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Novel decay laws for the one-dimensional reaction–diffusion model $A + A \to (2 - \epsilon)A$ as consequence of initial distributions

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Abstract. The effect of the initial particle distribution on the one-dimensional coagulation ($\epsilon = 1$) and annihilation ($\epsilon = 2$) reaction–diffusion models is studied analytically. With this aim, an exact expression for the particle number, $N(t)$, given explicitly in terms of the initial particle distribution, is derived. It is found that if the initial distribution has divergent first moments new decay laws occur. For the case of fractal distributions of dimension γ we obtain exactly the mean relative number of particles, $n(t) = \langle N(t)\rangle/\langle N(0)\rangle$. For long times it evolves as $n(t) \sim c_1\tau^{-\gamma/2} + c_2\tau^{-1/2} + c_3\tau^{-\gamma/2-1/2}$, with $\tau = 2Dt$. The existence of non-fractal initial distributions that lead to new decays is also discussed. As examples are considered an interparticle probability distribution of the form $p(r) \sim r^{-2}$ which yields $n(t) \sim a_1\tau^{-1/2}\ln(\tau) + a_2\tau^{-1/2}$ and a family of distributions of the form $p(r) \sim r^{-1}[\ln(r/r_0)]^{-1-\alpha}$, with $\alpha > 0$, which yields $n(t) \sim [\ln(\tau)]^{-\alpha}$. These results are tested by Monte Carlo simulations.

0. Introduction

Among the reactions limited by diffusion, the one-dimensional single species models of coagulation $A + A \to A$, and annihilation $A + A \to 0$, labelled with the index $\epsilon = 1, 2$ respectively: $A + A \to (2 - \epsilon)A$, have been extensively studied [1–15]. They are indeed the simplest models of reaction–diffusion and their main properties are well understood nowadays. While the classical kinetics rate equation predicts the same concentration decay $C(t) \sim t^{-1}$ for all spatial dimensions, the diffusion limitation introduces fluctuations in the local particle density [2, 3], leading to:

$$C(t) \approx \frac{1}{\epsilon}(2\pi Dt)^{-1/2} \tag{1}$$

for $d = 1$, as $t \to \infty$.

In this work we address a new source of fluctuations that can eventually not only change the course of the reaction dramatically but also this known long-time asymptotic decay, namely the effect of high fluctuations in the particle concentration at the beginning of the reaction. These high fluctuations will be modelled here by means of probability distributions with divergent moments. We will consider a one-dimensional lattice of unity spacing for comparisons with simulation results at all times. Let $N(t)$ be the number of particles at time t and $\langle N(t)\rangle$ its mean value, obtained over many realizations of the experiment. Let C_0 be the initial particle concentration as measured by $\langle N(0)\rangle$ divided by the total number of sites

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of the lattice. To obtain result (1) it is implicitly assumed that the existence of a well defined initial concentration $C_0 = \langle N(0)\rangle/L$, where L is the volume of the system measured by the number of lattice sites. What happens, however, if the *initial* particle distribution: (*a*) has a fractal dimension $0 < \gamma < 1$, for which the mean interparticle distance, $\langle r\rangle$, diverges; or (*b*) has a finite $\langle r\rangle$ but with high fluctuations around this mean value, such that its variance $\langle [r - \langle r\rangle]^2\rangle$ diverges?

In case (*a*), we have

$$\langle N(0)\rangle \sim L^{\gamma} \tag{2}$$

so that C_0 would vanish as $L^{-(1-\gamma)}$ for an infinitely large lattice. However, in experimental situations (in the laboratory as well as in computer simulations) one deals with systems of finite size, for which the problem is well posed by considering that C_0 depends parametrically on L, with $L < \infty$.

On the other hand, for case (*b*) there is a well defined (i.e. size-independent) initial concentration and thus it is to be expected that the long-time asymptotic result for homogeneous distributions, equation (1), remains unchanged. It will result that this is in fact the case; however the pure asymptotic regime establishes, at such long times, that it can hardly be reached in experimental situations and corrections to the pure asymptotic are necessary in order to describe the population decay along the main course of the reaction. We will focus on the relative mean number of particles, $n(t) \equiv \langle N(t)\rangle/\langle N(0)\rangle$, where the averages are understood over many realizations of the same experiment. We will find that in both cases the long-time asymptotics (1) changes into the new form

$$n(t) \approx \frac{1}{\epsilon}\begin{cases} c_1\tau^{-\gamma/2} + c_2\tau^{-1/2} + c_3\tau^{-\gamma/2-1/2} + \cdots & 0 < \gamma < 1 \\ \dfrac{1}{2\sqrt{\pi}}\tau^{-1/2}\ln(\tau) + \dfrac{1+\gamma^{\star}}{\sqrt{\pi}}\tau^{-1/2} + \cdots & \gamma = 1 \\ c_2\tau^{-1/2} + c_1\tau^{-\gamma/2} + c_3\tau^{-\gamma/2-1/2} & \text{for } 1 < \gamma < 2 \end{cases} \tag{3}$$

where $\tau = 2Dt$ and $\gamma^{\star}$ is the Euler constant. In equation (3) the leading terms are ordered from left to right.

