# Continuously varying exponents in reaction-diffusion systems

## LETTER TO THE EDITOR

# Continuously varying exponents in reaction–diffusion systems

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**Abstract.** We propose a simple reaction–diffusion model describing a class of competitive multi-species reactions. The model is exactly solvable at its upper critical dimension $d_u = 2$. The local moments of the component concentrations follow a power-law decay with exponents which vary continuously with system parameters. The exponents also have an underlying multifractal spectrum. The main results are supported by results from a numerical integration of the model.

Reaction-diffusion systems continue to attract the attention of many workers in the wider field of non-equilibrium phenomena [1]. This is due in part to their obvious relation to chemical kinetics, where a better understanding of scaling laws is desirable. However, the applicability of these model systems is really far wider since they may be considered as a natural description of many systems with spatial degrees of freedom along with dynamic competition among different species (such as the diverse examples of population dynamics, and monopole annihilation in the early universe). The most studied examples in the theoretical physics literature are the reactions A + A → inert and its close relative A + B → inert [2]. Each of these systems has an upper critical dimension $d_u$ (equal to 2 and 4, respectively) above which the scaling exponents are equal to predictions from naive power counting. Below $d_u$, the restrictions imposed from low-dimensional spatial diffusion become relevant and the exponents are dramatically changed. The simplest scenario is that of an initially homogeneous mixture of reagents decaying to some uniform asymptotic state. Renormalization-group calculations have recently been performed for this case, yielding exact values for the exponents describing the decay of the component concentrations [3].

In this letter we propose a model of a simple (and rather generic) three-component reaction–diffusion system. This model is found to have surprisingly rich scaling properties at its upper critical dimension. We shall motivate it here in the language of chemical kinetics, but we stress that its application is not limited to this field. We imagine the following reactions involving components A, B and C:

$$2A + C \xrightarrow{k_1} 2A$$
$$2B + C \xrightarrow{k_2} 2B \qquad\qquad (1)$$
$$A + B + C \xrightarrow{k_3} 3C.$$

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This system of reactions annihilates the component C in regions which are rich in either A or B. The component C can prosper only in regions which have sufficiently high amounts of both A and B. Therefore C acts as a tracer—marking out the complex boundaries separating the regions where A or B dominates. There are many potential applications of this model in population dynamics and related fields, since C is basically parasitic—it can only survive when its 'predators' A and B are *simultaneously* present, taking advantage of their mutual annihilation.

The translation of the chemical equations above into a mathematical model may be achieved at various levels of precision and sophistication; ranging from simple rate equations (with no spatial degrees of freedom) to a full description of the microscopic processes via a master equation formulation. The approach we shall persue here lies midway between these two extremes in that we shall neglect the intrinsic stochasticity of the dynamics, but we shall retain the spatial degrees of freedom in order to take account of possibly important effects arising from long-range spatial fluctuations. It is generally understood that there exist critical dimensions above which these types of approximations become valid. We expect the level of description used here to be sufficient above spatial dimension $d = 1$ since the basic reaction is *tri*-molecular [3]. We shall see that spatial fluctuations may be neglected for $d > 2$. The main results of this letter are for the case $d = 2$—the (upper) critical point of the model.

At this level of approximation the above reactions may be described by the following partial differential equations:

$$\partial_t a = D\nabla^2 a - k_3 a b \, \rho$$
$$\partial_t b = D\nabla^2 b - k_3 a b \, \rho \qquad \qquad (2)$$
$$\partial_t \rho = D'\nabla^2 \rho - k_1 a^2 \, \rho - k_2 b^2 \, \rho + 2k_3 a b \, \rho$$

where the concentration fields are $a = [A]$, $b = [B]$, and $\rho = [C]$, and $D$ is the diffusion constant for the A and B particles, whilst $D'$ is that for the C particles.

