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TOPICAL REVIEW

The non-equilibrium phase transition of the pair-contact process with diffusion

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Abstract

The pair-contact process $2A \to 3A, 2A \to \emptyset$ with diffusion of individual particles is a simple branching-annihilation process which exhibits a phase transition from an active to an absorbing phase with an unusual type of critical behaviour which had not been seen before. Although the model has attracted considerable interest during the past few years, it is not yet clear how its critical behaviour can be characterized and to what extent the diffusive pair-contact process represents an independent universality class. Recent research is reviewed and some standing open questions are outlined.

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(Some figures in this article are in colour only in the electronic version)

Contents

1. Introduction and history

The *pair-contact process with diffusion* (PCPD) is a classical reaction–diffusion process describing stochastically interacting particles of a single species which react spontaneously whenever two of them come into contact. In its simplest version, the PCPD involves two competing reactions, namely

$$\begin{aligned} &\text{fission:} && 2A \to 3A \\ &\text{annihilation:} && 2A \to \emptyset. \end{aligned}$$

In addition individual particles are allowed to diffuse. Moreover, depending on the specific variant under consideration, an exclusion principle or a similar mechanism may impose a restriction such that the particle density cannot diverge.

During the past four years the PCPD has attracted a lot of attention. The interest in this model is first motivated by the fact that the PCPD exhibits a non-equilibrium phase transition caused by the competing character of fission and annihilation. In the so-called *active phase*, the fission process dominates and the system evolves towards a fluctuating steady state characterized by a certain stationary particle density $\rho_s > 0$. In contrast, in the *absorbing phase* the annihilation process dominates and the density of particles decreases continuously until the system reaches a so-called *absorbing state* (for example the empty lattice) from where it cannot escape. Since absorbing states can only be reached but not be left, the process is generically out of equilibrium. The active and the absorbing phases are separated by a continuous phase transition with a non-trivial critical behaviour.

As we shall see, despite the simplicity of the PCPD, the properties of its phase transition(s) are quite involved and rather surprisingly, at the time of writing no clear consensus on its critical behaviour has been achieved. This makes the PCPD an ideal laboratory to explore the most advanced techniques from either field theory or simulation. On the other hand, due to the intensive recent research, the PCPD offers the possibility to introduce all these techniques as

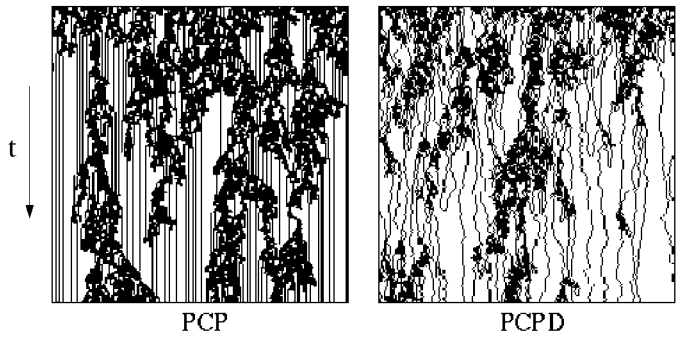

Figure 1. One-dimensional pair-contact process starting with a fully occupied lattice at criticality. Left: in the pair-contact process without diffusion solitary particles cannot diffuse, leading to frozen patterns of separated vertical lines. Right: in the PCPD, where individual particles are allowed to diffuse, offspring production can be restarted after long times when two diffusing particles meet, leading to a very different visual appearance of the process.

applied to the same model and thereby to critically appreciate their respective strengths and weaknesses.

The classification of non-equilibrium phase transitions from an active phase to an inactive phase with absorbing states is a challenging problem of contemporary statistical physics [1, 2]. Generally it is believed that such transitions belong to a finite number of universality classes with steady-state properties being characterized by a quartet $(\beta, \beta', \nu_\perp, \nu_\parallel)$ of critical exponents and certain universal scaling functions[3]. So far only a few universality classes are firmly established, the most important ones being directed percolation (DP) [4–7], the parity-conserving (PC) class of branching–annihilating random walks [8, 9], Z_2-symmetric transitions in the voter model [10, 11], the general epidemic process [12, 13] and absorbing phase transitions coupled to a conserved field [14–16]. The current interest in the PCPD is motivated by the perspective that it may represent yet another independent universality class of non-equilibrium phase transitions which had not been studied before. The asymptotic critical behaviour, however, seems to be masked by strong corrections to scaling so that it is not yet entirely clear how the transition in the PCPD should be characterized and classified. The purpose of this review is to summarize the present state of knowledge and to point out open questions.

The first investigation of this class of models considered the *non-diffusive* pair-contact process (PCP) [17, 18] with at most one particle per site. In this case individual particles are completely immobile so that activity can only spread in space by offspring production at empty nearest-neighbour sites. On a one-dimensional lattice, the PCP may be implemented by fission $\emptyset AA/AA\emptyset \to AAA$ and annihilation $AA \to \emptyset\emptyset$. A typical spacetime plot of a critical PCP is shown in the left panel of figure 1. Since solitary particles do not diffuse, any configuration of spatially separated particles is frozen. Therefore, on an infinite lattice the model has infinitely many absorbing states. More specifically, on a one-dimensional lattice with L sites and either periodic or free boundary conditions the model has 2^L states of which

$$N_{\mathrm{stat}}(L) \simeq N_0 g_+^L \qquad N_0 = \begin{cases} 1 & \text{periodic b.c.} \\ 1.17\ldots & \text{free b.c.} \end{cases} \tag{1}$$

[3] Only if a certain duality symmetry holds, will the *a priori* different [3] steady-state exponent β of the order parameter and β' of the survival probability agree.

are absorbing [19], where $g_+ = (1 + \sqrt{5})/2 \simeq 1.618$ is the golden mean (see appendix A). Numerical simulations in both one dimension (1D) [17, 20] and in 2D [21] have shown that the steady-state transition in the non-diffusive PCP belongs to DP. Although a rigorous proof is not yet available, recent numerical high-precision studies of universal scaling functions in various dimensions support this claim [22]. The result is remarkable since the PCP does not obey the assumptions of the so-called DP conjecture [23, 24], which states that under certain generic conditions any non-equilibrium phase transition into a *single* absorbing state should belong to DP. Spreading from a single seed, however, may show non-universal properties depending on the density and correlations of the surrounding particles [3, 25, 26]. To explain the observed critical behaviour in the PCP several field-theoretic approaches have been suggested [27, 28].

In the PCPD, where in addition to the binary PCP reactions individual particles are also allowed to diffuse, the situation is fundamentally different. Unlike the PCP without particle diffusion, the PCPD has only two absorbing states, $N_{\text{stat}} = 2$. These are the empty lattice and a homogeneous state with a single diffusing particle. Therefore, and in contrast to spreading processes such as DP, where diffusion does not alter the critical behaviour [29], introducing diffusion in the pair-contact process should be regarded as a *singular perturbation* which changes the structure of the absorbing phase. In fact, even the visual appearance changes drastically, as shown in the right panel of figure 1.

The pair-contact process *with* diffusion was already suggested in 1982 by Grassberger [30], who expected a critical behaviour 'distinctly different' from DP.[4] Fifteen years later the problem was rediscovered, under the name of 'annihilation–fission process', by Howard and Täuber [31], who proposed a bosonic field theory for the one-dimensional PCPD. Because of the bosonic nature of their model, the particle density is unrestricted and thus diverges in the active phase. Furthermore, since their field theory turned out to be non-renormalizable, no quantitative statements on the phase transition between the active and the inactive phases could be made. This triggered one of us (MH), together with J F F Mendes, to attempt a non-perturbative study of the 1D PCPD, formulated on a discrete lattice and with at most one particle per site. Starting from the master equation, rewritten as a matrix problem of an associated quantum Hamiltonian H, the longest relaxation time was obtained from the real part of the lowest eigenvalue of H and steady-state observables were found by forming matrix elements with the right ground state of H. The results were compared with those of a Monte Carlo simulation. While the estimates of the location of the transition were in reasonable agreement between the two methods, it turned out that for the longest chains ($L = 21$ sites) accessible, finite-size estimates for the critical exponents could not yet be reliably extrapolated towards the $L \to \infty$ limit [32]. As we shall see, even today the difficulties encountered in that first study are not yet completely overcome.

At that time, the likely solution to these difficulties appeared to be the investigation of larger lattices by adapting White's density-matrix renormalization group (DMRG) [33, 34] to non-equilibrium systems with non-Hermitian matrices H (for a recent review, see [35]). Kaulke and Peschel [36] used the DMRG to study biased diffusion, which leads to a q-symmetric Hamiltonian H which is similar to a symmetric matrix. The feasibility of the Hamiltonian approach using the DMRG for truly non-equilibrium systems without detailed balance was demonstrated with E Carlon and U Schollwöck, on a model in the DP class [37]. Equipped with this technique, we then returned to the investigation of a lattice model of the PCPD with an exclusion principle by density-matrix renormalization group methods [19]. This paper was

[4] He rather considered the process $2A \to 3A$, $3A \to A$, which is believed to exhibit the same type of phase transition as the PCPD.

followed by a long series of numerical and analytical studies [38–55] and released the still ongoing debate concerning the asymptotic critical behaviour of the PCPD at the transition. Until now a surprising variety of possible scenarios has been proposed, the main viewpoints being that the active-absorbing phase transition in the PCPD

- should represent a novel universality class with a unique set of critical exponents [38, 44, 48, 51],
- may represent *two different* universality classes depending on the diffusion rate [39, 52] and/or the number of space dimensions [53],
- can be interpreted as a cyclically coupled DP and annihilation process [40],
- could be regarded as a marginally perturbed DP process with continuously varying critical exponents [47],
- may have exponents depending continuously on the diffusion constant D [49, 56],
- may cross over to DP after a very long time [50, 54], and
- is perhaps related to the problem of non-equilibrium wetting in 1+1 dimensions [55].

Given these widely different and partially contradicting conclusions, it is clear that considerably more work will be needed to understand the behaviour of this so simple-looking model. In this review, we shall give an introduction to the PCPD, review the research done on it, and discuss these suggested scenarios in detail. We thereby hope to stimulate further research in order to finally understand the properties of this system.

2. Phenomenological scaling properties

It is well known that systems in the directed percolation universality class are usually characterized by the so-called DP conjecture [24, 30] which specifies certain conditions for DP critical behaviour. Similarly, experience suggests that the critical phenomenon observed in the PCPD is not restricted to a particular model, rather it is expected to appear in a large variety of models which are thought to be characterized by the following phenomenological features:

(i) Particles of a single species diffuse in a d-dimensional space.
(ii) The phase transition is driven by two competing *binary* reactions for particle creation and removal, i.e., two particles have to come into contact in order to be eliminated or to produce offspring.
(iii) There is a finite number of absorbing states of which at least one is reachable.
(iv) There are no unusual features such as quenched randomness or unconventional symmetries.

This means that the characteristic critical behaviour of the PCPD is also expected to exist in many other models, including e.g. generic reaction–diffusion processes of the form

$$\begin{array}{lll} \text{(a)} & 2A \to 3A & 2A \to \emptyset \\ \text{(b)} & 2A \to 3A & 2A \to A \\ \text{(c)} & 2A \to 4A & 2A \to A \\ \text{(d)} & 2A \to 3A & 3A \to \emptyset. \end{array}$$

All these models differ significantly from both DP and PC processes in two respects: firstly, processes in the DP class are unary processes, i.e. isolated particles can decay or trigger branching. The paradigmatic example is the contact process [4, 6] with the reactions $A \to 2A$, $A \to \emptyset$, exclusion on the lattice and possibly diffusion of single particles. In contrast, in the PCPD single diffusing particles cannot react unless they collide in pairs.

Secondly, in a typical system in the PC class such as $2A \to \emptyset$, $A \to 3A$, the parity of the total number of particles is conserved and there is at least one unary reaction while this is not so in the PCPD. In particular, all PCPD-like models have an inactive (or absorbing) phase, where either the annihilation process $2A \to \emptyset$ or else the coagulation process $2A \to A$ dominates. Therefore, in the inactive phase of the PCPD and related models the density $\rho(t)$ of particles decays algebraically as [57]

$$\rho(t) \sim \begin{cases} t^{-d/2} & \text{for} \quad d < 2 \\ t^{-1} \ln t & \text{for} \quad d = 2 \\ t^{-1} & \text{for} \quad d > 2. \end{cases} \tag{2}$$

This behaviour is quite distinct from the time dependence of the particle density for systems in the DP universality class, where the decay of $\rho(t)$ is exponential in time.

Studying the PCPD one has to distinguish between two fundamentally different types of models, namely, the *unrestricted* PCPD, where the number of particles per site is not constrained, and the *restricted* PCPD, where the particle number on any given site is effectively bounded[5]. This restriction can be implemented either as a hard constraint by an exclusion principle or as a soft constraint in the form of a higher order process for particle removal (such as $3A \to \emptyset$), which prevents the particle density from diverging. The difference between the two types is most pronounced in the active phase, where in the unrestricted case the particle density diverges while it saturates at a finite value in restricted variants. Since phase transitions with a well-defined particle density in the active phase are perceived as more natural, most studies consider the restricted PCPD.

In all recent studies of the restricted PCPD, it is assumed that the critical behaviour at the transition can be described in terms of the same scaling laws as found in other absorbing phase transitions, although possibly with a different set of critical exponents and scaling functions. For example, in a Monte Carlo simulation one usually measures the temporal evolution of the particle density starting from a homogeneous initial state (usually a fully occupied lattice). In this case, the particle density ρ is expected to obey the asymptotic scaling form

$$\rho(t, L, \epsilon) = t^{-\delta} f_\rho(t^{1/z}/L, \epsilon t^{1/\nu_\parallel}) \tag{3}$$

where L is the lateral system size, $\epsilon = p - p_c$ measures the distance from criticality and f_ρ is a scaling function with appropriate asymptotic behaviour. Here and in what follows a scaling limit $t \to \infty$, $L \to \infty$ and $\epsilon \to 0$ is implied. The exponent $\delta = \beta/\nu_\parallel$ describes the power-law decay of the density at criticality while $z = \nu_\parallel/\nu_\perp$ is the dynamical critical exponent. Apart from metric factors the scaling function and the critical exponents are determined by the universality class of the phase transition and the boundary conditions.

Alternatively one can start the process with an active seed, i.e. in the present case with a *pair* of particles at the origin. As usual in this type of simulation [23], one studies the survival probability P_s which scales as

$$P_s(t, L, \epsilon) = t^{-\delta'} f_{P_s}(Lt^{1/z}, \epsilon t^{1/\nu_\parallel}) \tag{4}$$

where $\delta' = \beta'/\nu_\parallel$. Similarly, the average number of particles averaged over all runs scales as

$$N(t, L, \epsilon) = t^{\eta} f_N(Lt^{1/z}, \epsilon t^{1/\nu_\parallel}) \tag{5}$$

and the mean-square spreading from the origin averaged over surviving runs is

$$R^2(t, L, \epsilon) = t^{2/z} f_{R^2}(Lt^{1/z}, \epsilon t^{1/\nu_\parallel}). \tag{6}$$

[5] These two variants are often referred to as *bosonic* and *fermionic* models. This nomenclature, however, is misleading since, e.g., models with a soft constraint are restricted but bosonic.

Here $\delta' = \beta'/\nu_\parallel$ is an independent exponent, although in the DP and the PC class the two exponents β and β' are equal[6]. The so-called initial-slip exponent η is related to the other exponents by the generalized hyperscaling relation [3, 58]

$$\eta = \frac{d}{z} - \delta - \delta'. \tag{7}$$

The definition of the survival probability in the PCPD is a little subtle. Clearly, the presence of a single particle as a criterion for survival is not sufficient since then $P_s(t)$ would tend to a constant. A natural definition, however, appears to be to consider a run as surviving as long as the system has not yet reached one of the two absorbing states, i.e. there have to be at least two particles in the system. A stronger condition is to require the presence of at least one *pair* in the system as advocated in [47, 49], see sections 4.3 and 5.2.

According to standard scaling theory the quartet of exponents $(\beta, \beta', \nu_\perp, \nu_\parallel)$ characterizes the universality class of the transition. For DP and PC transitions, where $\beta = \beta'$, the remaining three independent exponents in one spatial dimension have the values

$$\{\beta, \nu_\perp, \nu_\parallel\} \approx \begin{cases} \{0.276\,486(8) & 1.096\,854(4) & 1.733\,847(6)\} & \text{for DP [59]} \\ \{0.922(5) & 1.85(3) & 3.22(6)\} & \text{for PC [8].} \end{cases} \tag{8}$$

The central open question about the PCPD is whether it belongs to one of the known classes or whether it represents a novel universality class with an independent set of critical exponents.

3. Mean-field approaches

Mean-field theories are a convenient tool in order to obtain a first orientation about the possible critical behaviour of a statistical system. To be specific, we shall formulate the PCPD as a lattice model, where each site may either be empty or be occupied by a single particle. The model evolves by random-sequential dynamics according to the rules [19]

$$\begin{array}{lll} AA\emptyset, \emptyset AA \to AAA & \text{with rate} & (1-p)(1-D)/2 \\ AA \to \emptyset\emptyset & \text{with rate} & p(1-D) \\ A\emptyset \leftrightarrow \emptyset A & \text{with rate} & D \end{array} \tag{9}$$

where $0 \leqslant p \leqslant 1$ and $0 \leqslant D \leqslant 1$ are the control parameters. We are therefore treating a restricted version of the PCPD and shall comment on the unrestricted version as discussed in [31] as necessary.

