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Exact solution of a reaction–diffusion process with three-site interactions

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Abstract
The one-dimensional reaction diffusion process $AA \to A$ and $A\emptyset A \to AAA$ is exactly solvable through the empty interval method if the diffusion rate equals the coagulation rate. Independently of the particle production rate, the model is always in the universality class of diffusion–annihilation. This allows us to check analytically the universality of finite-size scaling in a non-equilibrium critical point.

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1. Introduction

The physics of non-equilibrium phase transitions in low dimensions is characterized by the presence of strong fluctuation effects which modify the properties of the steady-state and/or the long-time behaviour considerably with respect to simple kinetic equations (see [1–5] for recent reviews). However, and in contrast to equilibrium phase transition, most of the current understanding of non-equilibrium phase transitions comes from numerical studies of certain simple models. Integrable non-equilibrium systems are still very rare.

A model which has been met recently with a lot of interest is the one-dimensional pair contact process [6] with single-particle diffusion (PCPD). This model describes the interactions of a single species A of particles which can undergo the reactions $2A \to \emptyset$ and $AA\emptyset \to AAA$. If the diffusion constant $d = 0$, there are a huge number of steady states (for L sites of the order $\sim \phi^L$, where $\phi = (1 + \sqrt{5})/2$ is the golden mean [7]) and the steady-state phase transition between the active and the inactive phases is in the directed percolation universality class [6] (for $d = 0$, the mean pair density serves as the order parameter which is positive in the active phase and vanishes at the transition towards the inactive phase). On the other hand, for $d \neq 0$, there remain just two steady states. There is a general agreement on the location

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of the transition line between the active and the inactive phases (current studies apply either the density matrix renormalization group [7] or different Monte Carlo schemes [8, 9]) and that the entire inactive phase should be critical and in the diffusion–annihilation universality class [10]. However, so far there is no consensus on the exponents *at* the active–inactive transition.

In order to obtain a fresh view on this problem, we try to find a 'nearby' model where some analytical information might be available. In this paper, we shall study the following model: particles of a single species move along a one-dimensional lattice. Each site can be either empty ($\emptyset$) or else be occupied by a single particle (A). Between nearest-neighbour or next-nearest-neighbour sites the following reactions are allowed:

$$\begin{array}{lll} \text{diffusion:} & A\emptyset \leftrightarrow \emptyset A & \text{rate } d \\ \text{coagulation to the left:} & AA \to A\emptyset & \text{rate } d \\ \text{coagulation to the right:} & AA \to \emptyset A & \text{rate } d \\ \text{production:} & A\emptyset A \to AAA & \text{rate } 2d\lambda. \end{array} \tag{1}$$

The equality of the diffusion rate and the coagulation rates guarantees the solvability of the model for $\lambda = 0$ through the empty interval method [11].

As will be explained in the following section, the choice of this model is motivated by the equivalence of simple coagulation and annihilation. Considering the above model on a finite lattice with L sites and periodic boundary conditions, we shall show in section 3 that it is soluable through the finite-size empty interval method [12]. We obtain explicitly the long-time behaviour of the particle density and study the finite-size scaling of the leading relaxation time τ. We find that for all values of λ, the model remains in the universality class of pair annihilation and we discuss the physical reasons for this. While that does not provide any insight into the phase transition of the pair contact process, the fact that λ couples to an irrelevant operator allows us to test analytically the generalization [13] of Privman–Fisher universality of finite-size scaling amplitudes [14] in an exactly solvable non-equilibrium model. Section 4 summarizes our conclusions.

2. Motivation of the model

Although the present understanding of the phase transition in the PCPD is far from being complete, it is nearly possible to conjecture that the same type of transition occurs in a large variety of other models. More precisely, we expect such transitions to occur in models without parity conservation where: (a) solitary particles diffuse, (b) particle creation requires two particles and (c) particle removal requires at least two particles to meet at neighbouring sites. Examples of such reaction–diffusion processes include

$$2A \to 3A \qquad 2A \to A \tag{2}$$

$$2A \to 4A \qquad 2A \to A \tag{3}$$

$$2A \to 3A \qquad 3A \to \emptyset \tag{4}$$

$$2A \to 3A \qquad 3A \to A. \tag{5}$$

A particularly interesting candidate is the coagulation–production process (2). It is well known that coagulation $2A \to A$ and pair annihilation $2A \to \emptyset$ are equivalent and can be related by an exact similarity transformation (for reviews see [4, 5]). Assuming that this transformation does not entirely destroy the production process $2A \to 3A$ in the renormalization group sense, it is therefore natural to expect that the coagulation–production model exhibits the same type of phase transition as the PCPD.