There are some experimental situations in which these new decays are relevant. As is well known, the diffusion–annihilation reaction is formally related to the Ising model by identifying domain walls with particles [16–18]. Here the distribution of domain sizes can be of a fractal type for ferromagnetic (-electric) configurations. Therefore it could be of interest in the study of relaxation to the equilibrium of some substances such as potassium dihydrogen phosphate, KH_2PO_4, for which a one-dimensional ferroelectric structure with fractal aspects of the pentad Cantor set of Hausdorff dimension $\gamma \cong 0.756$ was recently reported [19, 20]. Another situation of interest is that of particles building up percolation clusters by being adsorbed on surfaces, after which they perform recombination reactions. Recently, in order to obtain information about the adsorption energy distribution on a catalytic surface, the measurement of the particle number decay along the entire course of the reaction was proposed [21]. It was found that the kinetics of the reaction $A + A \to 0$ is strongly influenced by energy correlations in the adsorptive field.

1. The model

The diffusion process will be modelled as a continuous-time random walk (CTRW) on a $d = 1$ lattice. The particles step to nearest-neighbour sites chosen with equal probability. Let $\psi(t)$ be the waiting time distribution (WTD). Pure diffusion with diffusivity D, i.e. with

a mean square displacement $\langle r^2(t)\rangle = 2dDt$, implies an exponentially distributed pausing time between steps:

$$\psi(t) = \lambda e^{-\lambda t} \qquad \hat{\psi}(u) = \int_0^\infty dt\, e^{-ut}\psi(t) = \frac{\lambda}{\lambda + u} \qquad \text{with } \lambda = 2dD. \tag{4}$$

This WTD leads exactly to a diffusion equation for the probability of finding a particle at position r if initially at $r = 0$ in the limit of continuum space: $\partial_t P(r,t) = D\partial_r^2 P(r,t)$.

Let $F(r,t)$ be the probability density for the *time* in which a random walker, starting at $r = 0$, reaches site r for the first time. For any lattice with translational invariance, it can easily be obtained in the Laplace representation [23, 24]. It can be written as

$$\hat{F}(r,u) = \hat{\eta}(u)^{-r} \qquad \text{with } \hat{\eta}(u) = 1 + (u/\lambda) + \sqrt{2(u/\lambda) + (u/\lambda)^2}. \tag{5}$$

2. An exact solution in terms of the initial distribution

In this section we will obtain an exact expression for $n(t)$ explicitly in terms of the *initial* interparticle distribution function (IPDF), $p(r)$. With this aim we will take advantage of the CTRW expression (5) in the exact results of Doering and ben-Avraham [5] (for coagulation) and of Spouge [6, 7] (for coagulation and annihilation) in one dimension. It is possible to recast their results in such a way that the relative concentration is written as a suitable average over the initial interparticle distance, r, of the survival probability of a *single pair* of particles:

$$n(t) = 1 - \int_0^t dt'\, \langle F_2(r,t')\rangle. \tag{6}$$

Here $F_2(r,t)$ is the probability density for the first encounter time, t, of two simultaneously mobile particles, which were at a distance r apart at time $t = 0$. In this notation, with the subscript '2' we would like to remark that this function refers to the *relative* motion of *two* particles. Therefore, as long as one deals with an exponential WTD, it follows from equation (5) with twice the hopping rate (i.e. 2λ in place of λ). In the Laplace representation, this amounts to taking

$$\hat{F}_2(r,u) = \hat{F}(r,u/2). \tag{7}$$

In equation (6), the average over r is given by [6]:

$$\langle F_2(r,t)\rangle = \int_0^\infty dr\, \beta(r) F_2(r,t) \tag{8}$$

with

$$\beta(r) = \begin{cases} p(r) & \text{for coagulation} \\ 2\displaystyle\sum_{k=1}^{\infty} (-1)^{k+1} p_k(r) & \text{for annihilation} \end{cases} \tag{9}$$

where $p(r)$ is the IPDF and $p_k(r)$ is the distribution for the distance of a typical particle to its kth neighbour *also at* $t = 0$ (i.e. $p_1(r) = p(r)$). We will consider an initial random distribution of particles with translational invariance modelled as a renewal process with IPDF $p(r)$. This means that the distances between next-neighbour particles are independent random variables with the same probability distribution, $p(r)$ (this is in fact the hypothesis in solution (6), see [5, 6]). In order to be more explicit, the probability density for the position, r, of the kth particle, $p_k(r)$, satisfies the recurrence relation

$$p_k(r) = \int_0^r dr'\, p(r - r') p_{k-1}(r'). \tag{10}$$

Then, in the Laplace representation, this density is readily obtained as

$$\tilde{p}_k(v) = \int_0^\infty \mathrm{d}r\, \mathrm{e}^{-vr}\, p_k(r) = [\tilde{p}(v)]^k. \tag{11}$$

Inserting (5) into (8) we obtain

$$\langle \hat{F}_2(r,u)\rangle = \int_0^\infty \mathrm{d}r\, \beta(r)\mathrm{e}^{-r\ln\hat{\eta}(u/2)} = \tilde{\beta}(v = \ln\hat{\eta}(u/2)) \tag{12}$$

with the Laplace representation (variable v) for the space: $\tilde{\beta}(v) = \int_0^\infty \mathrm{d}r\, \mathrm{e}^{-vr}\beta(r)$. From equation (9) it reads

$$\tilde{\beta}(v) = \begin{cases} \tilde{p}(v) & \text{for coagulation} \\ 2\tilde{p}(v)/[1+\tilde{p}(v)] & \text{for annihilation.} \end{cases} \tag{13}$$

