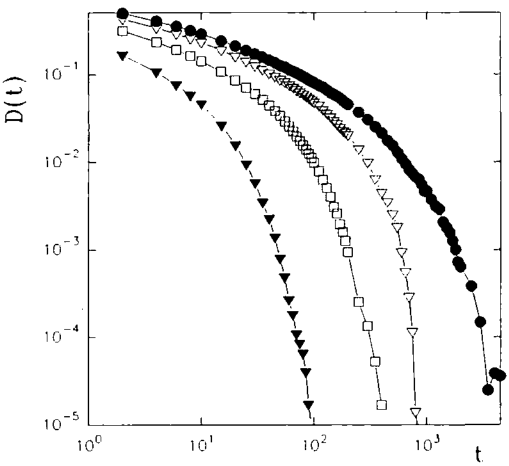

Fig. 1. Plot of $D(t)$ versus t obtained for $d=2$ and taking $D(0)=1$ for different Y-values. ▼ $Y=0.400$, □ $Y=0.450$, ▽ $Y=0.465$ and ● $Y=0.470$.

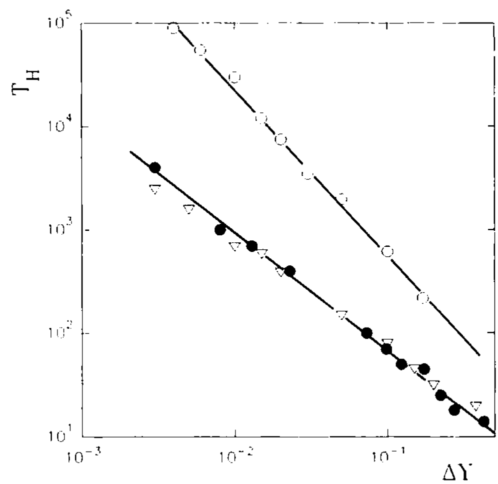

Fig. 2. Log-log plots of T_H versus ΔY, according to equation (2). Upper curve (○): data obtined taking $D(0)=1$ and for $d=1$. The straight line corresponds to a least square fit of the data and has slope $\alpha=1.62$. Lower curves: data corresponding to $d=2$ and obtained taking $D(0)=1$ (▽) and $D(0)=\theta_A$ (●). The straight line has slope $\alpha=1.08$. More details in the text.

healed within a finite time. However, the healing time (T_H) depends on Y and increases when approaching criticality (see, e.g., Fig. 1). In order to describe this finding, let us propose the following power law behavior:

$$T_H \propto (\Delta Y)^{-\alpha} \tag{2}$$

with $\Delta Y = Y_c - Y$. Figure 2 shows log–log plots of T_H versus ΔY corresponding to simulations in $d = 1$ and $d = 2$. For $d = 1$ a least square fit of the data gives $\alpha \cong 1.62 \pm 0.04$, where the error bars merely reflect the statistical error. For $d = 2$ we have also checked the dependence of T_H on the initial damage. Taking $D(0) = 1$, one obtains $\alpha \cong 1.04 \pm 0.04$, while taking $D(0) = \theta_A$, where θ_A is the concentration of A species on the lattice, one obtains $\alpha \cong 1.14 \pm 0.04$, where in both cases the error bars merely reflect the statistical error. The obtained result suggests that, at least for the analyzed examples, T_H is independent of $D(0)$. So we can assume $\alpha \cong 1.08 \pm 0.08$ as an average value for the exponent. For $Y > Y_c$ the lattice becomes irreversibly covered by A species, so the healing time is also the "poisoning" time $T_P = T_H$. It is found that T_P also diverges when approaching Y_c according to a power law similar to Eq. (2), i.e., $T_P \propto (Y - Y_c)^{-\alpha^*}$. The obtained exponents are $\alpha^* \cong 1.59 \pm 0.04$ ($d = 1$) and $\alpha^* \cong 1.02 \pm 0.04$ ($d = 2$), so within error bars one may conjectured that $\alpha = \alpha^*$.

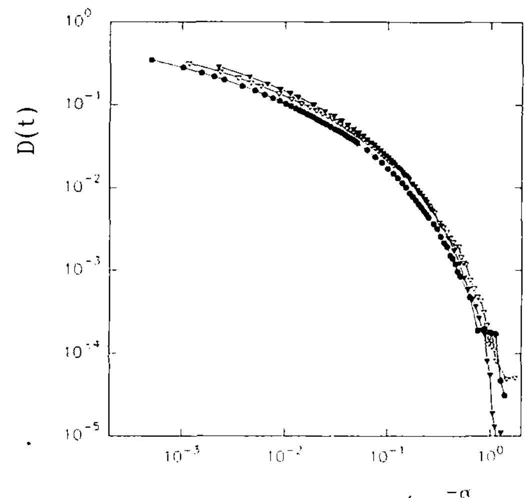

Fig. 3. Plot of $D(t)$ versus $t/\Delta Y^{-\alpha}$ ($\alpha = 1.62$) obtained for $d = 1$ and taking $D(0) = 1$ for different Y-values. ▼ $Y = 0.261$, ▽ $Y = 0.266$ and ● $Y = 0.270$.

The dependence of T_H on ΔY suggests that the time scale can be rescaled, in order to obtain data collapsing, according to

$$D(t) \propto t/\Delta Y^{-\alpha} \tag{3}$$

Figure 3 shows a plot of $D(t)$ versus the scaled time for $d=1$. The obtained results suggest the validity of equation (3) since data collapsing is acceptable.