This letter is concerned with exact results, and in order to achieve this we shall make two choices concerning the parameters in the model. Firstly, we shall take the rate constants $(k_1, k_2, k_3)$ to be equal, with value $k$. Secondly, we shall allow spatial diffusion only for the A and B particles. The C particles will be taken to be immobile ($D' = 0$). The relaxation of the above constraints makes the model intractable analytically. However, a numerical investigation into the properties of the full model is currently underway; in particular, the model is seen to develop a sharp phase transition (in the steady state) on variation of the rate constant $k_3$ with respect to $k_1$ and $k_2$. Details are expected to be presented in a future report [4].

Due to the symmetry between A and B particles, it suffices to consider only the concentration field: $\sigma = [A] - [B]$. The above equations then take the form

$$\partial_t \sigma = D\nabla^2 \sigma \qquad \partial_t \rho = -k\sigma^2 \rho \,. \qquad \qquad (3)$$

As an initial condition, we shall consider a uniform distribution of C particles, along with a random distribution (assumed to be Gaussian and delta correlated) for the A and B particles. The case of initially separated A and B particles forming a steady diffusion front of C particles will be treated in [4]. We therefore take $\rho(x, 0) = 1, \forall x$; and $\sigma(x, 0) = \sigma^0(x)$, where $\sigma^0$ is a Gaussian distributed random variable with zero mean and correlator $\langle \sigma^0(x)\sigma^0(x')\rangle = \Delta\delta(x - x')$.

At a purely formal level this problem reduces to calculating non-trivial statistics (connected with the $\rho$ field) in relation to the simple problem of the diffusion equation. The picture one should have in mind is that the $\rho$ field may only survive in the presence
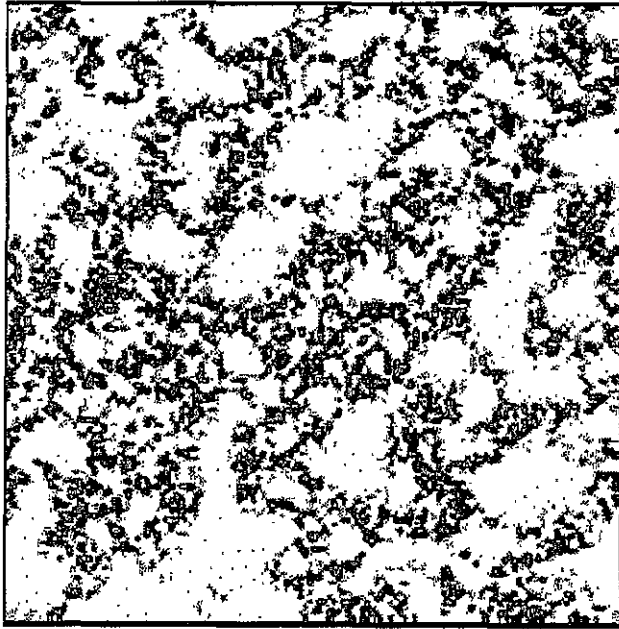
**Figure 1.** A contour plot of the density field $\rho$ from numerical integration of (3) for a system of size $128 \times 128$. Darker regions correspond to higher values of $\rho$.

of zero diffusion field (C particles prospering in regions rich in A *and* B). The contours of zero diffusion field are, however, constantly evolving (and coarsening) therefore leading to 'smearing' and long-term memory effects in the decay of the $\rho$ field. Figure 1 shows a contour plot of the density field $\rho$ for a system of size $128 \times 128$ at some late stage of the evolution.