Finally, returning to equation (6), the expression for the relative particle number is grasped as an explicit function of the initial distribution:

$$n(t) = \mathcal{L}_u^{-1}\left\{\frac{1}{u}[1-\tilde{p}(v=\ln\hat{\eta}(u/2))]\right\} \qquad \text{for } A+A\to A \tag{14}$$

$$n(t) = \mathcal{L}_u^{-1}\left\{\frac{1}{u}\frac{1-\tilde{p}(v=\ln\hat{\eta}(u/2))}{1+\tilde{p}(v=\ln\hat{\eta}(u/2))}\right\} \qquad \text{for } A+A\to 0 \tag{15}$$

where $\mathcal{L}_u^{-1}$ is the inverse Laplace operator acting on the complex variable u, i.e. $\mathcal{L}_u^{-1}\{\hat{f}(u)\} = f(t)$.

As an example of the application of this result, let us consider an initial distribution of one particle per lattice site. In this case $p(r) = \delta_{r,1}$, i.e. $\tilde{p}(v) = \mathrm{e}^{-v}$ and we readily obtain:

$$n(t) = \begin{cases} \mathrm{e}^{-4Dt}[I_0(4Dt) + I_1(4Dt)] & \text{for } A+A\to A \\ \mathrm{e}^{-4Dt} I_0(4Dt) & \text{for } A+A\to 0 \end{cases} \tag{16}$$

where $I_n(x)$ is the hyperbolic Bessel function. These are known results [4, 6, 8]. In figure 1 we see that there is a perfect agreement with simulations at all times.

3. Fractal initial distributions

In order to have a scaling with the system size of the form of (2) the initial distribution must be such that the particles build up a fractal pattern. This pattern can be a random or a deterministic fractal. In the following two sections we will consider both cases respectively.

3.1. Random fractals

We will consider random fractals generated as a renewal process along the line. Let $\chi_k(L)$ be the probability that exactly k particles lie inside a segment of size L. Then, the mean initial number of particles, $\langle N(0)\rangle$, within a segment of length L, is

$$\langle N(0)\rangle = \sum_{k=0}^{\infty} k\,\chi_k(L). \tag{17}$$

On the other hand, in terms of the probability $F(r)$, there are no particles within a distance r from the previous particle: $F(r) = 1 - \int_0^r \mathrm{d}r'\, p(r')$, the required probability $\chi_k(L)$ follows as

$$\chi_k(L) = \int_0^L \mathrm{d}r\, F(L-r)p_k(r). \tag{18}$$

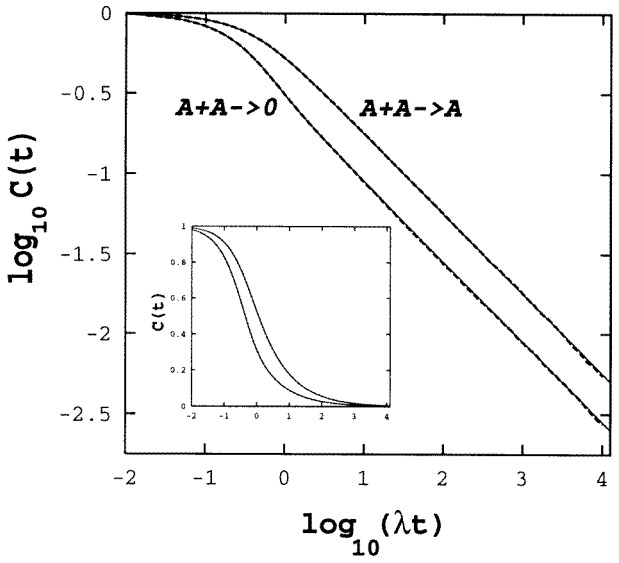

Figure 1. Evolution of the particle concentration for coagulation and annihilation, for initially one particle per site. Numerical simulations (broken curve) and theory, equation (16) (full curves). $N(0) = 30\,000$, 10 realizations.

In the Laplace representation, using (11), equation (18) becomes

$$\chi_k(v) = F(v)p_k(v) = \frac{1 - p(v)}{v}p(v)^k \tag{19}$$

and the sum in equation (17) is readily obtained as

$$\langle N(0)\rangle = \mathcal{L}_v^{-1}\left\{\frac{p(v)}{v(1 - p(v))}\right\}. \tag{20}$$

Provided the IPDF $p(r)$ has a finite first moment (the mean distance between the nearest-neighbour particles), $\langle r\rangle$, the long distance (small v) expansion of equation (20) yields $\langle N(0)\rangle \sim L/\langle r\rangle$ and the initial concentration is well defined. On the other hand, a fractal initial distribution is achieved if the IPDF is proportional to a stable law at long distances, i.e. $p(r) \sim r^{-1-\gamma}$. Let us consider the following form:

$$p(r) = \theta(r - r_0)\gamma r_0^{\gamma} r^{-1-\gamma} \tag{21}$$

where θ is the Heaviside step function and r_0 is the minimal nearest-neighbour particle distance (for example the lattice parameter).