All mean-field treatments must at some stage neglect some of the correlations present in a model. A systematic way of constructing a sequence of improving mean-field theories was devised by ben Avraham and Köhler [60] and extending earlier work [61, 62]. In their so-called (n, m)-approximation, they work with clusters of n sites. The approximation is made by factorizing the probabilities for configurations which occupy more than n sites in terms of n-site probabilities but in such a way that there is an overlap of m sites between adjacent clusters. More specifically, if $\mathfrak{A}$, $\mathfrak{B}$, $\mathfrak{C}$ are such overlapping clusters, and if $P(\mathfrak{A}|\mathfrak{B}) = P(\mathfrak{A})/P(\mathfrak{B})$ is the conditional probability to find $\mathfrak{A}$ for given $\mathfrak{B}$, the approximation $P(\mathfrak{ABC}) \approx P(\mathfrak{AB})P(\mathfrak{BC}|\mathfrak{B})$ is used. In this way, correlations up to n sites are taken into account. It is assumed throughout that the cluster probabilities $P(\mathfrak{A})$ are spatially translation invariant.

[6] In DP the equality is caused by a time-reversal symmetry [23] while for the PC class it is so far only observed numerically.

Table 1. Rates in the site approximation of the PCPD.

Reaction	$\Delta N_\bullet$	Rate
$\bullet\bullet\circ \to \bullet\bullet\bullet$	+1	$\frac{1}{2}(1-p)(1-D)\rho^2(1-\rho)$
$\circ\bullet\bullet \to \bullet\bullet\bullet$	+1	$\frac{1}{2}(1-p)(1-D)\rho^2(1-\rho)$
$\bullet\bullet \to \circ\circ$	−2	$p(1-D)\rho^2$

For example, consider a five-site cluster in the state $ABCDE$. In the (3, 1)- and (3, 2)-approximations, respectively, the probability $P(ABCDE)$ of this cluster is expressed as

$$\begin{aligned} P^{(3,1)}(ABCDE) &\approx P(ABC)P(CDE|C) = \frac{P(ABC)P(CDE)}{P(C)} \\ P^{(3,2)}(ABCDE) &\approx P(ABC)P(BCDE|BC) \approx P(ABC)\frac{P(BCD)P(CDE|CD)}{P(BC)} \\ &= \frac{P(ABC)P(BCD)P(CDE)}{P(BC)P(CD)}. \end{aligned} \tag{10}$$

Therefore, in the context of the $(3, m)$-approximation, the basic variables have to be constructed from the independent three-site probabilities.

It has been argued that the $(n, n-1)$-approximations are qualitatively the most reliable ones [60] and this conclusion has been generally accepted. In particular, the simplest of these schemes is the (1, 0)-approximation, which is also referred to as the *site approximation* ($N = 1$) or as *simple mean-field*. Similarly, the (2, 1)-approximation is called the *pair approximation* ($N = 2$) and the (3, 2)- and (4, 3)-approximations are referred to as *triplet* ($N = 3$) and *quartet* approximations ($N = 4$), respectively.

In what follows we shall denote an occupied site by $\bullet$ and an empty site by $\circ$. A three-site cluster $AA\emptyset$ will then be denoted as $\bullet\bullet\circ$ and has the probability $P(AA\emptyset) = P_{\bullet\bullet\circ}$. For notational simplicity, we shall only consider the one-dimensional case in this section.

3.1. Simple mean-field approximation for the particle density

The simplest mean-field approach considers only the single-site probabilities. If we let $\rho(t) = P_\bullet(t)$ and also assume that it is space independent, the rate equation for $\rho(t)$ is easily derived. In table 1 we collect those reactions from (9) which change the mean particle density, together with the change $\Delta N_\bullet$ in the number of occupied sites $N_\bullet$ by this reaction.

Adding the contributions to $\dot\rho$ and rescaling time $t \to t(1-D)^{-1}$ one easily finds

$$\frac{\mathrm{d}\rho(t)}{\mathrm{d}t} = (1-p)\rho(t)^2(1-\rho(t)) - 2p\rho(t)^2 \tag{11}$$

which implies the following large-time behaviour of the mean density [19]:

$$\rho(t) \simeq \begin{cases} \frac{1-3p}{1-p} + \mathfrak{a}\exp(-t/\tau) & \text{if} \quad p < 1/3 \\ \sqrt{3/4}\cdot t^{-1/2} & \text{if} \quad p = 1/3 \\ (3p-1)^{-1}\cdot t^{-1} & \text{if} \quad p > 1/3 \end{cases} \tag{12}$$

where $\tau = (1-p)/(1-3p)^2$ and $\mathfrak{a}$ is a constant which depends on the initial conditions. We see that the site approximation reproduces the intuitive expectation of a phase transition between an active phase, where $\rho(t) \to \rho_\infty > 0$ for large times, and an absorbing phase, where $\rho(t)$ vanishes in the $t \to \infty$ limit. We also see that throughout the absorbing phase, the

approach towards the steady state of vanishing particle density is algebraic, although mean-field theory is not capable of reproducing the correct decay $\rho(t) \sim t^{-1/2}$, which one would obtain in one dimension if the fluctuation effects neglected here were taken into account.

From the point of view of a continuum theory it is natural to introduce a coarse-grained particle density $\rho(\boldsymbol{x}, t)$ and to postulate a suitable rate equation. A reasonable rate equation should be given by[7]

$$\frac{\partial}{\partial t}\rho(\boldsymbol{x}, t) = b\rho^2(\boldsymbol{x}, t) - c\rho^3(\boldsymbol{x}, t) + D\nabla^2\rho(\boldsymbol{x}, t) \tag{13}$$

and we expect for a restricted model with the rates (9) that $b = 1 - 3p$ and $c = 1 - p$, see equation (11). On the other hand, for unrestricted models without any constraint on the occupation of a space point $\boldsymbol{x}$, one would have $c = 0$ [31] so that the mean particle density $\rho(\boldsymbol{x}, t)$ diverges in the active phase $b > 0$. Hence the cubic term with $c > 0$ can be interpreted to mean that a newly created particle requires some empty space to be put into. In later sections, we shall discuss variants of the PCPD with a soft constraint, generating effectively such a cubic term with $c > 0$. As we shall see this will lead to important consequences.

At first sight, one might believe that equation (11) contains with respect to (13) the further approximation that the space dependence of $\rho(\boldsymbol{x}, t) \mapsto \rho(t)$ is neglected. Still, both equations (11) and (13) lead to the same long-time behaviour of the density. To see this, choose some spatial domain Ω and consider the spatially averaged density

$$\overline{\rho}(t) = \frac{1}{|\Omega|}\int_{\Omega} \mathrm{d}\boldsymbol{x}\, \rho(\boldsymbol{x}, t) \tag{14}$$

where $|\Omega|$ denotes the volume of Ω and $\rho(\boldsymbol{x}, t)$ solves (13). Now, if $c > 0$ and $\overline{\rho}(0) > 0$ and with the boundary condition $\nabla\rho|_{\partial\Omega} = 0$, it can be shown rigorously [64] that there exists a constant b' so that $b'/b > 0$, and a positive constant c', which are both independent of $|\Omega|$ and of $\overline{\rho}(0)$ such that the inequalities

$$\begin{aligned} b\overline{\rho}(t)^2 - c'\overline{\rho}(t)^3 \leqslant \frac{\mathrm{d}\overline{\rho}(t)}{\mathrm{d}t} \leqslant b'\overline{\rho}(t)^2 - c\overline{\rho}(t)^3 \qquad & \text{if} \quad b \geqslant 0 \\ -|b'|\overline{\rho}(t)^2 - c'\overline{\rho}(t)^3 \leqslant \frac{\mathrm{d}\overline{\rho}(t)}{\mathrm{d}t} \leqslant -|b|\overline{\rho}(t)^2 - c\overline{\rho}(t)^3 \qquad & \text{if} \quad b \leqslant 0 \end{aligned} \tag{15}$$

hold true. In addition, one has in the quadratic mean the convergence $\rho(\boldsymbol{x}, t) \to \overline{\rho}(t)$ for large times [64]. Therefore, the time dependence of the averaged density $\overline{\rho}(t)$ can be bounded both from above and from below by a solution of the form (12). Hence we can conclude that the space dependence of $\rho(\boldsymbol{x}, t)$ is not essential for the long-time behaviour of the mean density, rather the crucial approximation in mean-field theories is made in neglecting correlations between the states of different sites.

Finally, a standard dimensional analysis of equation (13) (see [2]) yields the mean-field critical exponents

$$\beta^{MF} = 1 \qquad {\nu_\perp}^{MF} = 1 \qquad {\nu_\parallel}^{MF} = 2. \tag{16}$$

As will be discussed in section 6, these exponents are expected to be valid in $d \geqslant 2$ dimensions. In fact, high-precision simulations in 2D performed by Ódor *et al* [45] confirm this prediction within numerical errors and up to logarithmic factors for various values of the diffusion rate. In one spatial dimension, however, fluctuation effects are expected to be relevant, leading to different values. A better description of these fluctuation effects requires the consideration of larger clusters, going beyond the site approximation. These approaches will be discussed in the following subsections.

[7] We warn the reader that simple rate equations may not be at all adequate for the case of an unrestricted density, see [63] and section 6.

Table 2. Rates in the pair approximation of the 1D PCPD. In the last column, a symmetry factor coming from parity symmetry is included.

Reaction	$\Delta N_\bullet$	$\Delta N_{\bullet\bullet}$	Rate	
$\bullet\bullet\circ\circ \to \bullet\circ\bullet\bullet$	0	-1	$Duvw/\rho(1-\rho)$	$\times 2$
$\circ\bullet\circ\bullet \to \circ\circ\bullet\bullet$	0	$+1$	$Dv^3/\rho(1-\rho)$	$\times 2$
$\bullet\bullet\bullet\bullet \to \bullet\circ\circ\bullet$	-2	-3	$p(1-D)u^3/\rho^2$	
$\bullet\bullet\bullet\circ \to \bullet\circ\circ\circ$	-2	-2	$p(1-D)u^2v/\rho^2$	$\times 2$
$\circ\bullet\bullet\circ \to \circ\circ\circ\circ$	-2	-1	$p(1-D)uv^2/\rho^2$	
$\bullet\bullet\circ\bullet \to \bullet\bullet\bullet\bullet$	$+1$	$+2$	$\frac{1}{2}(1-p)(1-D)uv^2/\rho(1-\rho)$	$\times 2$
$\bullet\bullet\circ\circ \to \bullet\bullet\bullet\circ$	$+1$	$+1$	$\frac{1}{2}(1-p)(1-D)uvw/\rho(1-\rho)$	$\times 2$

3.2. The pair approximation: two transitions?

Treating the 1D PCPD in the pair approximation, we assume again that the probabilities $P(AB)$ are translation independent and furthermore that the system is left/right-invariant, namely $P_{\bullet\circ}(t) = P_{\circ\bullet}(t)$. Then, because of $P_\bullet = P_{\bullet\circ} + P_{\bullet\bullet}$ and $P_{\bullet\bullet} + 2P_{\bullet\circ} + P_{\circ\circ} = 1$, there are two independent variables which may be chosen as the particle density: $\rho(t) = P_\bullet(t)$ and the pair density $u(t) = P_{\bullet\bullet}(t)$.

We now illustrate the standard methods [1, 60] how to find the equations of motions for $\rho(t)$ and $u(t)$ in the pair approximation. Introduce the shorthand $v = P_{\bullet\circ} = \rho - u$ and $w = P_{\circ\circ} = 1 - 2\rho + u$. The reactions changing the number $N_\bullet$ of occupied sites of the number $N_{\bullet\bullet}$ of occupied pairs are listed with their rates in table 2, grouped into the separate contributions of the three reactions. In the last group, we only need to take into account those reactions $2A \to 3A$ which modify the particle configuration on a given site. Adding the contributions to $\dot\rho$ and $\dot u$, their equations of motion are easily derived [19]:

$$\dot\rho(t) = -2(1-D)pu(t) + (1-D)(1-p)(\rho(t) - u(t))\frac{u(t)}{\rho(t)} \tag{17}$$

$$\begin{aligned}\dot u(t) = {} & -(1-D)pu(t)\frac{2u(t)+\rho(t)}{\rho(t)} - 2D\frac{(\rho(t)-u(t))(u(t)-\rho(t)^2)}{\rho(t)(1-\rho(t))} \\ & + (1-D)(1-p)\frac{(\rho(t)-u(t))(1-u(t))u(t)}{\rho(t)(1-\rho(t))}.\end{aligned} \tag{18}$$

The pair approximation is the lowest order cluster approximation which allows the effects of diffusion to be treated explicitly. In particular, in the $D \to 1$ limit, the site approximation equation (11) is recovered for $\rho(t)$, while the pair density $u(t) = \rho(t)^2$.

The critical line is again at $p_c(D) = \frac{1}{3}$ for $D \geqslant \frac{1}{7}$, but if $0 \leqslant D < \frac{1}{7}$, one has $p_c(D) = \frac{1}{5}(1+3D)/(1-D)$. In addition, the scaling of both $\rho(t)$ and of $u(t)$—and similarly of their steady-state solutions ρ_∞ and u_∞—does depend on whether $D > \frac{1}{7}$ where $u \sim \rho^2$ or whether $D < \frac{1}{7}$ where $u \sim \rho$. The steady-state particle density $\rho_\infty \sim p_c(D) - p$ for all D, and if $D \neq \frac{1}{7}$ one has $u(t) \sim t^{-1}$ along the critical line. These results might suggest the existence of two distinct universality classes along the critical line, but since the pair approximation is the simplest cluster mean-field theory which permits study of the effect of particle diffusion at all, this conjecture certainly needs further verification.

In figure 2 the phase diagram of the 1D PCPD is shown. The pair approximation ($N = 2$) certainly is an improvement as compared to simple mean field ($N = 1$) but is still quite

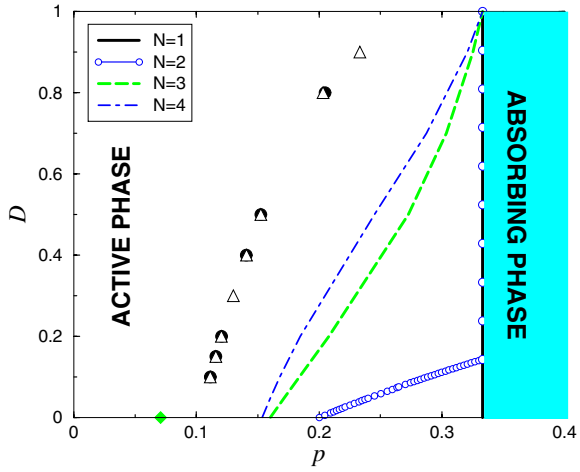

Figure 2. Phase diagram of the one-dimensional restricted PCPD with the rates as defined in equation (9), after [52]. The figure shows the boundary between the active and the absorbing phases according to cluster mean-field theory, ranging from site ($N = 1$) to quartet approximation ($N = 4$). The filled dots give values of $p_c(D)$ as found from the DMRG [19] and the open triangles those found in Monte Carlo simulations [65]. The grey diamond gives the critical point $p_c(0)$ of the PCP [21].

far from the exact location of $p_c(D)$ as obtained from DMRG calculations or Monte Carlo simulations which will be described in section 4.

3.3. Higher cluster approximations

In the pair approximation of the PCPD, the particle and pair densities in the steady state are related by $u_\infty = \rho_\infty(1 - 3p)/(1 - p)$. This means that the particle and pair densities have to vanish simultaneously which is certainly not true for the simple PCP without diffusion ($D = 0$), see section 1. This failure of the pair approximation can be overcome within the triplet approximation ($N = 3$). Consider first the PCP where $D = 0$ [22, 66]. Again assuming left/right symmetry, the independent variables may be chosen as $P_{\bullet\bullet\bullet}$, $P_{\bullet\bullet\circ}$, $P_{\bullet\circ\circ}$ and $P_{\bullet\circ\bullet}$. Now the critical point occurs at $p_c(0) \simeq 0.128$, where the steady-state pair density $u_\infty \sim p_c(0) - p$ vanishes linearly, but the critical particle density $\rho_{\infty,c} \simeq 0.23$ remains finite. These results have been extended up to the sextet approximation ($N = 6$) [67] and further to $N = 12$ [68] and remain qualitatively valid.

It is then natural to extend this study to the whole phase diagram. This was done in [52], including the quartet approximation ($N = 4$). As can be seen in figure 2 the kink in $p_c(D)$ observed in the pair approximation is absent for larger clusters. In addition, along the critical line, the steady-state particle density $\rho_\infty \sim p_c(D) - p$ for all values of $D > 0$, whereas $u_\infty \sim (p_c(D) - p)^2$ and this holds for both $N = 3$ and $N = 4$. This result strongly suggests that there is only one universality class along the critical line [52]. This finding is in agreement with simulational results, see section 4. A similar result had already been obtained before in the 2D process $2A \to \emptyset$, $2A \to 4A$ with single-particle diffusion [45].