In this letter we shall concentrate on calculating the local moments of the density $\rho$ defined by $\mu_r(t) \equiv \langle \rho^r \rangle$. We start by studying the system at the mean-field (MF) level. This amounts to replacing the right-hand side of (3b) by $-k\langle \sigma^2 \rangle \rho$. The mean-square fluctuations in $\sigma$ are easily evaluated from the diffusion equation giving $\langle \sigma^2 \rangle = \Delta (8\pi Dt)^{-d/2}$. We therefore have

$$\mu_r(t) = \begin{cases} \exp\left(-c_1 r t^{1-d/2}\right) & 0 < d < 2 \\ (t/t_0)^{-\gamma_r(\phi)} & d = 2 \\ c_2 & d > 2 \end{cases} \tag{4}$$

where $c_1$ and $c_2$ are constants, $\gamma_r(\phi) = r\phi/8\pi$ and $\phi = k\Delta/D$. So even at the MF level, the system shows quite rich behaviour. There is an upper critical dimension $d_u = 2$ above which the local moments of the density decay asymptotically to a constant. Below $d_u$ the moments decay as stretched exponentials. Exactly at $d_u$ the moments decay in power-law fashion with exponents which depend continuously on the system parameters through the quantity $\phi$. The exponents also have the striking property

$$\gamma_{r_1}(\phi_1) = \gamma_{r_2}(r_1\phi_1/r_2). \tag{5}$$

It is important to understand how much of the MF behaviour is relevant to the real evolution of the system. We shall tackle this question in the following way. Consider generalizing the system by changing $\sigma$ into an $n$-component vector $\sigma = (\sigma_1, \ldots, \sigma_n)$.

(We stress here, before continuing with the discussion, that the purpose of this generalization is to *motivate* an exact solution for *all* values of $n$, including $n = 1$ which corresponds to the original model (equation (3)). The $n$-component model should not be considered too seriously as an interesting model in its own right, at least in the context of reaction–diffusion systems.) .

We write the analogous model equations as

$$\partial_t \rho = -(k/n)\sigma_i\sigma_i\rho \qquad \partial_t\sigma_i = D\nabla^2\sigma_i . \tag{6}$$

The initial conditions are the same as in the scalar case, with the initial correlator for the $\sigma_i^0$ field being generalized to $\langle\sigma_i^0(x)\sigma_j^0(x')\rangle = \Delta\delta_{i,j}\delta(x - x')$. Therefore the components $\sigma_i$ evolve independently, although they are summed together in the effective decay rate of the $\rho$ field. The vector model defined above reduces to the original model defined in (3) for $n = 1$.

The motivation for this generalization is the following. An exact analysis of (6) reveals that the limit of $n \to \infty$ is formally equivalent to the MF approximation. One may therefore systematically expand around MF by expanding in the parameter $1/n$. It turns out that one can calculate this expansion to all orders. For $d > d_u$ one finds no corrections to the MF result—the moments still relax to constant values for large times. For $d < d_u$ one finds that the expansion is divergent for large times—indicating that the MF result is incorrect (for finite $n$). Improvement on MF may be effected by either an RG analysis of the present expansion technique, or by analysis of an eigenvalue expansion, which we shall outline later in this letter. For $d = d_u$, we shall find that each term of the expansion is relevant and that the power-law decay predicted by the MF approximation persists, but with a more complicated form for $\gamma_r(\phi)$. The expansion becomes divergent, however, for $r\phi > \pi/\ln 2$—in which case, a new technique is again required. In the remainder of this letter we shall restrict ourselves to $d = d_u(= 2)$ and concentrate on the evaluation of $\gamma_r(\phi)$ for $r\phi \leqslant \pi/\ln 2$. This letter is concerned with results, and we shall therefore only give the briefest outline of the evaluation of $\gamma_r(\phi)$. We plan to give a fuller account in a longer paper [4].