The mean distance between nearest-neighbour particles, diverges for $0 < \gamma < 1$ and reads as $\langle r\rangle = \gamma r_0/(\gamma - 1)$ otherwise. In the first case, equation (21) in (20) leads to

$$\langle N(0)\rangle \sim \frac{\sin[\pi(1 - \gamma)]}{\pi\gamma}L^{\gamma} \tag{22}$$

that is, we obtain a fractal distribution. In figure 2 we show a realization of the particle distribution along the lattice according to (21) for $\gamma = 0.8$. Despite the fact that the mean interparticle distance is infinite, the fluctuations are also infinite in such a way that a typical realization results in a non-empty lattice. $\langle r\rangle < \infty$ when $1 < \gamma < 2$, but r has infinitely large fluctuations around this mean value. In this case, as a measure of the

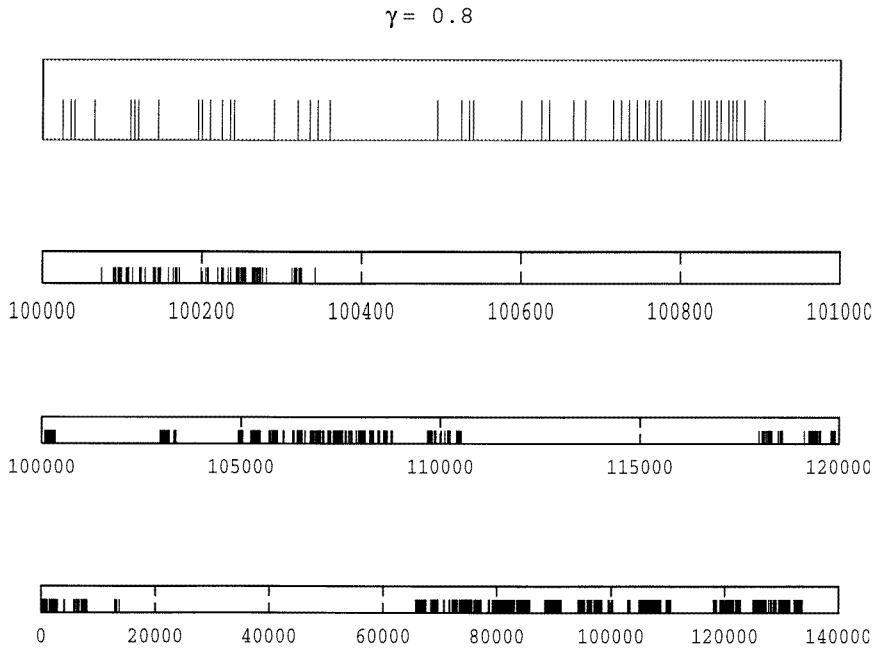

Figure 2. One realization of the initial distribution of particles generated as a fractal renewal process, equation (21). Each particle is marked with a vertical line. The first 140 000 lattice sites at different scales are shown. In the uppermost, individual lattice sites can be distinguished.

fluctuations of the initial particle distribution we can consider the second (centred) moment: $\langle (r - \langle r \rangle)^2 \rangle = \gamma r_0^2/[(\gamma - 1)^2(\gamma - 2)]$, which becomes finite only for $\gamma > 2$.

The Laplace representation of (21) reads as

$$\tilde{p}(v) = \mathrm{e}^{-(r_0 v)} - (r_0 v)^{\gamma} \Gamma(1 - \gamma; r_0 v). \tag{23}$$

Bringing this expression into equations (14), (15), studying the small u (long times) and small v (large distances) behaviours and using Tauberian theorems [25], we obtain the asymptotic form:

$$n(t) = \frac{1}{\epsilon}[c_1 \tau^{-\gamma/2} + c_2 \tau^{-1/2} - c_3 \tau^{-1/2-\gamma/2} + \cdots] \tag{24}$$

where $\tau = \lambda t = 2Dt$. The coefficients can be exactly computed (hereafter we take $r_0 = 1$, such that all distances are given in units of the lattice parameter):

$$c_1 = \frac{\Gamma(2-\gamma)}{(1-\gamma)\Gamma(1-\gamma/2)} \qquad c_2 = \frac{\gamma}{(\gamma-1)\sqrt{\pi}} \qquad \text{and} \qquad c_3 = \frac{5}{8}\frac{\gamma\Gamma(2-\gamma)}{\Gamma(1-\gamma/2)}. \tag{25}$$

This result shows a continuous transition around $\gamma = 1$, but it does not hold for $\gamma = 1$.

In particular, for the fractal case (a) $0 < \gamma < 1$, the leading term is:

$$n(t) \cong \frac{c_1}{\epsilon}\tau^{-\gamma/2} = \frac{1}{\epsilon}\frac{\Gamma(1-\gamma)}{\Gamma(1-\gamma/2)}(2Dt)^{-\gamma/2}. \tag{26}$$

This result reproduces the advanced form $t^{-\gamma/2}$ [15, 22] on the anomalous particle number decay for fractal initial distributions in one dimension. Moreover, for the first time, they give exactly the proportionality constants.