To summarize, the apparent presence of two universality classes for $D > 0$ should be an artefact of the pair approximation—at least in one dimension—and it has already been observed earlier that in some cases, cluster mean-field theories may indeed yield qualitatively incorrect phase diagrams [60]. Generically, in the PCPD some reactions involve three

neighbouring sites, and furthermore the explicit consideration of at least three neighbouring sites is required in order to become sensitive to the large number of absorbing states. Therefore it appears natural that cluster mean-field approximations which already neglect some of the correlations present in the reaction terms themselves are unlikely to be reliable (in fact, the site approximation may be too simplistic to yield anything but a single transition). Rather, the pair approximation is good enough to reveal the presence of a PCP transition for $D = 0$ which is distinct from the one which occurs for $D > 0$, but since three-site correlations are not treated correctly, the PCP transition might have been stabilized artificially even for some values $D > 0$. Similar considerations should apply to any interacting particle system where the interactions occur through the contact of at least two particles (see also section 6).

4. Numerical studies of the critical behaviour in one dimension

4.1. Density-matrix renormalization group study

Since the first non-perturbative study of the PCPD [19] was made using the reformulation of the problem through the quantum Hamiltonian formalism, we shall begin with a brief description of that method, see [2, 69, 70] for recent reviews. The starting point is provided by the master equation, cast into the form

$$\partial_t |P(t)\rangle = -H|P(t)\rangle \tag{19}$$

where $|P(t)\rangle = \sum_{\{\sigma\}} P(\{\sigma\}; t)|\{\sigma\}\rangle$ is the state vector of the system at time t, $|\{\sigma\}\rangle$ is the state vector of a particle configuration $\{\sigma\}$ on the lattice, and $P(\{\sigma\}; t)$ is the time-dependent probability of that configuration. For a chain of L sites with a maximal occupancy of one particle per site the *quantum Hamiltonian* H is a $2^L \times 2^L$ matrix with elements

$$\langle\{\sigma\}|H|\{\tau\}\rangle = -w(\tau \to \sigma) + \delta_{\sigma,\tau} \sum_{\{\upsilon\}} w(\tau \to \upsilon) \tag{20}$$

where $w(\tau \to \sigma)$ is the transition rate from the configuration $\{\tau\}$ to the configuration $\{\sigma\}$. Since the elements of the columns of H add up to zero, H indeed describes a stochastic process. From the condition of probability conservation $\sum_{\{\sigma\}} P(\{\sigma\}; t) = 1$ it follows that $\langle\mathfrak{s}|H = 0$, where $\langle\mathfrak{s}| = \sum_{\{\sigma\}} \langle\{\sigma\}|$ is a left eigenvector of H with eigenvalue 0. Since the particle reactions are generically irreversible, H is in general non-Hermitian and therefore it has distinct right and left eigenvectors, which we denote by $|0_r\rangle, |1_r\rangle, \ldots, |n_r\rangle$ and $\langle 0_l|, \langle 1_l|, \ldots, \langle n_l|$, respectively with the corresponding 'energy levels' $E_0, E_1, \ldots, E_n$ ordered according to $0 = E_0 \leqslant \mathrm{Re}\, E_1 \leqslant \cdots \mathrm{Re}\, E_n$. Clearly, $\langle n_l|m_r\rangle = 0$ if $E_n \neq E_m$ and we normalize states such that $\langle n_l|n_r\rangle = 1$. We also set $\langle\mathfrak{s}| = \langle 0_l|$.

Given the rates (9) of the PCPD, the associated quantum Hamiltonian H on a chain with L sites is easily constructed. The stationary states of the model correspond to right eigenvectors of H with vanishing eigenvalue. For the PCPD with $D > 0$ these are, for both periodic and free boundary conditions [19], the two absorbing states

$$\begin{aligned} |0_r\rangle &:= |\circ\circ\circ\cdots\circ\rangle \\ |1_r\rangle &:= \frac{1}{L}(|\bullet\circ\circ\cdots\circ\rangle + |\circ\bullet\circ\cdots\circ\rangle + \cdots + |\circ\circ\circ\cdots\bullet\rangle). \end{aligned} \tag{21}$$

Consequently, the first two eigenvalues E_0 and E_1 vanish so that the inverse relaxation time towards the absorbing state is given by the smallest 'energy gap' $\Gamma = \Gamma(p, D; L) := \mathrm{Re}\, E_2$. Finally, formally solving the master equation (19), the average value $\langle\mathfrak{O}\rangle(t)$ of an observable $\mathfrak{O}$ is given by

$$\langle\mathfrak{O}\rangle(t) = \langle\mathfrak{s}|\mathfrak{O}|P(t)\rangle = \sum_n \langle\mathfrak{s}|\mathfrak{O}|n_r\rangle\langle n_l|P(0)\rangle\, \mathrm{e}^{-E_n t} \tag{22}$$

where we tacitly assumed the completeness (and biorthogonality) of the right and left eigenvector systems. Although the quantum Hamiltonian formalism was originally introduced with the aim of relating non-equilibrium systems on infinitely long chains to integrable quantum systems, we are interested here in the numerical analysis of systems on *finite* chains with L sites. Then the long-time behaviour is given by the smallest inverse relaxation time $\tau = \xi_\parallel = \Gamma^{-1}$ with the following finite-size behaviour:

$$\Gamma \sim \begin{cases} \exp(-L/\xi_\perp) & \text{if} \quad p < p_c(D) \\ L^{-z} & \text{if} \quad p = p_c(D) \\ L^{-2} & \text{if} \quad p > p_c(D) \end{cases} \tag{23}$$

where $z = \nu_\parallel/\nu_\perp$ and $\xi_\perp \sim |p - p_c(D)|^{-\nu_\perp}$ is the spatial correlation length. For large lattices and $p \geqslant p_c(D)$, one expects that the lowest energies should satisfy a massless dispersion relation of the form $E(k) \sim k^z$, and since the lowest momenta should scale as $k_{\min} \sim L^{-1}$, the phenomenological scaling (23) is recovered.

Having found $\Gamma(p, D; L)$ on a sequence of finite lattices, one proceeds as usual, see [71] for a collection of reviews. The critical parameters (here $p_c(D)$ and z) are extracted by forming the logarithmic derivative

$$Y_L(p, D) := \frac{\ln[\Gamma(p, D; L+1)/\Gamma(p, D; L-1)]}{\ln[(L+1)/(L-1)]}. \tag{24}$$

However, since the entire absorbing phase is critical and therefore $\lim_{L\to\infty} \Gamma(p, D; L) = 0$ the habitual method of looking for the intersection of two curves $Y_L(p, D)$ and $Y_{L'}(p, D)$ cannot be applied [19]. Rather, the critical point $p_c(D)$ must be found by fixing d and L and finding the value of $p = p_L(D)$ which maximizes $Y_L(p, D)$ (see appendix B for further details). Then the sequence of estimates has to be extrapolated to $p_c(D) = \lim_{L\to\infty} p_L(D)$. Finally, for L large, one expects

$$Y_L(p, d) \simeq \begin{cases} -L/\xi_\perp & \text{if} \quad p < p_c(D) \\ -z & \text{if} \quad p = p_c(D) \\ -2 & \text{if} \quad p > p_c(D) \end{cases} \tag{25}$$

and one finally obtains $z = -\lim_{L\to\infty} Y_L(p_c(D), D)$ [19]. In addition an estimate of the order-parameter exponent $\beta/\nu_\perp$ can be obtained from the steady-state density profile at $p = p_c(D)$

$$\rho_L(\ell) = \langle \mathfrak{s}|\hat{n}(\ell)|0_r\rangle = L^{-\beta/\nu_\perp} f(\ell/L) \tag{26}$$

where $\hat{n}(\ell)$ is a particle number operator at site ℓ, and f is a scaling function. The double degeneracy of the ground state was lifted by adding a particle creation process $\emptyset \to A$ with a small rate p'. For estimates of the bulk exponent, one may set $\ell = L/2$ and $\rho_L(L/2) \sim L^{-\beta/\nu_\perp}$ as expected. On the other hand, if one sets $\ell = 1$, in the limit of $p' \to 0$ one has the scaling form $\rho_L(1) \sim L^{(\beta_1-\beta)/\nu_\perp}$ from which the surface critical exponent $\beta_1/\nu_\perp$ can be determined [37].[8]

The lowest eigenvalue Γ and the corresponding eigenvector are found from the non-symmetric DMRG algorithm [19, 37] on an open chain. In comparison with Monte Carlo simulations, the DMRG method as described here directly yields the steady state with a high numerical precision, does not suffer from a critical slowing-down in the vicinity of the critical point and for non-disordered systems does not require the use of a random-number generator. On the other hand, the number of lattice sites which can be treated is relatively restricted. For example, in [19] data for Γ_L with $L \lesssim 30$ sites and for ρ_L with $L \leqslant 48$ sites could be obtained.

[8] For models with a non-degenerate ground state, the use of a surface rate may be avoided by estimating the profile from $N(\ell) = \langle 1_l|\hat{n}(\ell)|1_r\rangle$. At criticality, the finite-size scaling forms $N(L/2) \sim L^{-\beta/\nu_\perp}$ and $N(1) \sim L^{-\beta_1/\nu_\perp}$ are expected [37, 72, 73].

Larger lattices with up to $L = 60$ sites have been obtained more recently [44, 54]. In the absorbing phase, however, the finite-size sequences converge very well and the accuracy of the estimated limits can be considerably enhanced through the *BST* extrapolation algorithm [74, 75]. The expected dynamical and order-parameter exponents $z = 2$ and $\beta/\nu_\perp = 1$ are recovered to high accuracy. On the other hand, along the critical line, the required finite-size extrapolations are affected by some ill-understood correction terms which preclude the use of sequence extrapolation algorithms. The final results for $p_c(D)$ and the exponents z and $\beta/\nu_\perp$ are collected in table 3. Since results for several values of D were obtained, a discussion of systematic effects on the estimates becomes possible.

While the values of $\beta/\nu_\perp$ are almost independent of D, the results for z show a considerable variation which was argued in [19] to come from a subtle finite-size correction. Taking mean values and comparing with the values of the other universality classes available at the time, namely directed percolation (DP) and the parity-conserved (PC) universality classes, the values of z and $\beta/\nu_\perp$ of [19] are far from those of DP but intriguingly close to those of PC (see table 3). Because of this surprising coincidence the possibility that the active–inactive transition of the PCPD might belong to the PC universality class emerged, in spite of the fact that there is no obvious counterpart for the parity conservation law in the PCPD, i.e. there is no symmetry separating the dynamics into two sectors [38]. In fact, in both cases the inactive phase is characterized by an algebraic decay of the density as $t^{-1/2}$. Moreover, both models have two absorbing states. Still, the unambiguous identification of a steady-state universality class requires the determination of four independent exponents (see [1–3]), rather than the two obtained in [19].

Indeed, small-scale Monte Carlo simulations [38, 39] seemed to confirm the DMGR results for $p_c(D)$ and, for D not too large, also the exponents z and $\beta/\nu_\perp$. However, either the exponent bound $\beta < 0.67$ [38] or the estimate $\beta \simeq 0.58$ [39] was significantly smaller than the expected PC value 0.92. In addition, the effective exponents δ' and η in seed simulations were shown to differ significantly from the expected PC values. These results rather suggested that the PCPD might be a novel non-equilibrium universality class, distinct from that of PC as well as DP processes.

4.2. High-precision Monte Carlo simulations

The first simulational study of the PCPD with sequential dynamics (the rates (9) were chosen for maximal efficiency) yielded the critical-point estimates [77]

$$p_c(0.1) = 0.1105(5) \qquad p_c(0.5) = 0.153(1) \tag{27}$$

which are in good agreement with later results shown in figure 2 and table 3. We point out that several inequivalent definitions of the critical threshold $p_c(D)$ are in use and only the definitions of the articles [19, 38, 47, 54] and of figure 5—which gives the results of [65]—are consistent with each other and equation (27). A systematic high-precision Monte Carlo simulation was performed by Ódor [39]. In order to implement the model on a parallel computer, he investigated a variant of the PCPD with *synchronous updates* on three sublattices. Depending on the value of the diffusion rate he found continuously varying exponents δ, β and η (see table 3), concluding that the process does not belong to the PC universality class. Instead the value of β seemed to jump from $\beta \approx 0.58$ for $0.05 \leqslant D \leqslant 0.2$ to smaller values at $D > 0.5$. This observation together with the aforementioned pair mean-field approximation led Ódor to the conjecture that the PCPD might belong to *two different* universality classes for low and high diffusion rates. Although it seems to be surprising how the choice of a rate can switch between two universality classes we note that a similar scenario has been observed in a certain two-species particle model [78], although the specific

Table 3. Summary of estimates for the critical exponents of the 1D PCPD. A star indicates that the control parameter is effectively fixed or defined in a different way. Several variants of models with differently defined critical thresholds $p_c(D)$ were used.

Reference	D	p_c	δ	$z = \frac{\nu_\parallel}{\nu_\perp}$	β	$\beta/\nu_\perp$	δ'	η
Carlon *et al* [19]	0.1	0.111(2)	–	1.87(3)	–	0.50(3)	–	–
	0.15	0.116(2)	–	1.84(3)	–	0.49(3)	–	–
	0.2	0.121(3)	–	1.83(3)	–	0.49(3)	–	–
	0.35	0.138(1)	–	1.72(3)	–	0.47(3)	–	–
	0.5	0.154(1)	–	1.70(3)	–	0.48(3)	–	–
	0.8	0.205(1)	–	1.60(5)	–	0.51(3)	–	–
Hinrichsen [38]	0.1	0.111 2(1)	0.25(2)	1.83(5)	<0.67	0.50(3)	0.13(2)	0.13(2)
Ódor [39]	0.05	0.250 78	0.273(2)	–	0.57(2)	–	0.004(6)	0.10(2)
	0.1	0.248 89	0.275(4)	–	0.58(1)	–	–	–
	0.2	0.248 02	0.268(2)	–	0.58(1)	–	0.004(6)	0.14(1)
	0.5	0.279 55	0.21(1)	–	0.40(2)	–	0.008(9)	0.23(2)
	0.9	0.432 4	0.20(1)	–	0.39(2)	–	0.01(1)	0.48(1)
Ódor [41]	0.2	0.179 75(8)	0.263(9)	–	0.57(1)	–	–	–
	0.4	0.264 7(1)	0.268(8)	–	0.58(1)	–	–	–
	0.7	0.352 8(2)	0.275(8)	–	0.57(1)	–	–	–
Park *et al* [42]	*	0.089 5(2)	0.236(10)	1.80(2)	0.50(5)	–	≈ 0.1	≈ 0.2
Noh and Park [47]	0.1	0.111 2(1)	0.27(4)	1.8(2)	0.65(12)	0.50(5)	0.09(2)	0.18(5)
Park and Kim [48] A	*	0.030 81(4)	0.241(5)	1.80(10)	0.519(24)	–	0.11(3)	0.15(3)
Park and Kim [48] B	*	0.287 35(5)	0.242(5)	1.78(5)	0.496(22)	–	0.13(3)	0.15(3)
Dickman	0.1	0.106 48(3)	0.249(5)	2.04(4)	0.546(6)	0.503(6)	–	–
and Menezes [49]	0.5	0.120 45(3)	0.236(3)	1.86(2)	0.468(2)	0.430(2)	–	–
	0.85	0.130 03(1)	0.234(5)	1.77(2)	0.454(2)	0.412(2)	–	–
Hinrichsen [50]	1	0.299 98(4)	0.22(1)	1.78(5)	–	–	0.13(1)	0.22(3)
Kockelkoren and Chaté [51]	*	*	0.200(5)	1.70(5)	0.37(2)	–	–	–
Ódor [52, 56]	0.05	0.104 39(1)	0.216(9)	2.0(2)	0.411(10)	0.53(7)	–	–
	0.1	0.106 88(1)	0.206(7)	1.95(1)	0.407(7)	0.49(2)	–	–
	0.2	0.112 18(1)	0.217(8)	1.95(1)	0.402(8)	0.46(3)	–	–
	0.5	0.133 53(1)	0.206(7)	1.84(1)	0.414(16)	0.41(2)	–	–
	0.7	0.157 45(1)	0.214(5)	1.75(1)	0.39(1)	0.38(2)	–	–
Barkema	0.1	0.111 05(5)	0.17	–	–	–	–	–
and Carlon [54]	0.2	–	0.17	1.70(3)	–	0.28(4)	–	–
	0.5	0.152 45(5)	0.17(1)	–	–	0.27(4)	–	–
	0.9	0.233 5(5)	0.17	1.61(3)	–	–	–	–
				Related models				
Hinrichsen [40]	1	0.692 9(1)	0.21(1)	1.75(10)	0.38(6)	–	0.15(1)	0.21(2)
Ódor [46]	*	0.325 3(1)	0.19(1)	1.81(2)	0.37(2)	–	–	–
Hinrichsen [76]	*	*	0.21(2)	1.75(2)	–	–	–	–
				Known universality classes				
DP [59]			0.1595	1.5807	0.2765	0.2521	0.1595	0.3137
PC [8]			0.286(2)	1.74(1)	0.922(5)	0.497(5)	0	0.286(2)

mechanism in these models is not obvious in the PCPD. We shall return to this problem in section 6.

As pointed out in [38] the unusual critical behaviour of the PCPD should be seen in a large variety of binary reaction–diffusion processes with absorbing states, in particular in the coagulation–fission process $2A \to 3A$, $2A \to A$. Simulating the coagulation–fission process with branching sidewards

$$\begin{array}{lll} AA\emptyset, \emptyset AA \to AAA & \text{with rate} & (1-p)(1-D)/2 \\ AA \to \emptyset A/A\emptyset & \text{with rate} & p(1-D)/2 \\ A\emptyset \leftrightarrow \emptyset A & \text{with rate} & D \end{array} \tag{28}$$

as well as a symmetric variant with offspring production in the middle of two particles

$$A\emptyset A \to AAA \qquad \text{with rate} \quad \lambda(1-p)(1-D). \tag{29}$$

Ódor [41] could confirm this expectation, provided that the diffusion rate is high enough. The observed exponents seemed to be in agreement with those of the PCPD for small diffusion rates, leading Ódor to the conjecture that the coagulation–fission process may belong to a single universality class.