One may write the exact solution of the diffusion equation for $\sigma_i$ in terms of the heat kernel $g(x, t) = (4\pi Dt)^{-1}\exp(-x^2/4Dt)$. Integrating the equation for $\rho$ then gives the exact expression

$$\mu_r(t) = \left\langle \exp\left(\frac{-kr}{n}\int_{t_0}^t dt_1 \int d^2y \int d^2y'\, g(y, t_1)g(y', t_1)\sigma_i^0(y)\sigma_i^0(y')\right)\right\rangle . \tag{7}$$

The required average is over a Gaussian distribution, so that in order to calculate $\mu_r(t)$, one must evaluate what is essentially a Gaussian path-integral. However, the calculation of the resulting determinant appears to be non-trivial due to the non-local structure of the covariance matrix. The determination of the eigenvalues of this matrix requires the solution of an integral equation which may be the best non-perturbative approach to analyse the cases of (i) $d < d_u$ and (ii) $d = d_u$ with $r\phi > \pi/\ln 2$. In this letter we shall pursue the expansion technique about the MF solution. We therefore expand the exponential in (7) and average each term separately. After averaging, it becomes clear that the expansion may be rewritten in terms of an effective generating function for connected averages, much the same as one uses in standard field theory. The connected averages in the present case are not cumulants, but completely connected cyclic averages of the random fields. In terms of these cyclic averages one has

$$\ln \mu_r(t) = (-r\phi/4\pi)\sum_{m=1}^\infty \Lambda_m(t)/m! \tag{8}$$

where

$$\Lambda_m(t) = (m-1)! \, (-r\phi/2\pi n)^{m-1} \int_{t_0}^{t} dt_1 \cdots \int_{t_0}^{t'} dt_m \, (t_1 + t_2)^{-1} \cdots (t_m + t_1)^{-1}. \tag{9}$$

On evaluating the cyclic time integrals one finds that all terms in the sum are proportional to $\ln(t/t_0)$ (with no corrections) and therefore the power-law decay $\mu_r(t) = (t/t_0)^{-\gamma_r}$ is still valid. The parameter $n$ labels the order of the expansion, but at this level is seen to simply scale the value of $\phi$—we shall henceforth take $n = 1$.

The exact form for the exponent $\gamma_r$ is found to be

$$\gamma_r(\phi) = r\phi/8\pi + (1/4) \sum_{p=0}^{\infty} (-1)^p \left( \frac{\ln[1 + a_p \, r\phi/\pi] - a_p \, r\phi/\pi}{a_p} \right) \tag{10}$$

where the numbers $\{a_p\}$ are given by

$$a_p = \int_0^1 du \, \frac{u^p}{(1+u)} = \frac{1}{2}\left[ \psi\left(\frac{p+1}{2}\right) - \psi\left(\frac{p}{2}\right) \right] \tag{11}$$

where $\psi(z)$ is the Psi, or digamma function [5]. This is the main result of the paper. From this exact result we see that $\gamma_r$ is still a function of $\phi$ only, and also that the relation shown in (5) still holds. However, we see that the property of 'gap' scaling ($\gamma_r \propto r$) which held at the MF level, is now lost.

The validity of (10) is restricted to $r\phi \leqslant \pi/\ln 2$ since the logarithm in the expression for $\gamma_r$ originates from a series expansion with radius of convergence $a_p \, r\phi/\pi = 1$. The largest member of the set $\{a_p\}$ is $a_0 = \ln 2$—hence the condition. However, it is possible that one may be able to analytically continue this expansion for larger values of $r\phi$ such that the above expression for $\gamma_r$ involving the logarithm is still valid. This possibility may only be verified through one of the alternative calculational procedures mentioned earlier.

To test our results, we have performed a numerical integration of the model equations (3). In order to measure averaged quantities with good precision we used a system of size $512 \times 512$. Figure 2 shows a log–log plot of the local moments $\mu_r$ versus time, for two choices of the system parameter $\phi$. It is clearly seen that the moments indeed decay in power-law fashion with exponents depending upon the parameter $\phi$; and also that the relation (5) is satisfied. A direct comparison of the measured values of $\gamma_1$ with the exact result (10) is shown in figure 3 for $0 < \phi \leqslant \pi/\ln 2$. Good agreement is seen for smaller values of $\phi$. As $\phi$ approaches the critical value $\pi/\ln 2$, the measured value of $\gamma_1$ deviates by about 10% from the exact result. This discrepancy is thought to be due to finite-size effects as evidenced by the improvement of the agreement between the exact result and the numerical prediction on increasing the system size to $1024 \times 1024$ (see figure 3). The exponents obtained numerically show no noticable discontinuity as $r\phi$ passes through $\pi/\ln 2$ indicating that the analytic continuation hypothesis for the form of $\gamma_r$ shown in (10) may be correct.