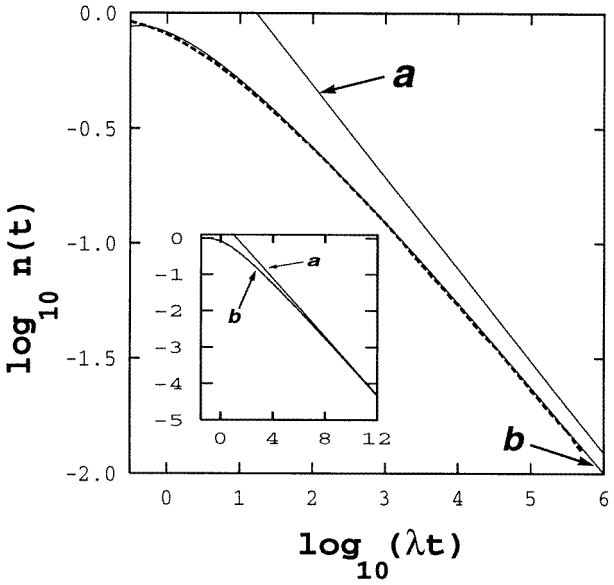

Figure 3. Relative particle number decay in numerical simulations of coagulation. $N(0) = 10\,000$, four realizations. Initially, particles form a random fractal with the nearest-neighbour distance generated according to equation (21) with $\gamma = 0.8$. The full curves correspond to the analytical predictions: (*a*) the long-time pure asymptotic given by equation (26) and (*b*) the exact solution, equation (14), computed after the numerical Laplace transform. The inset shows the slow convergence of the theoretical expression to its asymptotic.

In figure 3 we show numerical simulations (broken curves) for the coagulation reaction with particles whose initial positions were generated by means of a renewal process with IPDF (21), for $\gamma = 0.8$.

In figure 4 we show the corresponding comparision for annihilation. It is important to note that this *pure* asymptotic decay, equation (26) (curve '*a*' in the figures), establishes for times too long to be reached by the simulations. On the other hand, it is enough to take the first two terms in result (24) to obtain the correct decay along practically the whole course of the reaction.

In figure 5 we show the evolution of the IPDF as histograms generated from the same simulations as for figure 3. At variance with the case of homogeneous initial distributions [5, 12], here we see that the fractal distribution is preserved along the course of the reaction.

As an example of case (b) we have taken $1 < \gamma < 2$, such that $\langle r \rangle$ is finite but $\langle r^2 \rangle$ still diverges. In figures 6 and 7 we show simulation results for $\gamma = 1.2$ compared with our analytical expression (24). Note that now the leading terms are interchanged: the pure asymptotic is now

$$n(t) \cong \frac{1}{\epsilon} c_2 \tau^{-1/2} = \frac{\gamma}{\epsilon(\gamma - 1)} (2\pi Dt)^{-1/2} \tag{27}$$

which again occurs at very long times if $1 < \gamma < 2$, i.e. for initial distributions with infinitely large fluctuations around the mean initial concentration.

We should note that the appearance of decay laws other than the known form (1) is not a consequence exclusive of fractal distributions. In fact, taking $\gamma = 1$ and the same

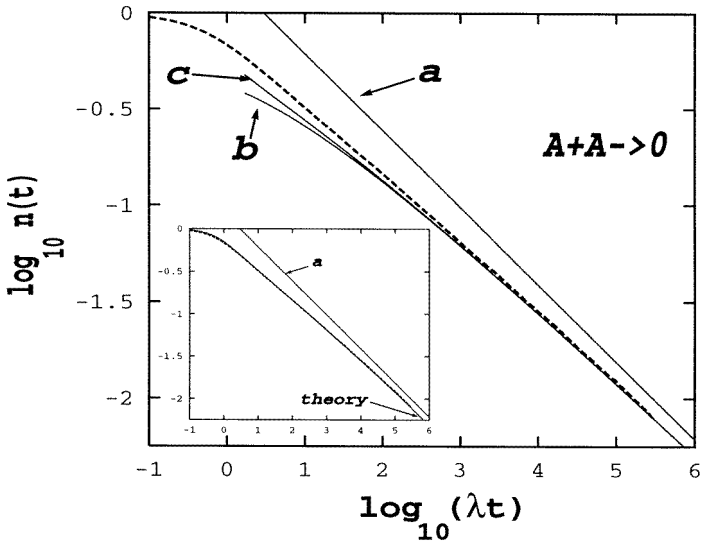

Figure 4. Annihilation reaction for a particle distributed initially as a random fractal with $\gamma = 0.8$, fixing the initial number of particles $N(0) = 80\,000$ and averaging over four realizations: (*a*) the leading term, equation (26); (*b*) taken the two first leading terms of equation (24); and (*c*) taken the three first leading terms given in expansion (24).

function $p(r)$, a similar expansion leads to the result

$$n(t) \cong \frac{1}{\epsilon}\left[\frac{\tau^{-1/2}}{2\sqrt{\pi}}\ln(\tau) + \frac{1+\gamma^{\star}}{\sqrt{\pi}}\tau^{-1/2} + \cdots\right] \tag{28}$$

which shows a non-neglectable logarithmic correction to the classical decay $\tau^{-1/2}$, see figure 8. Here $\gamma^{\star} = 0.577\,215\,6649\ldots$ is the Euler or Mascheroni constant.