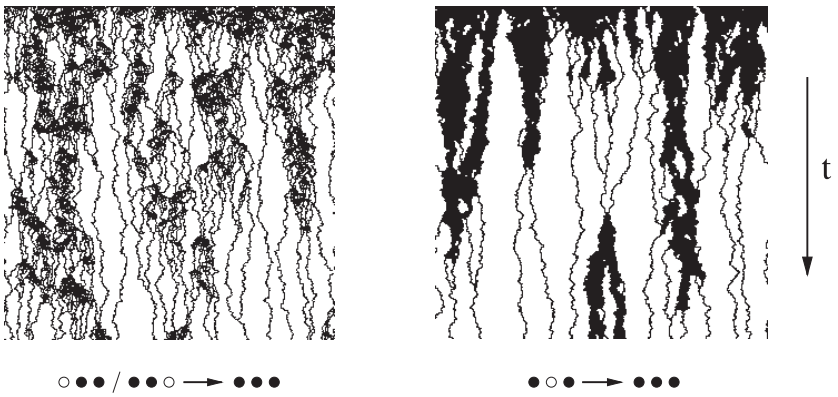

Figure 1. Typical temporal evolution of the coagulation–production process. Left, if particles are created to the left and to the right of a pair the system displays a phase transition similar to that observed in the PCPD. Right, if particles are created *between* two particles the model is always in the inactive phase. The figure shows a typical run for $\lambda = 100$.

It is important to note that the production process $2A \to 3A$ in one dimension can be implemented in two different ways. In the standard implementation particles are created to the left and to the right of a pair of particles:

$$\bullet\bullet\circ/\circ\bullet\bullet \to \bullet\bullet\bullet. \tag{6}$$

Together with the coagulation process this implementation of the model displays a non-equilibrium phase transition similar to the transition in the PCPD (see the left-hand panel of figure 1). In the other implementation of the production process, on which we will focus in this paper, a particle is created *between* two other particles:

$$\bullet\circ\bullet \to \bullet\bullet\bullet. \tag{7}$$

In this case the model displays a completely different behaviour. In particular, there is no phase transition. Rather the model is always in the inactive phase where the asymptotic behaviour is governed by the coagulation process. Even the visual appearance of clusters is clearly different in both cases, as demonstrated in figure 1. Obviously, the spatial arrangement of the production process is crucial on a one-dimensional chain. Similar hard-core effects can be observed in other one-dimensional models with three-site interactions [15].

Figure 2 illustrates why particle production between particles differs significantly from ordinary particle creation to the left and to the right. The figure sketches the temporal evolution of a pair of particles for a given realization of randomness. Without offspring production, the two particles diffuse until they meet and coagulate to a single particle. Adding the process (7), particles can only be created *between* the spacetime trajectories of these two particles. In other words, the pure coagulation process provides a 'skeleton'. The process (7) generates additional patches of high activity between two branches, while the skeleton itself remains unchanged. Moreover, there is no way for the particles to 'cross' the branches of the skeleton. Therefore, the asymptotic behaviour for $t \to \infty$ is governed by the pure coagulation process, i.e. we expect the density of particles to decay as $t^{-1/2}$.

As can be seen in the right-hand panel of figure 1, even for high values of λ most patches with high activity die out after a short time. New patches with finite lifetime can only be generated if two diffusing particles meet. As these events become rarer as time proceeds,

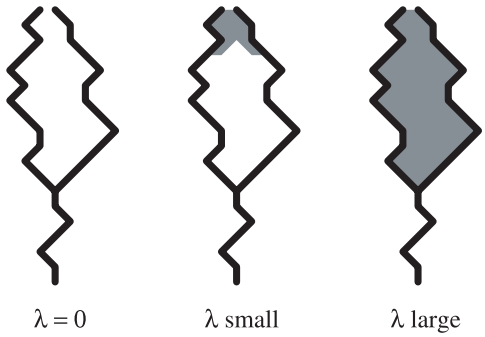

Figure 2. Schematic drawing of the temporal evolution of a pair of particles. For $\lambda = 0$ the two particles diffuse until they coagulate, forming a skeleton (bold lines). For $\lambda > 0$ particles are created between pairs of particles, forming a high-density region between the two branches. The skeleton itself remains unchanged.

it seems to be plausible (and will be proven below) that the model does not exhibit a phase transition.

Let us point out that the PCPD with production in the middle $A\emptyset A \to AAA$ and pair annihilation $AA \to \emptyset\emptyset$ does not have these special properties. Moreover, it is not exactly solvable and exhibits a phase transition similar to the standard PCPD.