Before concluding we shall briefly describe a multifractal analysis of our main result (equation (10)). We refer the reader to Halsey *et al* [6] for a thorough discussion of the following interpretation of multifractals (for a wider discussion, see also [7].) We have the basic result $\langle \rho(t)^r \rangle \sim (t_0/t)^{\gamma_r}$ with $\gamma_r(\phi)$ given above. As noted earlier, the moments of the density field do not obey simple 'gap' scaling as the exponents $\gamma_r$ are not proportional to $r$—this is a hallmark of multifractal scaling. Following [6] we regard the density field as a function on the space defined by the support of $t$, which in this case is just the real
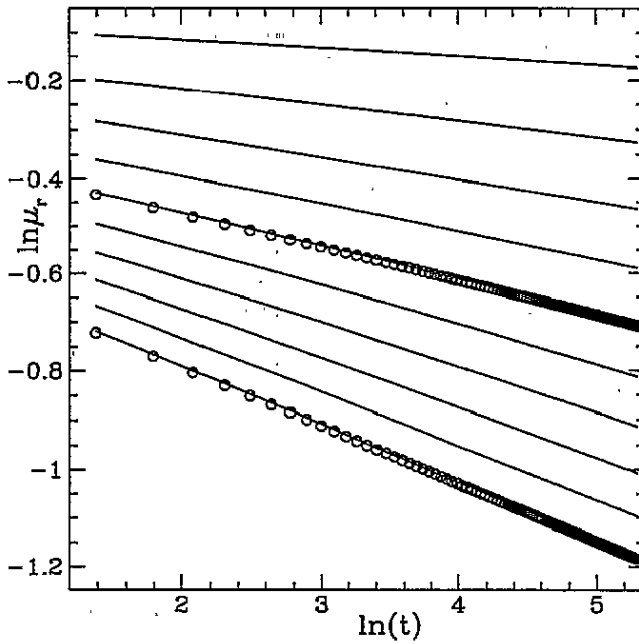
**Figure 2.** Log–log plot of the local moments $\mu_r(t)$ versus time, from a numerical integration of (3) for a system of size $512 \times 512$. The full curves are for $\phi = \pi/(10 \ln 2)$ with $r = 1, \ldots, 10$. The circles are for $\phi = \pi/(2 \ln 2)$ with $r = 1, 2$. In each case $r$ increases from top to bottom.
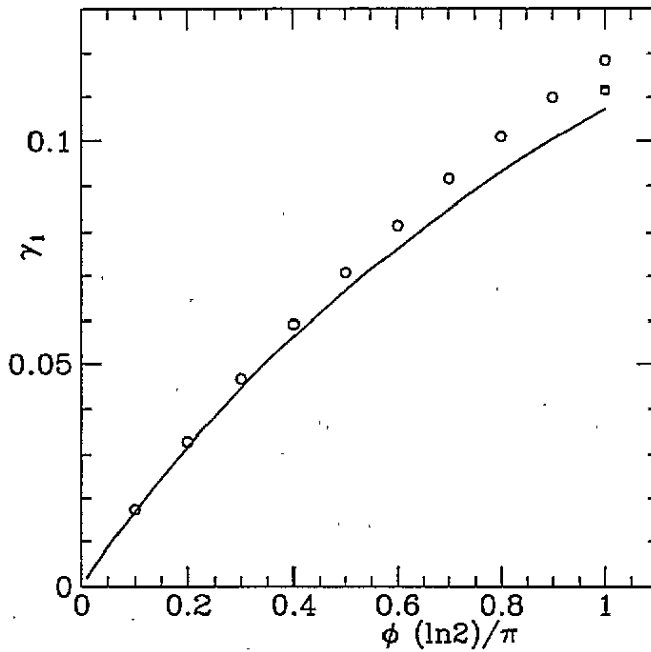