Still more surprising is another non-fractal distribution which also has divergent integer moments, recently introduced by Havlin and Weiss [26]:

$$p(r) \sim r^{-1}[\ln(r/r_0)]^{-1-\alpha} \qquad \text{with } \alpha > 0 \qquad \text{as } r \to \infty. \tag{29}$$

While for the IPDF proportional to a stable law, equation (21), moments of order less than γ will be finite, in this case now there are no finite positive moments. The logarithmic moments of order less than γ will be finite for the IPDF of equation (29). A similar analysis shows that the decay turns out to be

$$n(t) \sim \frac{1}{\epsilon}[\ln\tau]^{-\alpha}$$

at long times.

3.2. Deterministic fractals

As an example of a deterministic fractal structure we have taken a (generalized) Cantor set of base b constructed by placing one particle per site, dividing the lattice in b equal parts (b odd) and removing all particles of the central part. By repeating this procedure iteratively on each remaining part, the particles build up a pattern of fractal dimension $\gamma = \ln(b-1)/\ln(b)$. In order to implement this distribution we have numbered the lattice sites in base b (we have considered $b = 3, 5$) and assigned no particle to this site if in this

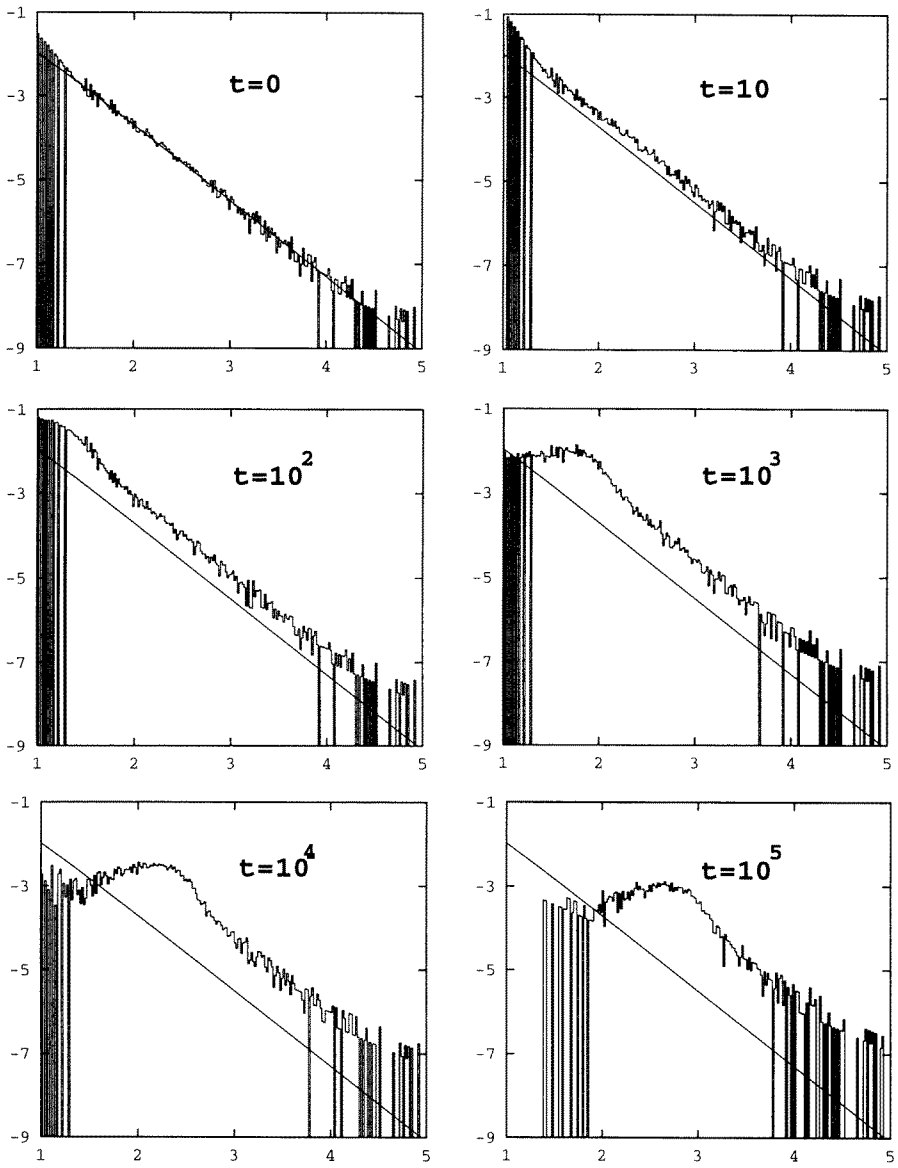

Figure 5. Histograms for the interparticle distance at the indicated times. They correspond to the simulations of figure 3. Both axis scales are logarithmic. The full line is the same in all figures, and shows the theoretical probability density, equation (21), from which the initial distribution was generated. These data correspond to a single realization in which the distance between the left-most and the right-most particle was also generated considering periodic boundary conditions. Note the appearence of finite size effects after a time of $t > 10^5$.

representation its lattice-site number contains the character $(b-1)/2$ (i.e. 1, 2 respectively), otherwise we assigned a particle to this site. In tables 1 and 2 we show the resulting scaling of the (initial) number of particles with the system size, L, for different sizes of lattice by using this algorithm.