It should be noted that the mechanism described above requires that the coagulation and diffusion rates are equal. In fact, by increasing the diffusion rate, the solvability is lost and a PCPD transition at a finite value of λ is recovered [16].

3. Exact solution

We consider the model (1) on a chain of L sites with periodic boundary conditions. The exact solution can be obtained through the generalization of the empty-interval method [11, 17] to finite lattices [12]. Since we are interested in working out spatially averaged values of the observables, we can assume translation invariance from the outset. Let $I_n(t)$ be the probability that n consecutive sites are empty at time t. Then the mean particle density is given by

$$\rho(t) = (1 - I_1(t))\, a^{-1} \tag{8}$$

where a is the lattice constant. The equations of motion for the $I_n(t)$ are

$$\begin{aligned} &I_0(t) = 1 \\ &\frac{\mathrm{d}I_1}{\mathrm{d}t}(t) = 2d\,[I_0(t) - 2I_1(t) + I_2(t)] - 2d\lambda\,[I_1(t) - 2I_2(t) + I_3(t)] \\ &\frac{\mathrm{d}I_n}{\mathrm{d}t}(t) = 2d\left[I_{n-1}(t) - 2I_n(t) + I_{n+1}(t)\right] \qquad 2 \leqslant n \leqslant L-1 \\ &I_L(t) = 0. \end{aligned} \tag{9}$$

Here the boundary condition $I_0(t) = 1$ allows one to take care of the coagulation process in the usual way, provided that the rates for coagulation and diffusion coincide [11, 12]. Obviously, the empty lattice

$$I_n(t) = 1 \qquad 0 \leqslant n \leqslant L \tag{10}$$

is a trivial stationary state which decouples from all other solutions. Therefore, we restrict our analysis to solutions with at least one particle. Since the last particle can never disappear, it

is impossible to have L consecutive empty sites for a chain with L sites, leading to the other boundary condition $I_L(t) = 0$. For $\lambda = 0$, equations (9) reduce to the known ones for simple coagulation with periodic boundary conditions [12].

In order to understand the λ-dependent term, consider the probability $P(n_1 n_2 n_3)$ of realizing the configuration $n_1 n_2 n_3$ at three neighbouring sites, where $n = \bullet$ indicates an occupied and $n = \circ$ an empty site. In particular, we have $P(\circ\circ\circ) = I_3$ and $P(\bullet\circ\circ) = P(\circ\circ\bullet) = I_2 - I_3$. In addition, summing over the states of the third site

$$P(\bullet\circ\bullet) + P(\bullet\circ\circ) = P(\bullet\circ) = I_1 - I_2 \tag{11}$$

which yields $P(\bullet\circ\bullet) = I_1 - 2I_2 + I_3$. The production of a particle between two others via the process $\bullet\circ\bullet \to \bullet\bullet\bullet$ only affects $I_1(t)$.

The equations of motion are solved through the ansatz

$$I_n(t) = \sum_{\omega} a_n(\omega)\, \mathrm{e}^{-2d\omega t} \tag{12}$$

which leads to the eigenvalue problem

$$\begin{bmatrix} 0 & 0 & 0 & \cdots & & & & 0 \\ 1 & -2-\lambda & 1+2\lambda & -\lambda & 0 & \cdots & & 0 \\ 0 & 1 & -2 & 1 & 0 & \cdots & & 0 \\ & 0 & 1 & -2 & 1 & 0 & \cdots & 0 \\ \vdots & & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ & & & 0 & 1 & -2 & 1 & 0 \\ & & & & 0 & 1 & -2 & 1 \\ 0 & \cdots & & & & 0 & 0 & 0 \end{bmatrix} \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \\ \vdots \\ \\ a_{L-1} \\ a_L \end{bmatrix} = -\omega \begin{bmatrix} a_0 \\ a_1 \\ a_2 \\ \\ \vdots \\ \\ a_{L-1} \\ a_L \end{bmatrix}$$

involving an $(L+1) \times (L+1)$ matrix $\hat{\Omega}$. The irreversible character of the stochastic process reflects itself in the fact that the matrix $\hat{\Omega}$ is not symmetric, while probability conservation implies that the sum of the elements in a row of $\hat{\Omega}$ vanishes. Because of these properties, the real part of the eigenvalues ω is non-negative.