The special case where the rates for coagulation and diffusion are equal, i.e. $D = p(1-D)/2$, can be solved exactly for any value of λ [43], using the well-known method of interparticle distribution functions [79]. As pointed out in [43], in this case the dynamics is special in so far as the fission process can only fill voids of an invariant skeleton of coagulating random walks. Unfortunately, in this case the active phase is inaccessible so that the exact solution does not provide any information about the critical exponents of a possible universality class of PCPD transitions, rather the system always crosses over to a decay of the form $\rho(t) \sim t^{-1/2}$. Nevertheless the solution reveals that the finite-size scaling of the relaxation times does not depend on the fission rate and thereby allows us to test a recent extension to non-equilibrium phase transitions [44] of the Privman–Fisher finite-size scaling forms [80].

Concerning the possibility of two universality classes or even continuously varying exponents, Park and Kim [48] showed by numerical simulations that in models, where the rates of diffusion and annihilation are tuned in such a way that the process without particle production would become exactly solvable, one obtains a well-defined set of critical exponents [48] (see table 3). In this sense, they argue, the transition in the PCPD may be considered as universal. Contrarily Dickman and Menezes [49] claim that the transition in the PCPD is non-universal. Their argument will be reviewed in the following subsection.

As a third possibility, one of us (HH) suggested an extremely slow crossover to DP [50]. Simulating a cellular automation of the PCPD which was originally introduced by Grassberger [65], it was argued that the scaling regime is not reached, even after six decades in time. Instead the effective exponents display a slow drift as time proceeds. Remarkably, all exponents seem to drift in the direction of DP values so that one cannot rule out that the critical behaviour of the (1+1)-dimensional PCPD may eventually tend to DP. According to these arguments the DP process manifests itself in the dynamics of pairs of particles, while the diffusing background of solitary particles becomes irrelevant as $t \to \infty$ (obviously, this mechanism should work exclusively in one spatial dimension while in higher dimensions the diffusive background may be increasingly relevant leading to an effective mean-field behaviour). Recently Barkema and Carlon [54] presented extrapolation results, arriving at a similar conclusion (see section 4.4). In contrast, a recent simulation of the PCPD with non-restricted occupancy per site performed by Kockelkoren and Chaté (see section 4.5) does not show such a drift, supporting the hypothesis of a single universality class distinct from previously known classes.

The DP hypothesis poses a conceptual problem, namely, how does the algebraic decay $\rho(t) \sim t^{-1/2}$ in the inactive phase comply with DP, where the decay is exponential? In this

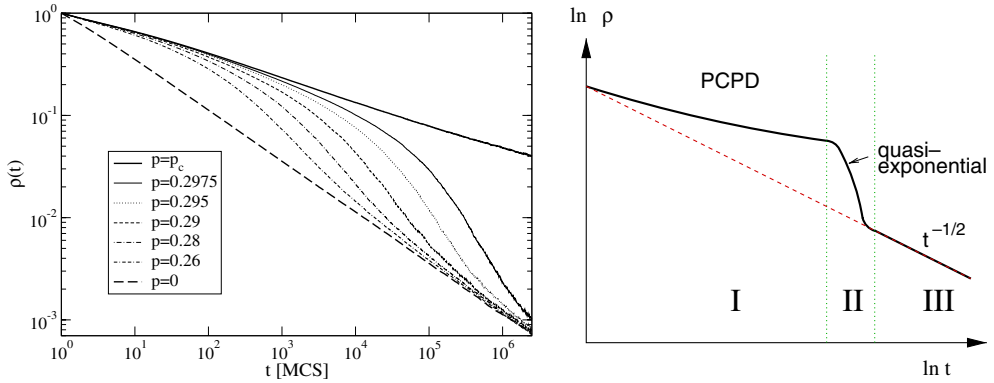

Figure 3. Left panel: decay of the particle density in the inactive phase for different values of p in comparison with the critical PCPD (bold line) and pure coagulation (dotted line). Right panel: sketch of the sudden decay of the particle density in the inactive phase (see the text). After [50].

context it is interesting to monitor the crossover of the particle density in a slightly subcritical PCPD. As shown in figure 3, there are three different temporal regimes. In the first regime (region I), the particle density decays very slowly as in a critical PCPD. After a characteristic time, however, the density decays rapidly (region II) until it crosses over to an algebraic decay $t^{-1/2}$ (region III). Remarkably, the amplitude of this asymptotic power law does *not* depend on $p - p_c$. Therefore, the breakdown in region II becomes more and more pronounced as the critical threshold is approached and might tend to a quasi-exponential decay in the limit $p \to p_c$.

4.3. Universal moments and amplitudes

Since the numerical values of the available exponents seem to vary between different universality classes, alternative diagnostic tools might be of value. Following [20], let us consider the order-parameter moments

$$m_n := \langle \rho^n \rangle \tag{30}$$

From the scaling arguments reviewed in section 2, it is known that ratios such as $m_4/m_2^2, m_3/m_1^3, m_3/(m_1 m_2)$ or m_2/m_1^2 should be universal. In fact, moment ratios are just special values of the scaling functions and hence their numerical values may be used, like the critical exponents, to identify the universality class of a given model. Further one may consider the cumulants [20]

$$K_2 := m_2 - m_1^2 \qquad K_4 := m_4 - 4m_3 m_1 - 3m_2^2 + 12 m_2 m_1^2 - 6m_1^4 \tag{31}$$

whose ratios K_4/K_2^2 and $K_2/m_1^2 = m_2/m_1^2 - 1$ should be universal as well.

For future reference, we reproduce in table 4 several universal moment ratios as obtained for the simple contact process (DP), for the pair-contact process without diffusion, and for a branching–annihilating random walk belonging to the parity-conserving class (PC). The numerical estimates were obtained at the critical point of finite-size systems by averaging over surviving quasi-stationary runs and extrapolating $L \to \infty$. Note that for the contact process, the order parameter is the particle density, whereas for the pair-contact process with $D = 0$, the order parameter is the *pair* density. While it had been known before that the static critical exponents of the DP and the PCP agree [17] the agreement of the moment ratios between the two models provides additional evidence in favour of the conjecture that the steady-state

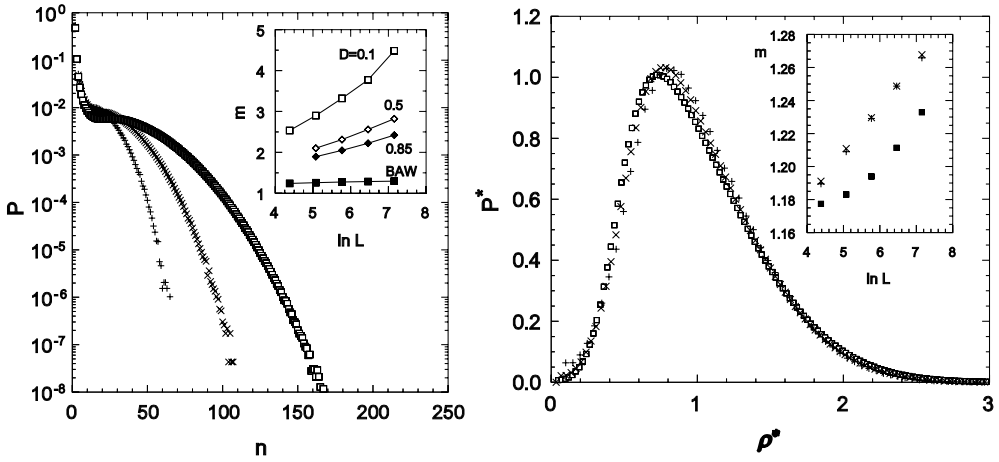

Figure 4. Left panel: probability distribution of the number of particles n at criticality, for $D = 0.1$ and +: $L = 80$; ×: $L = 160$; □: $L = 320$. The inset shows $m = m(\ln L)$ of the PCPD and also for the BAW. Right panel: scaling of the reduced probability distribution in the reactive sector and with the same symbols as before. The inset shows $m = m(\ln L)$ in the reactive sector of the PCPD, with ■: $D = 0.1$; +: $D = 0.5$; ×: $D = 0.85$. After [49].

Table 4. Some universal moment and cumulant ratios at criticality for the directed percolation universality class (DP), the pair-contact process (PCP) and the parity-conserving class (PC) for an infinite lattice in $d = 1, 2$ dimensions.

d	Model	m_4/m_2^2	m_3/m_1^3	$m_3/(m_1m_2)$	m_2/m_1^2	K_4/K_2^2	References
1	DP	1.554(2)	1.526(3)	1.301(3)	1.1736(2)	−0.505(3)	[20]
	PCP	1.558(2)	1.529(3)	1.303(3)	1.1738(2)	−0.493(3)	[20]
	PC				1.3340(4)		[49]
2	DP	2.093(8)	2.080(1)	1.569(1)	1.3257(5)	−0.088(4)	[20]
	PCP	2.07(1)	2.067(9)	1.56(1)	1.323(3)		[21]

transitions of the DP and the PCP are in the same universality class. On the other hand, the result for the branching–annihilating random walk (BAW) [8] which is in the PC class is clearly different, as expected. We are not aware of analogous data for any other interacting particle model but the building-up of a collection of data of these amplitudes in several universality classes should be helpful.

Having established that the method of universal moments is capable to distinguish between different universality classes, Dickman and Menezes [49] tried to apply the moment ratio method to the 1D PCPD and considered the universal ratio $m := \langle\rho^2\rangle/\langle\rho\rangle^2 = m_2/m_1^2$. Although several critical exponents could be determined from finite-size scaling, surprisingly they found for the moment ratio a logarithmic increase with the system size as $m \sim (\ln L)^\psi$ with $\psi \gtrsim 1$, see figure 4. No such behaviour is seen for the BAW. If this phenomenon persisted in the limit $L \to \infty$, it would collide with the scaling forms reviewed in section 2 from which one would deduce a scaling form

$$P(\rho; L) = \langle\rho\rangle\mathcal{P}(\rho/\langle\rho\rangle) \tag{32}$$

where $\mathcal{P}$ is a normalized scaling function. Indeed, as can be seen in figure 4, the particle distribution function does not scale (a similar result also holds for the pair distribution function).

Instead, the most probable particle number is always 2 and the distribution shows a tail which grows with L and generates the critical behaviour of the model.

In order to account for this, Dickman and Menezes [49] argue that the PCPD should be characterized by the simultaneous dynamics of isolated particles and colliding pairs (as is indeed rendered plausible by illustrations of the dynamics as in figure 1), and therefore propose to separate the model's states into a 'purely diffusive' sector and a 'reactive sector' which must contain at least a pair of particles. The idea is to restrict the analysis to the reactive sector by excluding all states without pairs when taking averages, but without modifying the dynamical rules (this was also proposed independently in [47]). The result is shown in the right panel of figure 4, where scaling behaviour in the reduced variables $\rho^* = \rho/\langle\rho\rangle$ and $P^* = \langle\rho\rangle P$ is obtained. Now, the form of P^* becomes quite similar to that of the non-diffusive PCP. In addition, the ratio m also becomes almost constant and with a value close to the estimates for DP, see figure 4. Still, as already noted in [49], neither the scaling collapse nor the L-independence of m is completely perfect and the origin of these deviations remains to be understood[9]. Although off-critical simulations lead to a clear scaling collapse and a DP-like exponent $\nu_\perp = 1.10(1)$ independently of D [49], other exponents maintain a weak D-dependence. When taking these results at face value, it implies a non-universality along the critical line and both the DP and the PC universality classes are excluded for the 1D PCPD [49]. However, one might wonder whether the estimates of the exponents could still be affected by some non-resolved correction-to-scaling term which would make the dependence on D only apparent. In any case, this study points to the large corrections to scaling which are present in the 1D PCPD and which render the extraction of universal parameters very difficult.

While the above universal moment ratios referred to a spatially infinite system, we now consider the case of a finite lattice of linear size L, e.g. a hypercube. For equilibrium systems, it is well known that the finite-size scaling of the correlation length leads to universal amplitudes, as reviewed in [81]. For non-equilibrium phase transitions, it has been argued that on a finite spatial lattice, the temporal correlation length $\xi_{\parallel,i}$ and the spatial correlation length $\xi_{\perp,i}$ should scale as [44]

$$\xi_{\parallel,i}^{-1} = L^{-z} D_0 R_i(C_1(p - p_c)L^{1/\nu_\perp}) \qquad \xi_{\perp,i}^{-1} = L^{-1} S_i(C_1(p - p_c)L^{1/\nu_\perp}) \tag{33}$$

where (for given boundary conditions) R_i and S_i are *universal* scaling functions, the index i refers to the observable $\mathfrak{O}_i$ of which the correlators are studied and the entire non-universality can be absorbed into the non-universal metric factors C_1 and D_0. In particular, the existence of the above scaling forms can be *derived* for systems in the directed percolation universality class [44]. For the convenience of the reader, the argument will be reproduced in appendix C. Consequently, the finite-size scaling amplitudes of the spatial correlation lengths $\xi_\perp^{-1}$ are universal, as are *ratios* of temporal correlation lengths $\xi_{\parallel,i}^{-1}/\xi_{\parallel,j}^{-1} = E_i/E_j$ which in turn are easily calculated from the spectrum of the quantum Hamiltonian H, as discussed above in section 4.1. Furthermore, from the scaling forms derived in appendix C it follows that the universality of the critical finite-size scaling amplitudes of $\xi_{\perp,i}$ is equivalent to the universality [44] of the moments

$$\left\langle r_\perp^n \right\rangle = \frac{\int_{\Omega(L)} \mathrm{d}^d \boldsymbol{r}_\perp \int_0^\infty \mathrm{d}r_\parallel r_\perp^n G(\boldsymbol{r}_\perp, r_\parallel; L/\xi_\perp)}{\int_{\Omega(L)} \mathrm{d}^d \boldsymbol{r}_\perp \int_0^\infty \mathrm{d}r_\parallel G(\boldsymbol{r}_\perp, r_\parallel; L/\xi_\perp)} = L^n \Xi(L/\xi_\perp) \tag{34}$$

of the pair connectivity $G(\boldsymbol{r}_\perp, r_\parallel)$ which is the probability that the sites $(\mathbf{0}, 0)$ and $(\boldsymbol{r}_\perp, r_\parallel)$ are connected by a direct path. Here $\Omega(L)$ is a d-dimensional hypercube of linear extent L and Ξ is a universal function the argument of which does not contain any non-universal metric

[9] Restricting to states with at least two pairs does not further reduce the apparent variation of m with L.

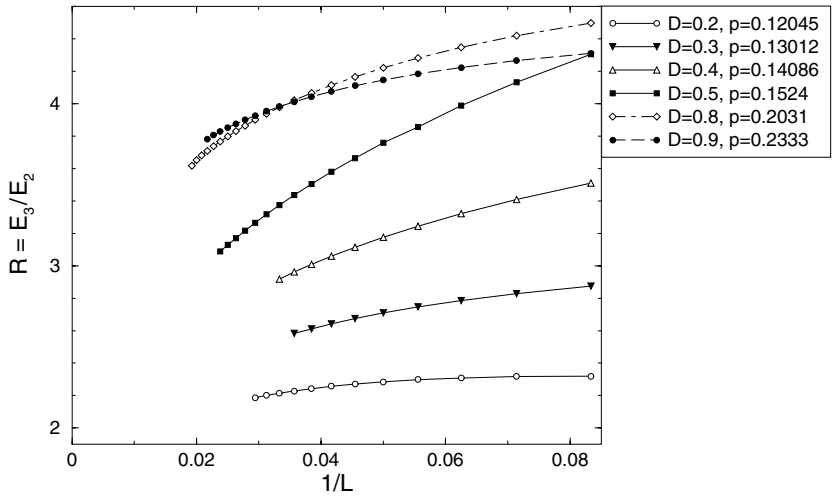

Figure 5. Universal ratio of finite-size scaling amplitudes of the relaxation times along the critical line in the 1D PCPD, for free boundary conditions. The values of $p_c(D)$ are from [65]. After [44].

factor. These universality statements have been confirmed in several exactly solvable models [43, 44]. In figure 5 we illustrate the universality of the amplitude ratio $R = E_3/E_2$ along the critical line in the 1D PCPD, as obtained from the DMRG. As observed before for the exponents, there appear to be some finite-size corrections which are sufficiently irregular such that the powerful sequence-extrapolation methods [75, 82] cannot be used. Still, inspection shows that for the smaller values of D (i.e. up to $D \lesssim 0.5$) the data seem to converge towards a limit $R_\infty \approx 2$ and its independence of D would confirm universality. On the other hand, for values of $D \gtrsim 0.8$, there appears to arise a large transient region and only for values of L larger than ≈ 50 sites might a convergence slowly set in. This is a cautionary example illustrating again that the truly asymptotic regime in the PCPD might set in very late and sometimes could be beyond the reach of currently available numerical methods.

At present, no finite-size data for the amplitude ratios (33) or (34) seem to be available for free boundary conditions in any non-equilibrium universality class. In this context we recall the well-known observation from critical equilibrium systems that universal amplitude ratios tend to vary considerably more between different universality classes than critical exponents usually do, see [81]. Finding reference values for these amplitudes in distinct non-equilibrium systems should be helpful.