3.2. Results for $d=3$

In three dimensions one has that the critical point of the BK model is close to $Y_C \cong 0.4985$. On the contrary than in lower dimensions one has damage spreading within the reactive regime, e.g., $0.42 < Y \leqslant Y_C$, while damage healing is observed roughly for $Y < 0.40$. So let us define the spreading critical point Y_S to be the Y value at which the frozen chaotic transition takes place. Close to Y_S we assume the following ansatz[14]

$$D(t) = t^{-\delta} F(\Delta t^{1/\nu}) \tag{4}$$

where $\Delta = Y - Y_S$, for large t the scaling function behaves as $F(x) \propto x^{\beta}$, and δ, ν and β are critical exponents. For $\Delta > 0$ and $t \to \infty$ one has that $D(t)$ take a stationary value independent of t, so $D(t) \propto \Delta^{\beta}$ and $\beta = \nu\delta$. Note that D is the appropriated order parameter and β the associated critical exponent[13]. For $\Delta = 0$ and $t \to \infty$ the damage should be healed according to a single power-law decay and consequently a log–log plot of $D(t)$ versus t should give a straight line. On the other hand, for $\Delta < 0$ ($\Delta > 0$) the cuves should veer downward (upward), respectively. This property will allow us to determine both Y_S and δ quite accurately. Following this procedure the best straight line is obtained for $Y_S \cong 0.4125 \pm 0.0025$ and a least square fit gives $\delta \cong 0.713 \pm 0.005$, where the error bars merely reflects the statistical error. After determining the spreading critical point we have studied its dependence on the initial damage. Figure 4 shows plots of $D(t)$ versus t obtained, just at Y_S, for three different values of the initial damage. Taking $D(0) = 0.5$ it is possible to fit the asymptotic behavior of $D(t)$ obtaining $\delta \cong 0.670 \pm 0.010$ which is consistent with the exponent determined taking $D(0) = 1$. Taking a rather small value of the initial damage, e.g., $D(0) = 0.01$, on observes that the asymptotic behavior of $D(t)$ approaches those obtained taking larger $D(0)$-values. So, at least within the studied range of $D(0)$-values, the dynamics of damage healing is independent of $D(0)$.

Once that Y_S has been determined one can also investigated the behavior of the damage within the chaotic phase. It is found that for $Y_S < Y < Y_C$ the damage reaches a stationary value $D = D(t \to \infty)$ which

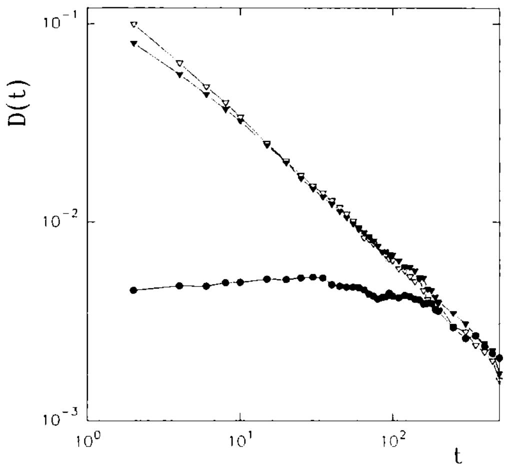

Fig. 4. Log–log plots of $D(t)$ versus t obtained, at $Y_S = 0.4125$, for different values of the initial damage: ∇ $D(0) = 1$, ▼ $D(0) = 0.5$ and ● $D(0) = 0.01$.

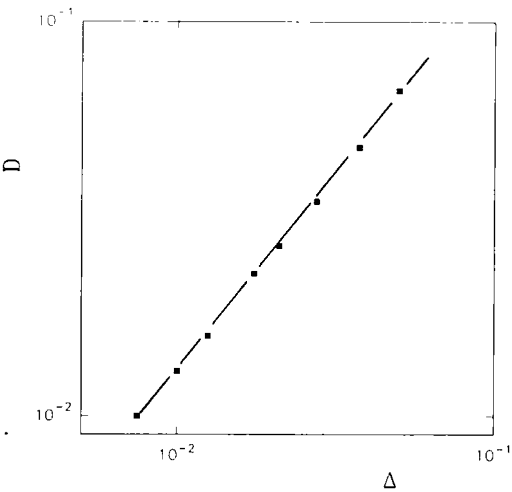

Fig. 5. Log–log plot of D versus Δ for the BK-model in three dimensions. The slope of the straight line is $\beta = 0.997$.

solely depends on Y, as expected from the scaling ansatz of equation (4). So, figure 5 shows that a log–log plot of D versus Δ exhibits linear behavior and by means of a least square fit one can determine the slope which gives for the order parameter critical exponent $\beta \cong 0.997 \pm 0.012$, where the error bars reflects the statistical error.

It should be stressed that the frozen-chaotic and the reactive-poisoning transitions take place at quite differential critical points, i.e., $Y_S \cong 0.4125$ and $Y_C \cong 0.4985$, respectively. Furthermore, the later belongs to the Directed Percolation universality class, with $\beta \cong 0.797$[21] while the former has a quite different order parameter critical exponent, e.g., $\beta \cong 0.997$. So, it becomes evident that DS introduces a new kind of dynamic critical behavior in the BK-model.

4. CONCLUSIONS

The spreading of a globally distributed damage is studied for the BK-model in 1, 2, and 3 dimensions. It is found that the maximum possible initial damage becomes healed in 1 and 2 dimensions for all Y-values, i.e., the system is immune in lower dimensions. However, a frozen-chaotic transition is found for $d = 3$ and it is located at a quite different critical point than the well known reactive-poisoning transition. Damage spreading introduce a new type of dynamic critical behavior whose nature depends on the dimensionality. $d = 3$ is the lower critical dimension for the onset of damage spreading in the BK-model.

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