**Figure 3.** The exponent $\gamma_1(\phi)$ versus $\phi$. The full curve is the exact result as given in (10). The circles are from numerical integration of (3) for a system of size $512 \times 512$. The single square data point at the critical value of $\phi$ is from numerical integration of a system of size $1024 \times 1024$.
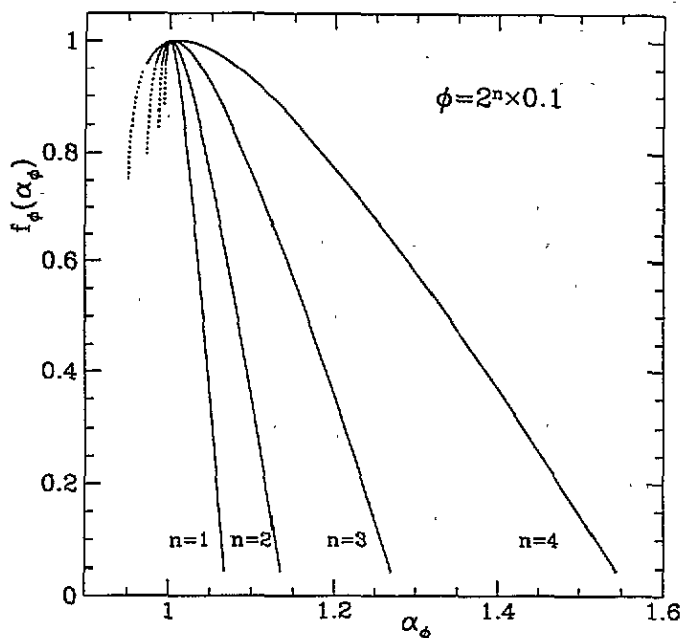
**Figure 4.** Multifractal scaling curves $f(\alpha)$ for values of $\phi = 2^n \times 0.1$ with $n = 1, 2, 3, 4$. The broken curves correspond to values of $r\phi > \pi/\ln 2$ for which the analytic expression (10) is not proven to hold.

(time) axis which has dimension equal to unity (this sounds pedantic, but in applications to spatial multifractality like DLA, the support—i.e. the cluster—is itself fractal.) We then define a measure with respect to this function

$$\mu(t^*) = \frac{\rho(t^*)}{\int\limits_{t_0}^{t} dt' \, \rho(t')} \tag{12}$$

with $t_0 < t^* < t$. One then postulates scaling of moments of the measure: $\int\limits_{t_0}^{t} dt' \, \mu(t')^r \sim (t_0/t)^{\tau_r}$. The two sets of exponents are related via [8]

$$\tau_r = \gamma_r - 1 + r(1 - \gamma_1). \tag{13}$$

The familiar function $f(\alpha)$ is generated from the exponents $\tau_r$ by the parametrization: $\alpha = d\tau/dr$ and $f = r\alpha - \tau$. For the present case, $f$ and $\alpha$ are both continuously dependent on the system parameter $\phi$—the explicit expressions are complicated and will not be written here. In figure 4 we present some sample $f(\alpha)$ curves for various values of $\phi$. These curves may not be collapsed by rescaling with respect to $\phi$.

In conclusion we have proposed and analysed a simple three-component reaction–diffusion model. It is found to have an upper critical dimension of 2, above which the density field $\rho$ relaxes to a non-zero value. Precisely at $d = 2$, one may solve the model exactly for a range of parameter values. One finds power-law decay of local moments of the density field $\mu_r$, with exponents $\gamma_r$ which are continuous functions of the system parameters, and which are also described by an underlying multifractal spectrum. It is of interest to determine the generality of this non-universal scaling in the wider class of multi-component reaction–diffusion systems.

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