4.4. Extrapolation techniques

In numerical simulations of the PCPD, there are two sources of uncertainty which cannot be separated easily. On the one hand, the critical PCPD shows unusually strong *intrinsic corrections* to scaling, on the other hand a possible error in the estimation of the critical point leads to additional *off-critical deviations* with an unknown functional form. Most numerical approaches assume that the first source of uncertainty can be neglected after sufficiently long simulation times. The critical point is then estimated by postulating power-law behaviour over the last few decades in time, indicated by a straight line in a log–log plot or saturating effective exponents. In the PCPD, however, the main risk lies in the possibility that the intrinsic corrections to scaling *at* criticality may still be present even after 10^6–10^8 time steps. Thus,

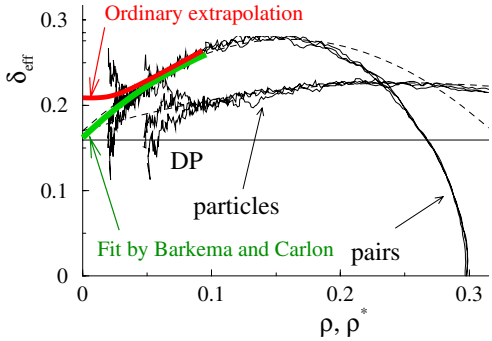

Figure 6. Extrapolation technique suggested by Barkema and Carlon (after [54]). Assuming algebraic corrections of the form (36) with $\gamma = \delta$ the curve of the effective exponent $\delta_{\rm eff}(t)$ should intersect with the vertical axis as a straight line (lower bold line). Ordinary extrapolations such as in [51], assuming that the scaling regime is actually reached within the simulation time, would correspond to the upper bold line, which becomes horizontal as $\rho(t) \to 0$.

looking for a power law over the last few decades of time, one may be tempted to 'compensate' the intrinsic scaling corrections by off-critical deviations in opposite direction, leading to a slightly biased estimate of the critical point and thereby to considerable systematic errors in the estimated critical exponents.

In order to solve this problem the two sources of corrections—intrinsic scaling corrections and off-critical deviations—have to be separated. One may try to do this by assuming a certain functional form for one of them and performing appropriate fits. The first attempt in this direction was made by Ódor [52], who postulates logarithmic corrections to scaling at criticality. For example, in the case of a temporally decaying particle density, where we expect an asymptotic power law $\rho(t) \sim t^{-\delta}$, he assumes the intrinsic scaling correction *at criticality* to be of the form

$$\rho(t) = \left[\frac{a + b\ln t}{t}\right]^{\delta} \tag{35}$$

where a and b are fit parameters. Using this technique Ódor obtained $\delta = 0.21(1)$ for various values of the diffusion rate between 0.05 and 0.7, favouring the scenario of a single independent universality class. Ódor also estimated the critical exponents in a two-dimensional PCPD, confirming the mean-field prediction in $d \geqslant 2$ dimensions.

Another extrapolation method was tried by Barkema and Carlon [54] in analysing high-quality data of a multispin Monte Carlo simulation. Unlike Ódor, they postulate algebraic scaling corrections of the form

$$\rho(t) = (1 + at^{-\gamma})t^{-\delta} \tag{36}$$

where a and γ have to be fitted appropriately. Although one would naively expect the exponent of the correction γ to be equal to 1, Barkema and Carlon present numerical evidence suggesting that $\gamma = \delta = \beta/\nu_{\perp}$. Based on this conjecture they propose to plot local slopes versus the density of particles. Using this representation the curve of local effective exponents should intersect with the vertical axis at $\rho = 0$ as a straight line, as sketched in figure 6. Applying this extrapolation method Barkema and Carlon argue that the critical exponents tend to those of DP, in agreement with the conclusions offered in [50] (they only quote the value of δ averaged over several values of D which is the one listed in table 3).

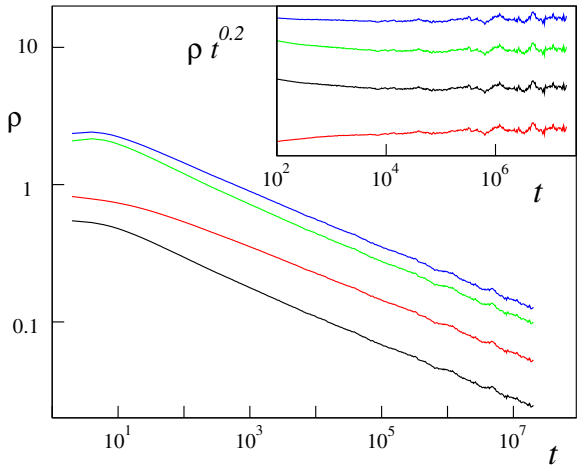

Figure 7. Soft-constraint model defined in [51] at criticality. From top to bottom are shown the decay of the particle density, the density of particles without solitary particles, the fraction of occupied sites and the fraction of occupied sites with at least two particles. Clean scaling behaviour is observed. After [51].

4.5. Restricted PCPD with a soft constraint

All variants of the PCPD discussed so far are restricted by hard-core exclusion, i.e. each site can be either empty or occupied by a single particle. Although these models are easy to implement numerically, they involve three-site interactions with some ambiguity concerning the spatial arrangement. In order to circumvent this problem, Kockelkoren and Chaté [51] proposed a surprisingly simple 'bosonic' model in which a soft constraint prevents the particle density in the active phase from diverging. The scaling arguments of the previous sections are expected to go through, and models with a soft constraint are expected to exhibit the same type of critical behaviour as the ordinary PCPD with hard-core exclusion, see also section 6.

Their model is defined as follows. Particles of a single species A evolve by synchronous updates in two sub-steps. Each site can be occupied by arbitrarily many particles. First the particles diffuse, i.e. all particles hop independently to a randomly chosen nearest neighbour. Then the pairs of particles react locally, either producing offspring or annihilating each other. To this end the population of n particles at a given site is divided into $\lfloor n/2 \rfloor$ pairs, which branch independently with probability $p^{\lfloor n/2 \rfloor}$ and annihilate otherwise. As a result, if n is very large, the fission process is exponentially suppressed, introducing effectively a soft constraint.

Unlike restricted variants of the PCPD, the model introduced by Kockelkoren and Chaté exhibits a surprisingly clean scaling behaviour, even when different order parameters are used (see figure 7). Since all reactions take place on single sites, the model seems to reach the scaling regime much faster than ordinary models with hard-core exclusion. These results led the authors of [51] to the conclusion that the PCPD represents a single universality class different from DP and PC, characterized by the critical exponent $\delta \approx 0.20$.

4.6. Surface critical behaviour

While most of the attempts in understanding the critical behaviour of the PCPD concentrated on bulk quantities, some information on surface critical exponents is also available. It

Table 5. Values of the surface exponent $\beta_1/\nu_\perp$ according to different methods for free and absorbing boundary conditions in some 1D models.

Model	Free	Absorbing	Method	References
PCPD	0.72(1)	1.11	DMRG, $D \lesssim 0.5$	[54]
DP	0.664(7)	–	Monte Carlo	[83]
	0.667(2)	–	DMRG	[37]
	0.6690(1)	–	Series	[84]
PC	0.73(1)	1.11(1)	Monte Carlo	[83]
	0.720(2)	1.10(1)	DMRG	[54]

is a well-established fact that in a semi-infinite system the critical behaviour near to the surface is in general different from that deep in the bulk, see [83] for a recent review. For example, in the steady state, the order-parameter density should scale near criticality as $\rho_b \sim (p - p_c)^\beta$ in the bulk but near the surface one expects $\rho_{surf} \sim (p - p_c)^{\beta_1}$ where β_1 is a surface critical exponent. The value of β_1 may further depend on the boundary conditions. Here we shall consider

(i) *free* boundary conditions, i.e. particles cannot cross the boundary.
(ii) *absorbing* boundary conditions, i.e. particles *at* the boundary may leave the system with a rate D. In other words, the boundary reaction $A \to \emptyset$ is added.

At criticality, one expects the finite-size scaling behaviour $\rho_{surf} \sim L^{-\beta_1/\nu_\perp}$ and techniques to calculate the boundary density are available [37]. For the PCPD, Barkema and Carlon [54] have obtained estimates for the exponent ratio $\beta_1/\nu_\perp$ and we list their results in table 5 together with results for the DP and PC universality classes for comparison. In the PCPD, estimates only converge for $D \lesssim 0.5$.

Taken at face value, the estimates of $\beta_1/\nu_\perp$ obtained for the PCPD appear actually to be compatible with those of the PC class but Barkema and Carlon carefully point out that their final estimates still depend on D, in particular for D large, and therefore may not yet give the correct asymptotic values.

5. Related models

5.1. Cyclically coupled spreading and annihilation

In order to characterize the essential features of the PCPD from a different perspective, one of us (HH) suggested interpreting the PCPD as a cyclically coupled DP and annihilation process [40]. The idea is to separate the dynamics of pairs and solitary particles, associating them with two species of particles A and B. The A, which stand for the pairs in the original PCPD, perform an ordinary DP process while the B represent solitary particles that are subjected to an annihilating random walk. Both subsystems are cyclically coupled by particle transmutation, as sketched in figure 8.

Such a cyclically coupled process was realized in [40] as a three-state model with random-sequential updates. Choosing particular rates it was shown that the process exhibits a phase transition with the same phenomenology as in the PCPD. Moreover, the values of the effective critical exponents

$$\delta = 0.215(15) \qquad z = 1.75(5) \qquad \nu_\parallel = 1.8(1) \tag{37}$$

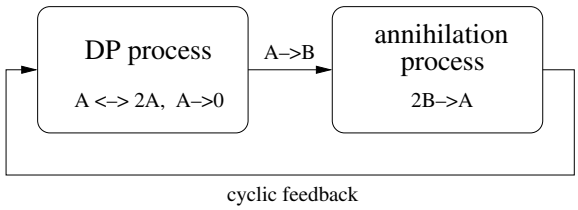

Figure 8. PCPD interpreted as a cyclically coupled DP and annihilation process.

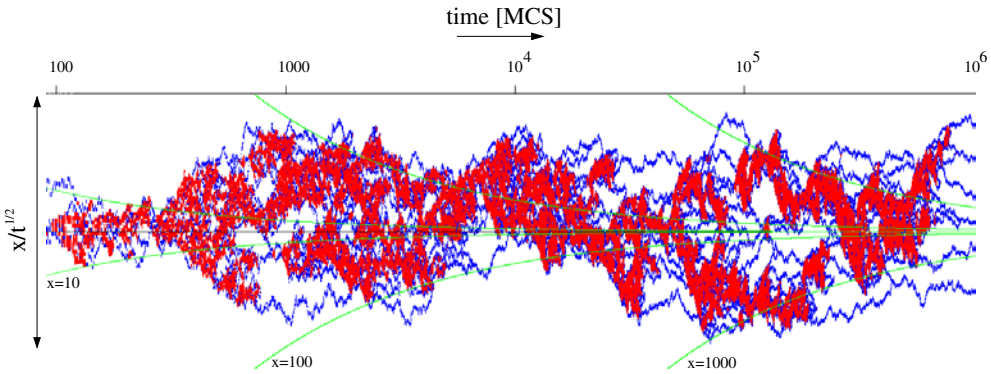

Figure 9. Typical spatio-temporal evolution of a binary spreading process starting from an initial seed. Particles of species A and B are represented as red and blue pixels, respectively. Plotting $x/L^{1/2}$ versus $\log_{10} t$ the figure covers four decades in time. As can be seen, patches of high activity (red) are connected by lines of diffusing B particles (blue) on all scales up to 10^6 time steps.

were found to be in fair agreement with other estimates for the PCPD. Recent simulations for various values of D between 0.1 and 1 suggest that the exponents should be independent of the diffusion constant [85]. These results indicate that cyclically coupled processes following the reaction–diffusion scheme in figure 8 display the same type of transition as the PCPD.

The separation into subprocesses illustrates an important feature of the PCPD, namely, the existence of two modes of spreading. As illustrated in figure 9, a typical spatio-temporal cluster is characterized by the interplay of a high-density mode dominated by self-reproducing and decaying A particles, and a low-density mode of solitary diffusing B particles. A similar interplay of high- and low-density patches can be observed in the critical PCPD, see figure 1.

Concerning the structure of a cluster a fundamental problem arises precisely at this point: as can be seen in figure 9, even after 10^6 time steps the solitary particles perform simple random walks over large distances. However, such a random walk is always characterized by the dynamic exponent $z = 2$, while all known simulations clearly indicate that the process as a whole spreads *superdiffusively*, i.e. $z < 2$. Therefore, the effective diffusion constant for solitary particles has to vary slightly under rescaling, meaning that a cluster such as in figure 9 cannot be scale invariant. Therefore it seems that the process is still far away from the asymptotic scaling regime, even after 10^6 time steps.

Table 6. Critical parameters of the generalized PCPD as defined in [47] for $D = 0.1$ as a function of r.

r	p_c	z	η	δ'	$\delta = \beta/\nu_\parallel$	$\nu_\perp$
0.00	0.046 87(2)	1.58(1)	0.314(6)	0.160(5)	0.159(1)	1.10(1)
0.25	0.055 05(5)	1.62(3)	0.29(1)	0.15(1)	0.173(5)	1.10(3)
0.50	0.066 36(4)	1.67(3)	0.26(1)	0.14(1)	0.197(3)	1.10(3)
0.75	0.083 15(5)	1.75(5)	0.20(2)	0.13(2)	0.230(5)	1.17(5)
1.00	0.111 2(1)	1.7(1)	0.18(5)	0.09(2)	0.27(4)	1.30(10)

5.2. Interpolating between DP and PCPD

A different explanation of the apparent non-universality in the PCPD was suggested by Noh and Park [47], who claim that the violations of scaling can be traced back to a long-term memory effect mediated by the diffusive background of single particles. To show this, they introduce a generalized version of the PCPD, as follows. Each site of the lattice can be either empty or occupied by a single particle and the following reactions are admitted

$$\begin{aligned} AA &\to \emptyset\emptyset && \text{with rate} \quad (1-D)\,p \\ AA\emptyset, \emptyset AA &\to AAA && \text{with rate} \quad (1-D)(1-p)/2 \end{aligned} \tag{38}$$

$$\begin{aligned} A\emptyset\emptyset &\to \emptyset A\emptyset && \text{with rate} \quad D \\ A\emptyset A &\to \emptyset AA && \text{with rate} \quad Dr \\ A\emptyset A &\to \emptyset\emptyset\emptyset && \text{with rate} \quad D(1-r) \end{aligned} \tag{39}$$

which allows one to interpolate between the DP fixed point at $r = 0$ and the critical behaviour of the PCPD at $r = 1$. In this model the branching probability depends on whether a collision is caused by a previous branching process or by diffusion. In addition, one restricts the calculation of averages to the sector where at least one pair (rather than two isolated particles) is present, in analogy with [49]. Since $r = 1$ in this model is not a special point, one may hope that corrections to scaling are more easy to control for $0 < r < 1$ and that the results could be extended to $r = 1$ at the end.

Dynamic and static exponents are found from simulations at several values of r and some of the results of [47] are listed in table 6. As a consistency check, the exponent values are used to test the hyperscaling relation equation (7) and full agreement is observed.

Comparison with table 3 shows that for $r = 0$, these results are in excellent agreement with the DP values while for $r = 1$, they fall within the range of values of the PCPD determined with different methods. In contrast to the limit $D \to 0$, where the exponents change abruptly, the exponents seem to vary smoothly when r is taken to zero. Based on these numerical observations Noh and Park [47] conclude that the transition in the PCPD may correspond to a line of fixed points with continuously varying exponents. As a possible explanation they suggest considering the long-term memory imposed by solitary diffusing particles as a marginal perturbation of the underlying field theory.

5.3. Parity-conserving PCPD

As the PC class compared to DP exemplifies that an additional parity-conservation law may change the universality class of an absorbing phase transition the question arises whether the

same happens in binary spreading processes. To answer this question in the context of the PCPD parity-conserving process

$$2A \to 4A \qquad 2A \to \emptyset \tag{40}$$

was studied [42]. Surprisingly it turns out that parity conservation does not change the nature of the phase transition, i.e., one observes the same phenomenological behaviour as in the PCPD with comparable effective critical exponents $\delta \simeq 0.23(1)$ and $z = 1.80(5)$.

To understand this observation, we note that there is another well-known example where parity conservation is irrelevant, namely, the annihilation process $2A \to 0$ as compared to the coagulation process $2A \to A$, which are known to belong to the same universality class. This is due to the fact that the even sector and the odd sector in the parity-conserving process $2A \to 0$ are essentially equivalent since in both of them the particle density decays algebraically until the system is trapped in an absorbing state (namely, the empty lattice or a state with a single diffusing particle). The present model is similar in so far as both sectors have an absorbing state. In contrast, in the PC class only one of the sectors has an absorbing state, leading the authors of [42] to the conclusion that parity conservation changes universality whenever one of the two sectors has no absorbing state.