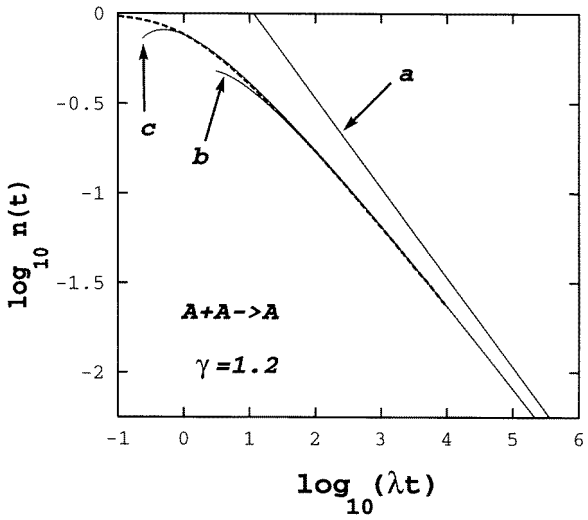

Figure 6. The same as figure 3 but for $\gamma = 1.2$: (a) the leading term, equation (27); (b) taken the two first leading terms and (c) taken the three first leading terms given in equation (24). Here is $N(0) = 50\,000$, three realizations.

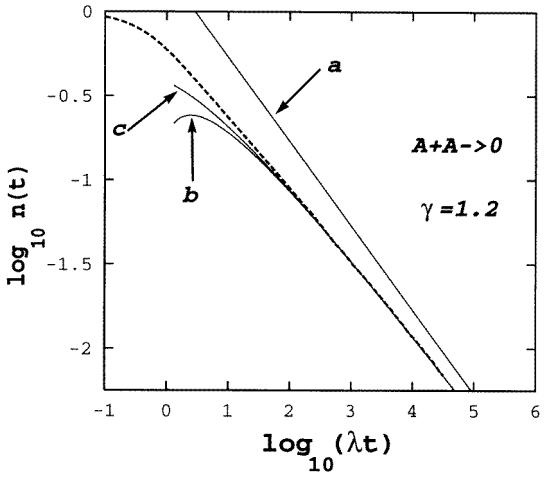

Figure 7. The same as figure 6 ($\gamma = 1.2$) for the annihilation reaction. Here is $N(0) = 50\,000$, three realizations.

In figure 9 we show the simulation results for the coagulation reaction with particles initially placed on the lattice building up Cantor sets of bases $b = 3, 5$ generated up to levels 14, 9 shown in tables 1 and 2 respectively. As a comparison, the case of initially one particle per site is also shown in the bottom curve. The full lines, as reference, show the pure asymptotics $n(t) \sim t^{-\gamma/2}$. Note that this asymptotics establishes after a few steps of the particles. In this respect, the evolution of the particle number for random and deterministic fractals are very different, despite the fact that both share the same pure asymptotics.

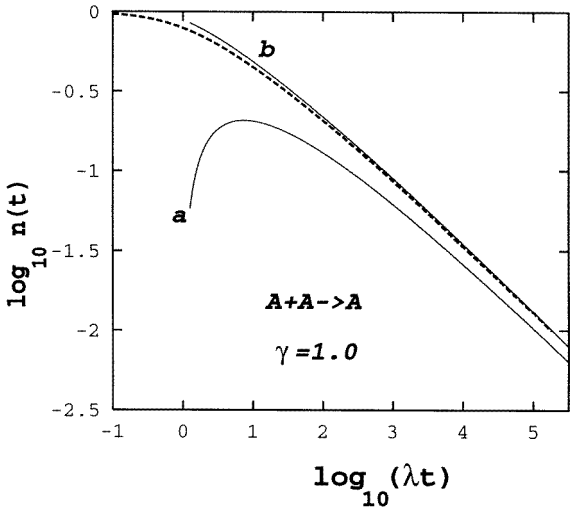

Figure 8. Coagulation reaction: same as figure 3 for $\gamma = 1$: (a) the leading term, $\frac{1}{2\sqrt{\pi}}\tau^{-1/2}\ln(\tau)$; ($b$) taken the two first leading terms shown in equation (28). Here is $N(0) = 50\,000$, three realizations.

Table 1. Cantor set of base $b = 3$ and dimension $\gamma = \ln(2)/\ln(3) = 0.630\,929\,75\ldots$.

$N(0)$	L	$\log_3(N(0))$	$\log_3(L)$	$\gamma = \log_3(N(0))/\log_3(L)$
2	3	0.630 929 75	1	0.630 929 75
4	9	1.261 859 51	2	0.630 929 75
8	27	1.892 789 26	3	0.630 929 75
16	81	2.523 719 01	4	0.630 929 75
32	243	3.154 648 77	5	0.630 929 75
64	729	3.785 578 52	6	0.630 929 75
128	2 187	4.416 508 27	7	0.630 929 75
256	6 561	5.047 438 03	8	0.630 929 75
512	19 683	5.678 367 78	9	0.630 929 75
1 024	59 049	6.309 297 54	10	0.630 929 75
2 048	177 147	6.940 227 29	11	0.630 929 75
4 096	531 441	7.571 157 04	12	0.630 929 75
8 192	1594 323	8.202 086 80	13	0.630 929 75
16 384	4782 969	8.833 016 55	14	0.630 929 75

4. Conclusions

We have found new decay laws which appear as a consequence of a high inhomogeneity in the initial distribution. Considering the great number of works dedicated to the study of these reactions, this aspect had not received enough attention [15, 22].