It is easy to see that the solution

$$a_n(0) = 1 - n/L \qquad \omega = 0 \tag{13}$$

describes the steady state with a single diffusing particle. Therefore, the model has *two* steady states, one corresponding to the empty lattice and the other one being the translation-invariant superposition of all single-particle states with an average density $\rho_{\mathrm{av}} = 1/L$. For the relaxational modes with $\omega > 0$ the boundary condition $I_0(t) = 1$ implies that $a_0(\omega) = 0$. Similarly, the other boundary condition $I_L(t) = 0$ implies $a_L(\omega) = 0$. Therefore, we go over to an eigenvalue problem involving an $(L-1) \times (L-1)$ matrix if $\omega \neq 0$

$$\begin{bmatrix} -2-\lambda & 1+2\lambda & -\lambda & 0 & \cdots & & 0 \\ 1 & -2 & 1 & 0 & \cdots & & 0 \\ 0 & 1 & -2 & 1 & 0 & & \\ \vdots & \ddots & \ddots & \ddots & \ddots & \ddots & \vdots \\ & & 0 & 1 & -2 & 1 & 0 \\ & & & 0 & 1 & -2 & 1 \\ 0 & \cdots & & & 0 & 1 & -2 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \\ \vdots \\ \\ a_{L-2} \\ a_{L-1} \end{bmatrix} = -\omega \begin{bmatrix} a_1 \\ a_2 \\ \\ \vdots \\ \\ a_{L-2} \\ a_{L-1} \end{bmatrix}. \tag{14}$$

Equation (14) is solved through the ansatz

$$a_n(\omega) = A\mathrm{e}^{\mathrm{i}kn} + B\mathrm{e}^{-\mathrm{i}kn} \qquad \omega \neq 0 \tag{15}$$

which leads to the dispersion relation

$$\omega = \omega(k) = 2(1 - \cos k) \tag{16}$$

and the allowed values k are obtained by inserting the ansatz (15) into the first line of equation (14) and taking the boundary condition $a_L(\omega) = 0$ into account. This leads to a system of two equations,

$$A\left(\lambda\left(\mathrm{e}^{\mathrm{i}k} - 2\mathrm{e}^{2\mathrm{i}k} + \mathrm{e}^{3\mathrm{i}k}\right) + 1\right) + B\left(\lambda\left(\mathrm{e}^{-\mathrm{i}k} - 2\mathrm{e}^{-2\mathrm{i}k} + \mathrm{e}^{-3\mathrm{i}k}\right) + 1\right) = 0$$

$$A\mathrm{e}^{\mathrm{i}kL} + B\mathrm{e}^{-\mathrm{i}kL} = 0$$

which has a non-trivial solution if k is a solution of

$$\tan kL = \frac{4\lambda \sin(2k)\sin^2(k/2)}{4\lambda\cos(2k)\sin^2(k/2) - 1}. \tag{17}$$

We call the solutions of (17) k_m, where $m = 0, 1, \ldots, L-1$. Having found these, we can write the final result for the empty interval probabilities $I_n(t)$ in the form

$$I_n(t) = \left(1 - \frac{n}{L}\right) + \sum_{m=0}^{L-1} C_m \sin\left(k_m(n-L)\right)\, \mathrm{e}^{-2d\omega_m t} \tag{18}$$

where $\omega_m = \omega(k_m) = 2(1 - \cos k_m)$ and the C_m are real constants which must be determined from the initial conditions. For example, for an initially fully occupied lattice, one has $I_n(0) = \delta_{n,0}$. If we insert the values of k_m into (18) and use (8), we obtain the average particle density as a function of time.

Closed-form solutions of (17) exist for $\lambda = 0$ and $\lambda \to \infty$. We find $k_m = m\pi/L$ for $\lambda = 0$ and $k_m = m\pi/(L-2)$ for $\lambda \to \infty$, respectively. For general values of λ, we have

$$k_m = \frac{m\pi}{L} - \frac{2\pi^3\lambda m^3}{L^4} + \cdots \qquad m = 0, 1, \ldots, L-1. \tag{19}$$

Since the asymptotic scaling of the $k_m \sim L^{-1}$ is the same for λ finite and for $\lambda = \infty$, even the point $\lambda = \infty$ cannot be interpreted as being a transition point towards a different phase.

From equations (18) and (19) we see that the *exact* inverse leading relaxation time τ is given by

$$\tau^{-1} = 2d\omega(k_1) \simeq 2d\pi^2 L^{-2}\left(1 + \mathrm{O}(L^{-2})\right). \tag{20}$$

In other words, the finite-size scaling amplitude

$$A := \lim_{L\to\infty} L^2\tau_L^{-1} = 2d\pi^2 \tag{21}$$

is independent of the particle production rate λ, confirming the hand-waving arguments presented in section 2. We point out that the value of A is equal to the value of the finite-size scaling amplitude of the leading relaxation time in the entire inactive phase in the pair contact process [13]. An analogous universality holds for the entire spectrum of relaxation times $\tau_m^{-1} = 2d\omega(k_m)$.