5.4. Multicomponent binary spreading processes

In order to search for further possible generalizations, Ódor [46] investigated different variants of binary production–annihilation processes with several species of particles, in particular the reaction–diffusion processes

$$\begin{array}{lllll} \text{(a)} & AB \to ABA & 2A \to \emptyset & BA \to BAB & 2B \to \emptyset \\ \text{(b)} & 2A \to 2AB & 2A \to \emptyset & 2B \to 2BA & 2B \to \emptyset. \end{array}$$

Process (a) seems to exhibit the same type of critical behaviour as the PCPD, while in process (b) the phase transition takes place at zero branching rate, where the exponents are different, e.g. $\beta = 2$. However, it would be misleading to conclude that process (b) indeed represented a different universality class, rather the model is designed in such a way that the non-trivial transition, which possibly belongs to the same class as the PCPD, is shifted to an inaccessible region of the parameter space. Detecting a transition at zero branching rate does not necessarily mean that all realizations of the same reaction–diffusion scheme will yield such a trivial transition.

5.5. Roughening transition driven by the PCPD

As demonstrated in [76] the PCPD may also play a role in a special class of models for interface growth which exhibit a roughening transition. The idea follows an earlier work by Alon *et al* [86, 87], where a deposition–evaporation model with a DP-related roughening transition was introduced. Later it was shown that by depositing dimers instead of monomers one obtains a different type of roughening transition which is related to the PC class [88, 89].

As a key property of all these models, desorption is only allowed at the *edges* but not from the middle of deposited plateaux. Therefore the actual bottom layer of the interface, once it has been completed, cannot evaporate again which leads effectively to an absorbing phase transition at the bottom layer. Using this interpretation the pinned phase, where the interface is smooth, corresponds to the active phase of the underlying spreading process. However, if the growth rate is increased above a certain critical threshold the interface eventually detaches, meaning that the bottom layer enters an 'absorbing' state.

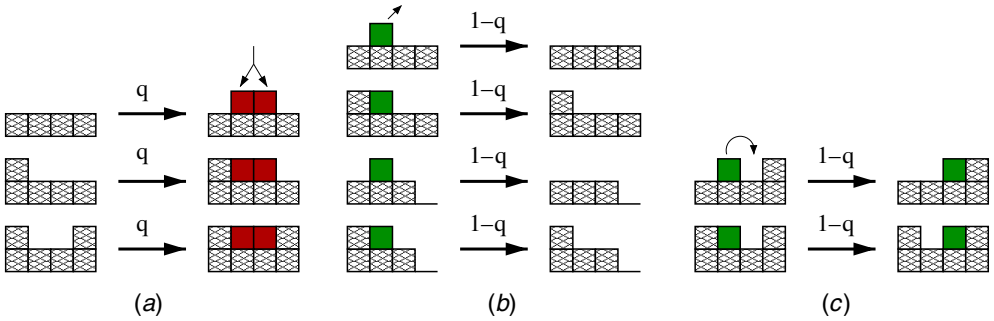

Figure 10. Dynamic rules of the PCPD-driven growth process: (*a*) deposition of a dimer at the sites i and $i + 1$. (*b*) Evaporation of a monomer from the right edge of a terrace at site i. (*c*) Hopping of a monomer between two adjacent islands, moving the hole between the islands in the opposite direction. In all cases the spatially reflected rules (not shown here) have to be included as well.

In order to study a PCPD-driven roughening transition one has to introduce appropriate dynamic rules that mimic a binary spreading process at the bottom layer. These rules involve three different physical processes, namely, deposition of dimers, surface diffusion and evaporation of diffusing monomers (see figure 10). The dimers are deposited horizontally on pairs of sites at equal height, leading to the formation of islands. These islands are stable in the interior but unstable at the edges, where monomers are released at a certain rate. The released monomers diffuse on the surface until they either attach to another island or evaporate back into the gas phase. In the limit of a very high evaporation rate a released monomer is most likely to evaporate unless it immediately attaches to an *adjacent* island at the next site, effectively moving the hole between the two islands in the opposite direction.

In order to explain how the growth model is related to the PCPD, let us consider the dynamic processes at the bottom layer (the spontaneously selected lowest height level of the interface). Interpreting sites at the bottom layer as particles A of a spreading process, the dynamic rules listed in figure 10 can be associated with certain reactions of the particles. For example, the deposition of a dimer corresponds to pairwise annihilation $2A \to \emptyset$, while evaporation of a monomer can be viewed as the creation of a particle A. However, in the present model atoms can only evaporate at the edge of a terrace followed by two bottom layer sites, hence rule (*b*) in figure 10 has to be interpreted as a fission process $2A \to 3A$. Otherwise, if there is only one such bottom layer site next to the edge, rule (*c*) applies which corresponds to a random walk of a single particle A. Thus the processes at the bottom layer resemble the dynamic rules of the PCPD. Clearly, this correspondence is not rigorous, especially because of second-layer nucleations. However, as in the case of DP- and PC-related growth models, the correspondence is expected to be valid asymptotically.

In the case of DP-related growth processes, the behaviour at the first few layers above the bottom layer can be described by a unidirectionally coupled hierarchy of DP processes [90]. Similarly the dynamics at higher levels in the growth process in figure 10 is expected to be related by a unidirectionally coupled sequence of PCPDs, which has not been investigated so far.

6. Field-theoretic approaches

Since the numerical simulations as a whole remain inconclusive, it is important to find and analyse a suitable field theory that describes the phase transition in the PCPD. So far there

are two important contributions in this direction. Some time ago Howard and Täuber [31] proposed a field theory for the unrestricted PCPD, while recent attempts to devise a field theory for the restricted case turned out to be unsuccessful [91]. Moreover, in a recent paper the pair correlation function in the unrestricted PCPD has been derived exactly by Paessens and Schütz [53], leading to non-trivial and surprising results. The purpose of this section is to summarize the present state of knowledge.

6.1. Field theory of the unrestricted case

Consider the unrestricted PCPD which is defined by the reaction–diffusion scheme

$$2A \xrightarrow{\mu} \emptyset \qquad 2A \xrightarrow{\nu} A \qquad 2A \xrightarrow{\sigma} 3A \tag{41}$$

where μ, ν and σ are the rates for annihilation, coagulation and fission, respectively. In the continuum limit (see e.g. [92]) the classical master equation of this process corresponds to the field-theoretic action

$$S = \int \mathrm{d}^d \boldsymbol{x} \int \mathrm{d}t [\hat{\phi}(\partial_t - D\nabla^2)\phi - \mu(1-\hat{\phi}^2)\phi^2 - \nu(1-\hat{\phi})\hat{\phi}\phi^2 + \sigma(1-\hat{\phi})\hat{\phi}^2\phi^2] \tag{42}$$

where D is the diffusion rate while $\hat{\phi}(x,t)$ and $\phi(x,t)$ can be thought of as particle creation and annihilation operators. Shifting the response field by $\hat{\phi} = 1 + \bar{\phi}$ the action can also be written as

$$S = \int \mathrm{d}^d \boldsymbol{x} \int \mathrm{d}t [\bar{\phi}(\partial_t - D\nabla^2)\phi + (2\mu + \nu - \sigma)\bar{\phi}\phi^2 + (\mu + \nu - 2\sigma)\bar{\phi}^2\phi^2 - \sigma\bar{\phi}^3\phi^2]. \tag{43}$$

Since higher order terms will be generated under renormalization group (RG) transformations, it is convenient to write the action in the general form

$$S = \int \mathrm{d}^d \boldsymbol{x} \int \mathrm{d}t \left[\bar{\phi}(\partial_t - D\nabla^2)\phi + \sum_{p=1}^{\infty}\sum_{q=2}^{\infty} \Lambda_{p,q}\bar{\phi}^p\phi^q \right] \tag{44}$$

taking all possible reactions into account which are at least binary, i.e. quadratic in ϕ. In this notation the bare coupling constants of the unrestricted PCPD are given by

$$\Lambda_{1,2} = 2\mu + \nu - \sigma \qquad \Lambda_{2,2} = \mu + \nu - 2\sigma \qquad \Lambda_{3,2} = -\sigma \tag{45}$$

while all other *bare* coupling constants (but not necessarily the renormalized ones) vanish. Regarding the first two terms $\bar{\phi}\phi^2$ and $\bar{\phi}^2\phi^2$ a simple power-counting analysis yields the upper critical dimension

$$d_\mathrm{c} = 2 \tag{46}$$

at which the dynamical critical exponent $z = 2$. In the annihilation phase, the coupling constants and the fields carry the dimensions

$$[\Lambda_{p,q}] = \kappa^{2-(q-1)d} \qquad [\phi] = \kappa^d \qquad [\bar{\phi}] = 1 \tag{47}$$

where κ denotes an arbitrary momentum scale. Hence for given q all contributions with p running from 1 to ∞ are *equally relevant* and the usual renormalization group scheme in terms of a finite series of Feynman diagrams cannot be applied. At the critical point, however, the dimensions of the fields are given by $[\phi] = [\bar{\phi}] = \kappa^{d/2}$ [93].

In [31] the field theory was found to be non-renormalizable so that no quantitative information on critical exponents can be obtained. Nevertheless it is possible to compute the critical point of the unrestricted PCPD exactly. To this end we note that the transition expressed in bare parameters takes place at $2\mu + \nu = \sigma$, where the cubic term $\bar{\phi}\phi^2$ in the

shifted action vanishes [31]. Since there is no way to generate this contribution under RG transformations to *all* orders, fluctuation effects do not influence the location of the transition, hence

$$2\mu + \nu = \sigma \tag{48}$$

determines the critical line to all orders of perturbation theory. In the inactive phase $2\mu + \nu < \sigma$ annihilation and/or coagulation eventually dominate, leading to an asymptotic decay as $t^{-d/2}$ for $d < 2$, while in the supercritical regime $2\mu + \nu > \sigma$ the particle density grows rapidly and diverges within finite time. Consequently, there is no stationary state in the supercritical regime.

6.2. Attempts towards a field theory of the restricted PCPD

Recently van Wijland, Täuber and Deloubrière proposed and studied a field theory for the restricted case. Their results, however, turned out to be unphysical [91], suggesting that a different field-theoretic approach is needed.

The starting point of the theory of Wijland *et al* was to extend the field-theoretic action (42) by an additional mechanism which prevents the field ϕ from diverging in the supercritical regime. This mechanism may be implemented as a soft constraint by adding a reaction of the form $3A \to pA$ with $p \leqslant 2$. For example, the reaction $3A \xrightarrow{\tau} \emptyset$ would lead to an additional contribution $-\tau(1 - \hat{\phi}^3)\phi^3$ in the action (42), corresponding to the bare coupling constants

$$\Lambda_{1,3} = 3\tau \qquad \Lambda_{2,3} = 3\tau \qquad \Lambda_{3,3} = \tau. \tag{49}$$

Alternatively, the restriction may be incorporated directly in the field-theoretic action by inserting exponential damping factors, whose purpose is to 'switch off' the reactions when a certain particle density is exceeded [94]. To this end each reaction term is multiplied by an exponential function $\exp(-nv\hat{\phi}\phi)$, where $n = \max(p, q)$ is the maximal number of particles involved in the respective reaction and v is an additional coupling constant. When applied to the PCPD, one is led to the unshifted action

$$S = \int \mathrm{d}^d x \int \mathrm{d}t [\hat{\phi}(\partial_t - D\nabla^2)\phi - \mu(1 - \hat{\phi}^2)\phi^2 \,\mathrm{e}^{-2v\hat{\phi}\phi} - \nu(1 - \hat{\phi})\hat{\phi}\phi^2 \,\mathrm{e}^{-2v\hat{\phi}\phi} + \sigma(1 - \hat{\phi})\hat{\phi}^2\phi^2 \,\mathrm{e}^{-3v\hat{\phi}\phi}]. \tag{50}$$

Roughly speaking, the constant v determines the field amplitude needed to declare a location in spacetime (representing a site) as occupied. Since the argument of the exponential function has to be dimensionless and $[\hat{\phi}\phi] = \kappa^d$ the coupling constant v is irrelevant, allowing the exponential functions to be expanded. To first order in v this gives rise to the additional nonzero bare coupling constants

$$\begin{aligned} \Lambda_{1,3} &= v(3\sigma - 4\mu - 2\nu) \\ \Lambda_{2,3} &= v(9\sigma - 6\mu - 4\nu) \\ \Lambda_{3,3} &= v(9\sigma - 2\mu - 2\nu) \\ \Lambda_{4,3} &= 3\sigma v \end{aligned}$$

while higher order contributions lead to additional non-vanishing bare coupling constants of the form $\Lambda_{p,q} \propto v^{q-2}$.

In the inactive phase all terms of the leading series $\Lambda_{p,2}$ are marginal and thus have to be retained while all terms of higher order are irrelevant. In order to handle the series of marginal contributions, Wijland *et al* studied the corresponding generating function $G(x) = \sum_{p=1}^{\infty} \Lambda_{p,2}\phi^2\bar{\phi}^p$, recasting the flow equations of all coupling constants $\Lambda_{p,2}$ into

a single functional renormalization group equation for the renormalized counterpart of G. Alternatively, one may work at the critical point, where the naive field dimensions of ϕ and $\bar{\phi}$ are equal, leading to a renormalizable field theory [93]. Although a fixed point was shown to exist, it turned out to be unreachable from any physically meaningful initial condition. In addition, the fixed point itself is characterized by a negative variance of the order parameter fluctuations, which would have been unphysical as well. Finally, the critical exponents, in particular the exact result $z = 2$, would have been incompatible with the existing numerical estimates which clearly indicate that $z < 2$.

The failure suggests that a field-theoretic action in terms of a *single* coarse grained field ϕ (and its associated response field $\bar{\phi}$) may be incapable of describing the properties of the restricted PCPD. In fact, a single field for the density of particles may fail to describe the complex spatio-temporal interplay of particles and pairs, questioning the validity of the continuum limit on which equation (50) is based. Instead it may be more promising to devise a field theory based on two different fields for single particles and pairs, separating the two dynamical modes in a similar way as in the cyclically coupled models of section 5.1. However, a consistent formulation of such a field theory is not yet known.

6.3. On the impossibility of a Langevin equation for the PCPD

Langevin equations are very popular in non-equilibrium statistical physics because of their intuitive simplicity and their enormous success in well-known systems such as DP. Therefore it has become customary to deal with phenomenological or even guessed Langevin equations even when a rigorous derivation is not available. For example, in the context of the PCPD several authors [31, 51, 55, 95] have been discussing a Langevin equation of the form

$$\frac{\partial}{\partial t}\rho(\boldsymbol{x},t) = (\sigma - 2\mu)\rho^2(\boldsymbol{x},t) - c\rho^3(\boldsymbol{x},t) + D\nabla^2\rho(\boldsymbol{x},t) + \rho(\boldsymbol{x},t)\xi(\boldsymbol{x},t) \tag{51}$$

where $\xi(\boldsymbol{x},t)$ is a white Gaussian noise with zero mean and the correlations

$$\langle \xi(\boldsymbol{x},t)\xi(\boldsymbol{x}',t')\rangle = (4\sigma - 2\mu)\delta^{(d)}(\boldsymbol{x}-\boldsymbol{x}')\delta(t-t'). \tag{52}$$

This Langevin equation, if indeed realized, would be particularly appealing since it can be related to the problem of non-equilibrium wetting [55]. However, as a mesoscopic description a Langevin equation assumes that all features of the process, in particular all particle–particle correlations, could be captured in terms of a single coarse-grained particle density. This works only in few cases (e.g. in DP), but not in the case of the PCPD, where anticorrelations produced by the annihilation/coagulation process play an important role.

In this context it is useful to recall that a Langevin equation can be derived from the field-theoretic action by transforming the terms of the form $\bar{\phi}^2\phi^q$ into a noise and computing the functional derivative with respect to the response field $\bar{\phi}$. This procedure requires that terms involving cubic or higher order powers of the response field are fully irrelevant. However, in the case of the PCPD cubic terms of the form $\bar{\phi}^3\phi^q$ have to be retained in the action. Therefore, any attempt to describe the PCPD by a Langevin equation misses the physics of these terms and thus should lead to wrong results. In addition, one would have to add an additional term $\xi_D(\boldsymbol{x},t)$ on the rhs of the Langevin equation accounting for diffusive noise with the correlations

$$\langle \xi_D(\boldsymbol{x},t)\xi_D(\boldsymbol{x}',t')\rangle = -D\rho(\boldsymbol{x},t)\nabla^2\delta^{(d)}(\boldsymbol{x}-\boldsymbol{x}')\delta(t-t') \tag{53}$$

which is expected to play an important role in the PCPD. However, it is at present not clear what consequences the inclusion of such an additional term would have [93].

6.4. Pair correlation functions in the unrestricted PCPD at criticality

A different approach has been followed by Paessens and Schütz [53] and leads to a non-trivial, unexpected result. They consider the *unrestricted* version of a generalized PCPD with the reactions

$$\begin{array}{lll} mA \to (m+k)A & \text{with rate} & \nu \\ pA \to (p-l)A & \text{with rate} & \mu \\ A\emptyset \leftrightarrow \emptyset A & \text{with rate} & D. \end{array} \tag{54}$$

Models of this kind may be thought of as realizing a bosonic field theory such as in [31] and are specified by four integers (m, p, k, l) and three rates ν, μ and D. Paessens and Schütz start from the master equation (19) and rewrite the quantum Hamiltonian H in terms of spacetime-dependent creation and annihilation operators $a^\dagger(\boldsymbol{x}, t)$ and $a(\boldsymbol{x}, t)$ such that the particle operator $n(\boldsymbol{x}, t) = a^\dagger(\boldsymbol{x}, t)a(\boldsymbol{x}, t)$. In what follows, the averages

$$\langle n(\boldsymbol{x}, t)\rangle = \langle a(\boldsymbol{x}, t)\rangle \qquad \langle n(\boldsymbol{x}, t)^2\rangle = \langle a(\boldsymbol{x}, t)^2\rangle + \langle a(\boldsymbol{x}, t)\rangle \tag{55}$$

will be considered. Specializing to the case $m = p$, the critical line between the absorbing phase and the active phase (with an infinite particle density) is located at $\mu_c = \nu k/l$. For $\mu = \mu_c$, the spatially averaged particle density $|\Omega|^{-1}\int_\Omega \mathrm{d}\boldsymbol{x}\langle a(\boldsymbol{x}, t)\rangle = \rho_0$ is a constant, where Ω is a spatial domain with volume $|\Omega|$. Remarkably, it turns out that at criticality and for $m = p$, the system of equations of motion for the variables $\{\langle a(\boldsymbol{x}, t)\rangle, \langle a(\boldsymbol{x}, t)a(\boldsymbol{y}, t)\rangle\}$ closes if either $m = 1$ or $m = 2$ [53].