We have considered in detail two types of fractal initial particle distribution. First a random fractal generated as a renewal process along the line, such that it is completely specified by the interparticle probability distribution function (IPDF), $p(r)$. Using CTRW expressions for the first-passage-time density in the method of solution given by Spouge [6], we have obtained the relative mean number of particles, $n(t) = \langle N(t)\rangle/\langle N(0)\rangle$ as an explicit function of $p(r)$ (see equations (14), (15)).

Table 2. Generalized Cantor set of base $b = 5$ and dimension $\gamma = \ln(4)/\ln(5) = 0.861\,353\,12\ldots$.

$N(0)$	L	$\log_5(N(0))$	$\log_5(L)$	$\gamma = \log_5(N(0))/\log_5(L)$
4	5	0.861 353	1	0.861 353 116 146
16	25	1.722 706	2	0.861 353 116 146
64	125	2.584 059	3	0.861 353 116 146
256	625	3.445 412	4	0.861 353 116 146
1 024	3 125	4.306 765	5	0.861 353 116 146
4 096	15 625	5.168 118	6	0.861 353 116 146
16 384	78 125	6.029 471	7	0.861 353 116 146
65 536	390 625	6.890 824	8	0.861 353 116 146
262 144	1953 125	7.752 178	9	0.861 353 116 146

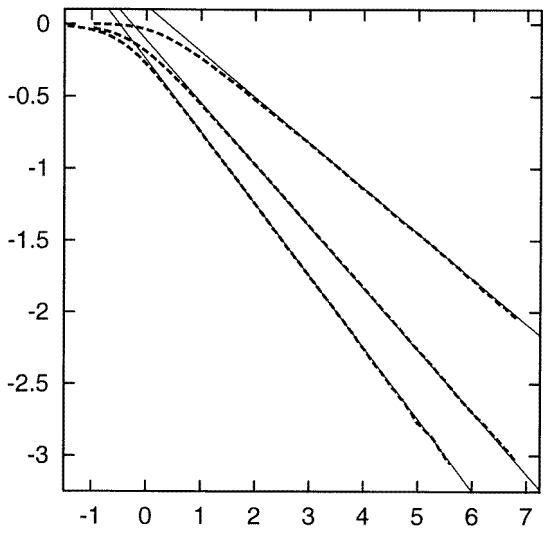

Figure 9. Log_{10}–$\log_{10}$ plot of $n(t)$ for the coagulation reaction with particles forming a deterministic fractal at $t = 0$ (axis are as in previous figures). From the top to the bottom: for a Cantor set of base $b = 3$ ($\gamma = \ln(2)/\ln(3) = 0.63$), for a Cantor set of base $b = 5$ ($\gamma = \ln(4)/\ln(5) = 0.86$) and (as a reference) for one particle per site. In all cases the broken curves correspond to simulations (two realizations) and the full lines show the asymptotics: $t^{-\gamma/2}$ for the Cantor sets and equation (1) for one particle per site.

Taking a distribution proportional to a stable law at large distances: $p(r) \sim r^{-1-\gamma}$; $\gamma > 0$ we found that for long times $n(t) \sim c_1(2Dt)^{-\gamma/2} + c_2(2Dt)^{-1/2} + c_3(2Dt)^{-\gamma/2-1/2}$, with the factors c_1, c_2, c_3 given exactly in equation (25). For $0 < \gamma < 1$ (a fractal distribution) the leading term is $t^{-\gamma/2}$ at variance with the characteristic decay $t^{-1/2}$. However, even for $1 < \gamma$, for which a mean initial concentration C_0 does exist, if $\gamma < 2$ the fluctuations in the spatial distribution of particles diverges. As a consequence, the expected asymptotics (1) does not suffice to describe the long-time decay and at least the first two leading terms: $n(t) \sim c_2(2Dt)^{-1/2} + c_1(2Dt)^{-\gamma/2}$ must be considered.

We have also considered particles building up a Cantor set at $t = 0$, of dimension $\gamma = \ln(2)/\ln(3)$ and a generalized Cantor set of dimension $\gamma = \ln(4)/\ln(5)$ as examples of deterministic fractals. We found that the asymptotic decay $N(t) \sim t^{-\gamma/2}$ establishes at

earlier times, without the large transients found for random fractals.

Finally, we pointed out that the appearance of anomalous decay laws are not a consequence of exclusively fractal initial distributions, but of the non-existence of first moments of this distribution. As an example, taking the IPDF $p(r) \sim r^{-1}[\ln(r/r_0)]^{-1-\alpha}$, $\alpha > 0$ we obtained the novel decay $n(t) \sim [\ln(2Dt)]^{-\alpha}$.

We consider that it is important to be aware of these effects, in order to interpret experimental results, where departures of the known decays could be the sign of an exotic spatial distribution.

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