Starting with a fully occupied lattice, the leading relaxation time is proportional to the time needed to reach the steady state (13) with density $\rho(\infty) = 1/L$, see equation (18). As an immediate consequence (see section 4), the asymptotic decay of the particle density has to be independent of λ as well. To verify this prediction, we performed Monte Carlo simulations. As shown in figure 3, the production process affects the curves only in a limited time window. Eventually all curves converge, demonstrating the universality of the long-time behaviour with respect to λ.

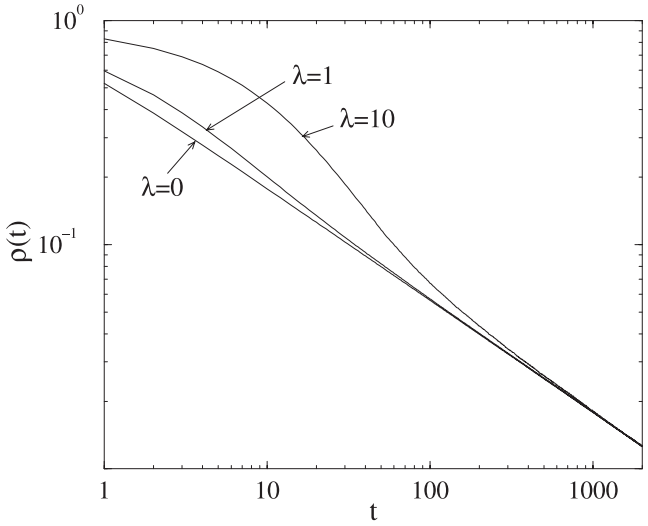

Figure 3. Particle density as a function of time for various values of λ. All curves converge to a single one, demonstrating the irrelevance of the parameter λ.

4. Conclusions

We have seen that in our solvable coagulation–production model (2), the finite-size scaling of the relaxations times τ_m and of the steady-state particle density ρ is independent of λ. We have also shown how to understand this in a physical way. In addition, this result can also be understood in the context of a recent extension [13] of the Privman–Fisher scaling forms [14] (see [18] for a review) to the steady states of non-equilibrium phase transitions below their upper critical dimension. In particular, for a one-dimensional reaction–diffusion system of finite length L, the relaxation times τ_m should scale as (using the same notation as in [13])

$$\tau_m^{-1} = C_0 L^{-z}\ R_m\left(0, C_2 h L^{1+z-\beta/\nu_\perp}\right)\Big|_{h=0} \tag{22}$$

and the steady-state particle density as

$$\rho = C_2 L^{-\beta/\nu_\perp} Y'\left(0, C_2 h L^{1+z-\beta/\nu_\perp}\right)\Big|_{h=0} \tag{23}$$

where β, $\nu_\perp$, z are the order parameter, correlation length and dynamical exponents, R_m and Y' are universal scaling functions, h parametrizes an external source of particles, and C_0, C_2 are non-universal constants [13]. For the diffusion-coagulation model at hand (when $\lambda = 0$), it is known that $z = 2$ and that the time scale can be fixed by choosing $C_0 = d$ [19]. The λ independence of all the τ_m is therefore consistent with the expected universality of the R_m. Furthermore, the steady-state density is given by $\rho(\infty) = 1/L$, which implies that even the generically non-universal constant C_2 does not depend on λ and that $\beta/\nu_\perp = 1$. A simple scaling argument then shows that, in the limit $L \to \infty$, also the time-dependent density

$$\rho(t) = \sum_m \rho^{(m)} \mathrm{e}^{-t/\tau_m} \underset{t\to\infty}{\simeq} \rho_0 (dt)^{-\delta} \tag{24}$$

where $\delta = \beta/\nu_\parallel = \beta/(\nu_\perp z) = \frac{1}{2}$ and the constant ρ_0 is λ-independent. That is indeed what we observe from figure 3.

Recall that in the pair contact process similar arguments demonstrate that C_0 is not renormalized through the effects of the interactions (see [10, 13] and references therein).

However, the universality of the amplitude A in the pair contact process could only be established numerically [13]. On the other hand, the universality of the relaxation times in the annihilation–coagulation model $2A \to \emptyset$, A is trivial because of a similarity transformation which reduces the model to simple diffusion–annihilation. We have therefore obtained the first non-trivial analytic confirmation of the universality of the finite-size scaling amplitudes of the correlation length.

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