The case $m = 1$ is a 'bosonic' version of the ordinary contact process and has been considered as a model for biological clustering [63, 96]. It can be shown that the fluctuations $\langle a(\boldsymbol{x}, t)^2\rangle$ of the particle density diverge for $t \to \infty$ in dimensions $d \leqslant 2$, while they remain finite for $d > 2$ [53, 63].

The PCPD is described by the case $m = 2$. After a time rescaling $t \mapsto t/(2D)$, and assuming translation-invariant initial conditions, consider the pair correlator

$$F(\boldsymbol{r}, t) := \langle a(\boldsymbol{x}, t)a(\boldsymbol{x} + \boldsymbol{r}, t)\rangle \tag{56}$$

(which is independent of $\boldsymbol{x}$) and the reduced coupling

$$\alpha := \frac{\nu}{D}\frac{k(k+l)}{2}. \tag{57}$$

Then, under the stated conditions, the following equation holds on a hypercubic lattice:

$$\frac{\partial}{\partial t}F(\boldsymbol{r}, t) = \sum_{i=1}^{d}[F(\boldsymbol{r} - \boldsymbol{e}_i, t) + F(\boldsymbol{r} + \boldsymbol{e}_i, t) - 2F(\boldsymbol{r}, t)] + \delta_{r,\boldsymbol{0}}\,\alpha F(\boldsymbol{0}, t) \tag{58}$$

where $\boldsymbol{e}_i$ is the unit vector in the ith direction. If as initial condition one takes a Poisson distribution $F(\boldsymbol{r}, 0) = \rho_0^2$, one obtains the following Volterra integral equation:

$$F(\boldsymbol{r}, t) = \rho_0^2 + \alpha\int_0^t \mathrm{d}\tau\, b(\boldsymbol{r}, t - \tau)F(\boldsymbol{0}, \tau) \tag{59}$$

$$b(\boldsymbol{r}, t) = \mathrm{e}^{-2dt}I_{r_1}(2t)\cdots I_{r_d}(2t) \tag{60}$$

where I_r is a modified Bessel function of order r. For $\boldsymbol{r} = \boldsymbol{0}$, the same equation describes the kinetics of the mean spherical model (see [97–99]), but it is not yet clear if there is a deeper reason for this relationship or whether it merely occurs by accident. The exact solution leads to the following long-time behaviour, at $\mu = \mu_c$ [53]:

$$F(\boldsymbol{0}, t) \sim \begin{cases} \exp(t/\tau) & \text{if} \quad \alpha > \alpha_c \\ t^\nu & \text{if} \quad \alpha = \alpha_c \\ F_\infty & \text{if} \quad \alpha < \alpha_c \end{cases} \tag{61}$$

where α_c is a known critical value such that $\alpha_c = 0$ for $d \leqslant 2$ but it is finite for $d > 2$, in addition $\tau = C_d \left(\frac{\alpha-\alpha_c}{\alpha}\right)^{-1/\nu}$, the exponent $\nu = d/2 - 1$ for $2 < d < 4$ and $\nu = 1$ for $d > 4$, $F_\infty = \rho_0^2(1 - \alpha/\alpha_c)^{-1}$ and C_d is a known constant. As can be seen the two-point correlator diverges for large times if the reduced rate α is large enough. This result can be generalized to yield $F(\boldsymbol{r}, t)$ exactly, with a similar conclusion. In particular, one obtains the dynamical exponent $z = 2$ [53].

Since α measures the relative importance between the reaction and the diffusion rates, the result (61) means that for $d > 2$ at high values of D the distribution of the particle density along the critical line is relatively smooth and changes through a 'clustering transition' (which occurs at a tricritical point) to a rough distribution for small values of D. This transition manifests itself in the variance $\sigma(t)^2 := \langle n(\boldsymbol{x}, t)^2\rangle - \langle n(\boldsymbol{x}, t)\rangle^2$ and not in the mean density $\langle n(\boldsymbol{x}, t)\rangle$ which is purely diffusive and has a constant average. A convenient order parameter of the clustering transition is F_∞^{-1} [53]. On the other hand, for $d \leqslant 2$ there is a single transition along the critical line.

These exact results for the bosonic PCPD [53] surprisingly agree with the conclusions of pair mean-field theory and with the numerical results of [39] which suggested the presence of two distinct transitions along the critical line. That scenario had, in the light of more recent simulations in 1D, somewhat fallen into disfavour, see section 3. In fact, in hindsight one observes that the existing cluster approximations of the PCPD all explicitly restrict to clusters of a linear shape. At the level of the pair approximation, at most two-site clusters need be considered and there is no qualitative difference between one and several space dimensions. On the other hand, beginning with the triplet approximation, the geometrical shape of the clusters also becomes important and one will have to distinguish between linear clusters such as $\bullet\circ\bullet$ or $\bullet\bullet\bullet\circ$ (in 1D *only* such clusters occur) and nonlinear ones as $\begin{smallmatrix}\bullet\\ \circ\bullet\end{smallmatrix}$ or $\begin{smallmatrix}\bullet\bullet\\ \bullet\circ\end{smallmatrix}$ which are meant to indicate more complicated geometrical forms as they will only occur for $d \geqslant 2$. Indeed, truly three-dimensional clusters arise for the first time in the quartet approximation ($N = 4$). The triplet and higher approximations of the form as discussed in section 3 only take *linear* clusters into account and should hence be expected to be more adapted to a truly one-dimensional system than the pair approximation. Then a single transition along the critical line should be expected for the $N \geqslant 3$ approximation while the different result of the pair approximation might be related to the existence of two transitions for $d > 2$.

It would be very interesting to see whether two transitions exist along the critical line for the restricted PCPD in $d \geqslant 3$ dimensions. The interaction terms in existing field-theory studies might be too close to the site approximation to be able to see this and a study based on the master equation is called for.

7. Possible generalizations

7.1. Higher order processes

As shown in the preceding sections, the unusual critical behaviour of the PCPD is related to the fact that only *pairs* of particles can react while individual particles form a diffusing background. Therefore, as an obvious generalization, it is near at hand to study higher order processes such as

$$nA \to (n+1)A \qquad nA \to \emptyset \qquad (n \geqslant 3). \tag{62}$$

Table 7. Estimates for the critical exponents of the 1D triplet process TCPD.

References	δ	z	β	$\nu_\parallel$
Park *et al* [95]	0.32(1)	1.75(10)	–	2.5(2)
Kockelkoren and Chaté [51]	0.27(1)	1.8(1)	0.90(5)	–
Ódor [45]	0.33(1)	–	0.95(5)	–

Without diffusion, the number of absorbing steady states increases exponentially with the lattice size L. For example, for the triplet process ($n = 3$) and in one dimension, we find

$$N_{\text{stat}}(L) \simeq N_0 g^L \qquad N_0 = \begin{cases} 1 & \text{periodic b.c.} \\ 1.137\ldots & \text{free b.c.} \end{cases} \tag{63}$$

absorbing steady states, where $g \simeq 1.839\ldots$ (see appendix A). On the other hand, with single-particle diffusion, only n absorbing steady states remain.

The central question is whether such a system still exhibits a non-trivial phase transition. As a first naive approach, the simple mean-field equation

$$\frac{\partial}{\partial t}\rho(\boldsymbol{x}, t) = b\rho^n(\boldsymbol{x}, t) - c\rho^{n+1}(\boldsymbol{x}, t) + D\nabla^2\rho(\boldsymbol{x}, t) \tag{64}$$

predicts the mean-field exponents

$$\beta^{MF} = 1 \qquad {\nu_\perp}^{MF} = n/2 \qquad {\nu_\parallel}^{MF} = n \tag{65}$$

in sufficiently high space dimensions, including DP ($n = 1$) and the PCPD ($n = 2$) as special cases. The question posed here is whether the higher order processes, in particular the diffusive triplet-contact process (TCPD) with $n = 3$, still displays non-trivial critical behaviour in one spatial dimension.

The TCPD was introduced in [95], where numerical simulations seemed to indicate possible non-trivial behaviour at the transition. This point of view was confirmed by Kockelkoren and Chaté [51], who established the 1D TCPD as an independent universality class and with an upper critical dimension $d_c = 1$. However, Ódor [100] questioned this claim by showing that the simulation results are compatible with mean-field exponents combined with appropriate logarithmic corrections (see table 7).

Even more confusing are the findings for the quadruplet contact process $n = 4$. In [51] the expected mean-field exponents are obtained while Ódor finds numerical evidence for the presence of fluctuation effects [100]. The origin of these discrepancies is not yet understood. However, while comparing the results one should keep in mind that the model used by Kockelkoren and Chaté is particularly suitable to simulate higher order processes. In their model the reactions are local for any n, while in models with hard-core exclusion extended strings of n particles have to line up before they can react.

7.2. Towards a general classification scheme

Extending these studies Kockelkoren and Chaté [51] suggested that transitions in a reaction–diffusion process of the form

$$mA \to (m + k)A \qquad nA \to (n - l)A \tag{66}$$

can be categorized according the orders m, n of creation and removal, while the numbers k and l determine additional symmetries such as parity conservation. In terms of m, n, they propose the general classification scheme shown in table 8. In addition they investigate the

Table 8. General classification scheme of absorbing phase transitions in the 1D models (66) as proposed by Kockelkoren and Chaté [51] and modified after [102].

	n			
m	1	2	3	4
1	DP	DP/PC	DP	DP
2	DP	PCPD	PCPD	PCPD
3	DP	DP	TCPD	TCPD
4	DP	DP	DP	?

rôle of parity conservation in more detail, finding that such a symmetry does *not* alter the universality class whenever *every* sector includes an absorbing state. This conjecture is in agreement with the observation of [42] that an additional parity conservation does not change the critical behaviour of the PCPD (see [101] for recent evidence of a PCPD transition in the diffusive $2A \to 3A, 4A \to \emptyset$ system, where $m = 2, n = 4$).

8. Summary and outlook

In spite of intensive and prolonged efforts, the critical behaviour of the one-dimensional PCPD is not yet understood. It is surprising to see that the field-theoretical and numerical methods used to study the PCPD transition have led to such wildly different conclusions as listed in section 1. It appears that almost the only piece of information for which different methods obtain the same result is the location $p_c(D)$ of the critical point (if applicable at all). This continuing discrepancy is all the more astonishing because the same techniques yield nicely consistent results when applied to models in the DP or PC universality classes. By itself, this observation is a clear indication of a subtlety in the behaviour of the PCPD which is not present in those other models.

Specifically, at present there seems to be some majority opinion, based on numerical work, in favour of a single new universality class along the critical line and characterized by critical exponent values of the order

$$\delta \approx 0.2 \qquad z \approx 1.7-1.8 < 2 \qquad \eta \approx 0.5 \qquad \beta/\nu_\perp \approx 0.5. \tag{67}$$

On the other hand, a recent analytical study [53] of the bosonic field theory finds a dynamical exponent $z = 2$ and a single universality class along the critical line, at least in one dimension. Their value of $z = 2$ clearly is in disagreement with the numerical results from fermionic models. At the time of writing, it is not clear how this should be explained.

Besides the majority opinion, several alternative scenarios have been proposed. These include the possibility of more than one transition along the critical line (which is known to be exact for the unrestricted bosonic version in $d > 2$ dimensions), continuously varying exponents and even the cross-over to directed percolation after very long times. The last possibility would mean that the diffusive background of solitary particles would become irrelevant in the limit $t \to \infty$ which goes against the current understanding of bosonic field theory.

All in all, we are not (yet) able to decide between the several scenarios proposed. Pending further insight, the reader might find some comfort in a quotation of 'Thales'

> Sei ruhig – es war nur gedacht. *J W Goethe, Faust II (1830)*

or alternatively with

> It were not best that we should all think alike; it is the difference of opinion which makes horseraces. *M Twain, Pudd'nhead Wilson (1894)*

We look forward to future insightful studies shedding more light on the so simple-looking PCPD.

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Appendix A. The absorbing states in the pair-contact process

Consider the 1D pair-contact process on a lattice with L sites. We derive the number of absorbing steady states $N_{\rm stat}(L)$ given in equation (1), following [19]. The main ingredient is that any state which only contains isolated particles is an absorbing steady state.

First, we consider free boundary conditions. Obviously, $N_{\rm stat}(1) = 2$ and $N_{\rm stat}(2) = 3$. Now fix the leftmost site. If it is occupied, its neighbour must be empty in order to obtain a steady state and it remains to consider an open chain of $L - 2$ sites. On the other hand, if the leftmost site is empty, one considers the remaining open chain of $L - 1$ sites. We thus have the recursion

$$N_{\rm stat}(L) = N_{\rm stat}(L-2) + N_{\rm stat}(L-1). \tag{A.1}$$

Because of the initial conditions,

$$N_{\rm stat}(L) = F_{L+1} = \frac{g_+^{L+2} - g_-^{L+2}}{g_+ - g_-} \tag{A.2}$$

is the $(L+1)$th Fibonacci number, where $g_\pm = (1 \pm \sqrt{5})/2$.

On the other hand, for periodic boundary conditions, we fix one of the sites. If that site is occupied, both its left and right nearest neighbours must be empty and we are left with an *open* chain of $L - 3$ sites. But if that site is empty, we are left with an open chain of $L - 1$ sites. Therefore

$$N_{\rm stat}^{\rm (per)}(L) = N_{\rm stat}(L-3) + N_{\rm stat}(L-1) = g_+^L + g_-^L. \tag{A.3}$$

From these results we recover (1) for L sufficiently large.

In general, $N_{\rm stat}(L)$ is found from its generating function $\mathcal{G}(z) = \sum_{L=0}^{\infty} N_{\rm stat}(L) z^L$. For the kind of application at hand, $\mathcal{G}(z) = z(2+z)/(1-z-z^2)$ is a simple rational function of z and its coefficients can be obtained in a closed form as follows.

Lemma. *Let $P(z)$ and $Q(z)$ be polynomials of orders p and q, respectively and let $p < q$. If one has in addition $Q(z) = q_0(1 - z\rho_1)\cdots(1 - z\rho_q)$ such that the ρ_i are pairwise distinct for $i = 1, \ldots, q$ and q_0 is a constant, then*

$$f(z) = \frac{P(z)}{Q(z)} = \sum_{n=0}^{\infty} f_n z^n \qquad f_n = -\sum_{j=1}^{q} \frac{\rho_j^{n+1} P(1/\rho_j)}{Q'(1/\rho_j)}. \tag{A.4}$$

In [103] this is proved in an elementary way, here we give a function-theory proof which easily generalizes to the case when $Q(z)$ has multiple zeros. We have

$$f_n = \frac{1}{n!} f^{(n)}(0) = \frac{1}{2\pi \mathrm{i}} \oint_{\mathcal{C}} \mathrm{d}w \frac{f(w)}{w^{n+1}} = \frac{1}{2\pi \mathrm{i}} \oint_{\mathcal{C}'} \mathrm{d}u \frac{u^n P(1/u)}{u Q(1/u)}$$

where we have set $u = 1/w$. The contour $\mathcal{C}$ is a circle around the origin with a radius smaller than the convergence radius of $f(z)$ and $\mathcal{C}'$ encloses all the points ρ_j, $j = 1, \ldots, q$. Since $p < q$, there is no singularity at $u = 0$ and the only singularities of $u^{-1} f(1/u)$ are the simple poles located at $u = \rho_j$. If we concentrate on the singularity at $u = \rho_1$, we have $uQ(1/u) = (u - \rho_1) q_0 \prod_{j=2}^{q} (1 - \rho_j/u)$ such that the product is regular at $u = \rho_1$. On the other hand, the derivative $Q'(1/\rho_1) = -\rho_1 q_0 \prod_{j=2}^{q} \left(1 - \rho_j/\rho_1\right)$. Therefore, close to $u \simeq \rho_1$, we have

$$uQ(1/u) \simeq -(u - \rho_1) \frac{Q'(1/\rho_1)}{\rho_1}.$$

From the residue theorem and summing over all simple poles of $f(z)$ the assertion follows.

Other processes can be treated similarly. As an example, consider the triplet-contact process without diffusion as introduced in section 7.1. Absorbing states are those without any triplet of neighbouring occupied sites. On a 1D lattice with free boundary conditions and L sites, we have the recursion

$$N_{\mathrm{stat}}(L) = N_{\mathrm{stat}}(L-1) + N_{\mathrm{stat}}(L-2) + N_{\mathrm{stat}}(L-3) \tag{A.5}$$

together with the initial conditions $N_{\mathrm{stat}}(1) = 2$, $N_{\mathrm{stat}}(2) = 4$ and $N_{\mathrm{stat}}(3) = 7$. Therefore the generating function is $\mathcal{G}(z) = z(2 + 2z + z^2)/(1 - z - z^2 - z^3)$ and its coefficients are easily read off. For periodic boundary conditions, we find

$$N_{\mathrm{stat}}^{(\mathrm{per})}(L) = N_{\mathrm{stat}}(L-1) + N_{\mathrm{stat}}(L-3) + 2N_{\mathrm{stat}}(L-4). \tag{A.6}$$

For L sufficiently large, we thus arrive at equation (63).

Appendix B. On finite-size scaling techniques

In systems like the PCPD, where the critical line separates a non-critical ordered phase from a critical disordered phase, the analysis of finite-size data needs some modifications with respect to the usual situation, where both the ordered and the disordered phases are non-critical. To be specific, we shall discuss here the finite-size scaling of the lowest gap Γ of the quantum Hamiltonian H, see section 4, and following [19]. As usual, we begin with the finite-size scaling form

$$\Gamma_L(p) = L^{-z} f((p - p_{\mathrm{c}}) L^{1/\nu_\perp}) \tag{B.1}$$

where p is the control variable which measures the distance to the critical point p_{c} (the dependence on D is suppressed throughout) and f is assumed to be continuously differentiable. One expects the asymptotic behaviour, see equation (23)

$$\Gamma_L(p) \sim \begin{cases} \mathrm{e}^{\sigma L} & \text{if} \quad p < p_{\mathrm{c}} \\ L^{-2} & \text{if} \quad p > p_{\mathrm{c}} \end{cases} \tag{B.2}$$

where $\sigma = \sigma(p)$ is a constant. In the usual case, one would have instead $\Gamma_L(p) \sim \Gamma_\infty$ for $p > p_{\mathrm{c}}$. From (B.2), one finds for the scaling function

$$f(\mathfrak{z}) \sim \begin{cases} \exp(-A|\mathfrak{z}|^{\nu_\perp}) & \text{if} \quad \mathfrak{z} \to -\infty \\ \mathfrak{z}^{(z-2)\nu_\perp} & \text{if} \quad \mathfrak{z} \to +\infty \end{cases} \tag{B.3}$$

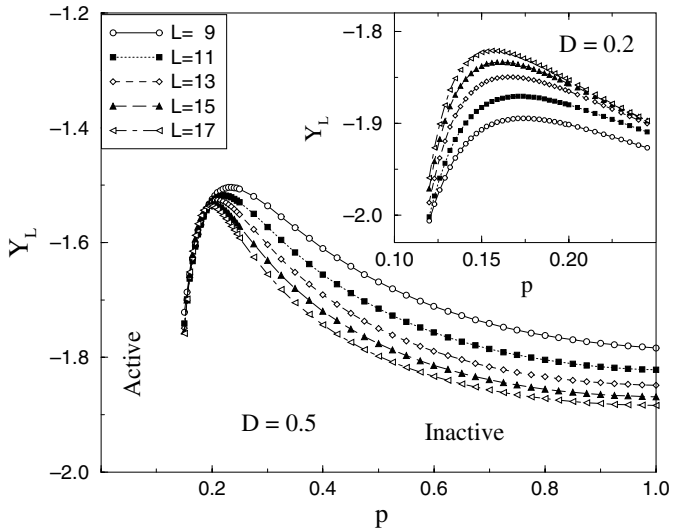

Figure 11. Plot of the function $Y_L(p)$ in the 1D PCPD as a function of p for several lattice sizes L and $D = 0.5$. The inset shows the case $D = 0.2$. After [19].

where A is a positive constant. Therefore, since $f(\mathfrak{z}) > 0$, it follows that for $z < 2$ the scaling function f must have a maximum at some finite value $\mathfrak{z}_{\max}$. Next, the logarithmic derivative (24) becomes

$$Y_L = -z + \frac{\ln[f(\mathfrak{z}_+)/f(\mathfrak{z}_-)]}{\ln[(L+1)/(L-1)]} \tag{B.4}$$

where $\mathfrak{z}_\pm = (p - p_c)(L \pm 1)^{1/\nu_\perp}$. Furthermore, it is easy to see that in the scaling limit $p \to p_c$ and $L \to \infty$ such that $\mathfrak{z} = (p - p_c)L^{1/\nu_\perp}$ is kept fixed, one has

$$\lim \frac{\mathrm{d}Y_L}{\mathrm{d}p} \simeq \begin{cases} L^{1/\nu_\perp} A(2-\nu_\perp)(-\mathfrak{z})^{\nu_\perp - 1} & \text{if} \quad \mathfrak{z} \to -\infty \\ L^{1/\nu_\perp}(z-2)\mathfrak{z}^{-1} & \text{if} \quad \mathfrak{z} \to +\infty. \end{cases} \tag{B.5}$$

Provided that $z < 2$ and $\nu_\perp < 2$, there *must* exist a finite $\mathfrak{z}^*$ such that $\mathrm{d}Y_L/\mathrm{d}p|_{\mathfrak{z}=\mathfrak{z}^*} = 0$. However, since

$$Y_L(\mathfrak{z}^*) = -z + \frac{1}{\nu_\perp}\frac{\mathfrak{z}^* f'(\mathfrak{z}^*)}{f(\mathfrak{z}^*)} \tag{B.6}$$

that maximum value of Y_L *cannot* be used to estimate the dynamical exponent z [19]. Rather, one has to form first a sequence of estimates p_L of the critical point p_c from the above extremum criterion which should converge according to $p_L \simeq p_c + \mathfrak{z}^* L^{-1/\nu_\perp}$. Having found p_c, estimates of z can finally be obtained from equation (25).

We finally point out that the habitual method of intersecting two curves $Y_L(p)$ and $Y_{L'}(p)$ for two lattice sizes L, L' does not work in general. For example, it is known for the 1D PCPD with free boundary conditions, that the curves $Y_L(p)$ do not intersect for different values of L [19]. We illustrate this in figure 11.

Appendix C. On universal amplitudes in non-equilibrium criticality

We recall the phenomenological scaling arguments about universal scaling amplitudes in non-equilibrium critical points and derive equations (33) and (34) for systems in the directed

percolation universality class, following [44]. We shall denote time by $r_\parallel$ and space by $r_\perp$. The distance from the steady-state critical point is measured by t, and h denotes an external field (e.g., for directed percolation $t = p - p_c$ and h is the rate of a process $\emptyset \to A$). We shall assume translation invariance throughout. The arguments involves tracing the non-universal metric factors, generalizing a similar by now classic line of thought for equilibrium systems [80]. This is most conveniently done in the bulk first before finally introducing lattices of finite extent.

Physical quantities of interest are the mean particle density ρ, the survival probability P and the pair connectedness function $G = G(r'_\perp, r'_\parallel; r_\perp, r_\parallel)$, which is defined as the probability that the sites $(r'_\perp, r'_\parallel)$ and $(r_\perp, r_\parallel)$ are connected by a direct path [1, 2]. Because of translation invariance $G = G(r'_\perp - r_\perp, r'_\parallel - r_\parallel)$. These quantities are expected to satisfy the scaling behaviour

$$\begin{aligned}
\rho(r_\perp, r_\parallel; t, h) &= b^{-x_\rho}\rho\left(\frac{r_\perp}{b}, \frac{r_\parallel}{b^z}; tb^{y_t}, hb^{y_h}\right) = D_{1\rho}\xi_\perp^{-x_\rho}\mathcal{E}^\pm\left(\frac{r_\perp}{\xi_\perp}, D_0\frac{r_\parallel}{\xi_\perp^z}; D_2 h|t|^{-y_h/y_t}\right)\\
P(r_\perp, r_\parallel; t, h) &= b^{-x_P}P\left(\frac{r_\perp}{b}, \frac{r_\parallel}{b^z}; tb^{y_t}, hb^{y_h}\right) = D_{1P}\xi_\perp^{-x_P}\mathcal{F}^\pm\left(\frac{r_\perp}{\xi_\perp}, D_0\frac{r_\parallel}{\xi_\perp^z}; D_2 h|t|^{-y_h/y_t}\right)\\
G(r_\perp, r_\parallel; t, h) &= b^{-x_G}G\left(\frac{r_\perp}{b}, \frac{r_\parallel}{b^z}; tb^{y_t}, hb^{y_h}\right) = D_{1G}\xi_\perp^{-x_G}\mathcal{G}^\pm\left(\frac{r_\perp}{\xi_\perp}, D_0\frac{r_\parallel}{\xi_\perp^z}; D_2 h|t|^{-y_h/y_t}\right)
\end{aligned} \tag{C.1}$$

where the x are scaling dimensions and $y_{t,h}$ renormalization group eigenvalues (in particular $y_t = 1/\nu_\perp$), the D are non-universal metric factors, $\mathcal{E}, \mathcal{F}, \mathcal{G}$ are universal scaling functions where the index distinguishes between the cases $t > 0$ and $t < 0$, $\xi_\perp = \xi_0|t|^{-\nu_\perp}$ is the spatial, $\xi_\parallel = \xi_\perp^z / D_0$ is the temporal correlation length and z is the dynamical exponent.

In the steady state, and for $h = 0$, one expects $\rho \sim t^\beta$ and $P \sim t^{\beta'}$. In general, the two exponents β and β' are distinct from each other. For spatial translation invariance, the dependence on $r_\perp$ drops out for both ρ and P and in the steady state (i.e. $r_\parallel \to \infty$) one has

$$\begin{aligned}
\rho(t, h) &= D_{1\rho}\xi_0^{-\beta/\nu_\perp}\widetilde{\mathcal{E}}^\pm\left(D_2 h|t|^{-y_h/y_t}\right)|t|^\beta\\
P(t, h) &= D_{1P}\xi_0^{-\beta'/\nu_\perp}\widetilde{\mathcal{F}}^\pm\left(D_2 h|t|^{-y_h/y_t}\right)|t|^{\beta'}
\end{aligned} \tag{C.2}$$

where $x_\rho = \beta/\nu_\perp$, $x_P = \beta'/\nu_\perp$ and $\widetilde{\mathcal{E}}^\pm = \lim_{r_\parallel\to\infty}\mathcal{E}^\pm$ and similarly for $\mathcal{F}$. We also consider the auto-connectedness (that is $r_\perp = r'_\perp$) in the steady state

$$G(0, \infty; t, h) =: G(t, h) = D_{1P}\xi_0^{-x_G}\widetilde{\mathcal{G}}^\pm(D_2 h|t|^{-y_h/y_t})|t|^{x_G\nu_\perp}. \tag{C.3}$$

In the active phase ($t > 0$), the surviving clusters will create an average density $\sim |t|^\beta$ in the interior of the spreading cone. Therefore, the auto-connectedness should in the steady state saturate at the value [3]

$$G(t, h) = \rho(t, h)P(t, h). \tag{C.4}$$

Comparison of the scaling forms then yields, setting $h = 0$,

$$x_G = (\beta + \beta')/\nu_\perp \qquad D_{1G} = D_{1\rho}D_{1P}\frac{\widetilde{\mathcal{E}}^\pm(0)\widetilde{\mathcal{F}}^\pm(0)}{\widetilde{\mathcal{G}}^\pm(0)}. \tag{C.5}$$

Usually, $x_G = d - \theta z$ is expressed in terms of the initial critical slip exponent θ [104], which makes it apparent that the expression (C.5) is in fact a generalized hyperscaling relation, see [3].

Next, we consider the total mass M of the cluster, given by

$$M(t,h) := \int_{\mathbb{R}^d} \mathrm{d}^d r_\perp \int_0^\infty \mathrm{d}r_\parallel G(r_\perp, r_\parallel; t, h) = \frac{D_{1G}}{D_0} \xi_\perp^{\gamma/\nu_\perp} \overline{\mathcal{G}}^{\pm}(D_2 h |t|^{-y_h/y_t}) \tag{C.6}$$

where equation (C.1) was used and $\overline{\mathcal{G}}^{\pm}$ is a new universal function related to $\mathcal{G}^{\pm}$. Also

$$\gamma = d\nu_\perp + \nu_\parallel - \beta - \beta' \tag{C.7}$$

which is the analogue of the hyperscaling relation of equilibrium systems.

While the discussion so far has been completely general, we now appeal to two properties which are valid for systems in the directed percolation universality class, but need not be generically valid. First, we consider a directed percolation process in the presence of a weak field h (physically, h parametrizes the rate of a particle creation process $\emptyset \to A$). A site at a given time becomes active if it is connected with at least one active site in the past, where a particle was created by the field. The number of such sites is equal to the cluster size, the probability of becoming active is given by the density

$$\rho(t,h) \simeq 1 - (1-h)^{M(t,h)} \simeq hM(t,h) \tag{C.8}$$

for h small. Therefore,

$$M(t,0) = \left.\frac{\partial \rho(t,h)}{\partial h}\right|_{h=0}. \tag{C.9}$$

Comparison with the scaling forms for ρ and M leads to

$$y_h/y_t = \beta + \gamma \qquad D_{1P} = D_0 D_2 \xi_0^{-(\beta+\gamma)/\nu_\perp} \mathcal{A}^{\pm} \tag{C.10}$$

where $\mathcal{A}^{\pm}$ is an universal amplitude. Second, directed percolation is special in the sense that there is a 'duality' symmetry which can be used to show that [23]

$$\rho(t,h) = P(t,h). \tag{C.11}$$

As a consequence, $\beta = \beta'$ and $D_{1\rho} = D_{1P}$ for directed percolation and we thus have, combining equations (C.2), (C.6) and (C.10),

$$\begin{aligned} \rho(t,h) &= D_0 D_2 \xi_0^{-d-z} |t|^{\beta} \hat{\mathcal{M}}_1^{\pm}(D_2 h |t|^{-\beta-\gamma}) \\ M(t,h) &= D_0 D_2^2 \xi_0^{-d-z} |t|^{-\gamma} \hat{\mathcal{M}}_2^{\pm}(D_2 h |t|^{-\beta-\gamma}) \end{aligned} \tag{C.12}$$

with universal functions $\hat{\mathcal{M}}_n^{\pm}(x) = \mathrm{d}^n \hat{\mathcal{M}}^{\pm}(x)/\mathrm{d}x^n$ and where the hyperscaling relation equation (C.7) has been used. Finally, we define a new function $\mu = \mu(t,h)$ by $\rho(t,h) = \partial \mu(t,h)/\partial h$, which implies

$$\mu(t,h) = D_0 \xi_0^{-d-z} |t|^{(d+z)\nu_\perp} \hat{\mathcal{M}}^{\pm}(D_2 h |t|^{-\beta-\gamma}). \tag{C.13}$$

In particular we have because of $\xi_\parallel = \xi_\perp^z / D_0$ that

$$\mu(t,0) \xi_\perp^d(t,0) \xi_\parallel(t,0) \underset{t \to 0}{\to} \text{univ. constant} \tag{C.14}$$

again quite analogous to an equilibrium result, see [80].

At last, we consider a geometry of finite size L in space but of infinite extent in time. As usual in finite-size scaling [80], we postulate that in this finite geometry merely the scaling functions are modified

$$\hat{\mathcal{M}}_n^{\pm} = \hat{\mathcal{M}}_n^{\pm}\left(D_2 h |t|^{-\beta-\gamma}; L\xi_\perp^{-1}\right) \tag{C.15}$$

and without introducing any further metric factor. Indeed, we can then scale out L and, because of equation (C.14), arrive at the scaling forms (33). The universality of the moment ratio (34) is obtained from the analogous extension of (C.1) as follows:

$$\begin{aligned}\left\langle r_\perp^n \right\rangle &= \frac{\int_{\Omega(L)} \mathrm{d}^d r_\perp \int_0^\infty \mathrm{d}r_\parallel r_\perp^n G(r_\perp, r_\parallel; L/\xi_\perp)}{\int_{\Omega(L)} \mathrm{d}^d r_\perp \int_0^\infty \mathrm{d}r_\parallel G(r_\perp, r_\parallel; L/\xi_\perp)} \\ &= \xi_\perp^n \frac{\int_{\Omega(L/\xi_\perp)} \mathrm{d}^d r_\perp \int_0^\infty \mathrm{d}r_\parallel r_\perp^{n-x_G} \mathcal{G}^\pm(r_\perp, r_\parallel; L/\xi_\perp)}{\int_{\Omega(L/\xi_\perp)} \mathrm{d}^d r_\perp \int_0^\infty \mathrm{d}r_\parallel r_\perp^{-x_G} \mathcal{G}^\pm(r_\perp, r_\parallel; L/\xi_\perp)} \\ &= \xi_\perp^n \bar{\Xi}_n(L/\xi_\perp) \\ &= L^n \Xi_n(L/\xi_\perp) \end{aligned} \tag{C.16}$$

where $\Omega(L)$ is a d-dimensional hypercube of linear extent L and $\bar{\Xi}_n$ and Ξ_n are universal functions.

References

[1] Marro J and Dickman R 1999 *Non-Equilibrium Phase Transitions in Lattice Models* (Cambridge: Cambridge University Press)

[2] Hinrichsen H 2000 Non-equilibrium critical phenomena and phase transitions into absorbing states *Adv. Phys.* **49** 815

[3] Mendes J F F, Dickman R, Henkel M and Marques M C 1994 Generalized scaling for models with multiple absorbing states *J. Phys. A: Math. Gen.* **27** 3019

[4] Harris T E 1974 Contact interactions on a lattice *Ann. Prob.* **2** 969

[5] Kinzel W 1983 Percolation structures and processes *Ann. Isr. Phys. Soc.* vol 5, ed G Deutscher, R Zallen and J Adler, (Bristol: Adam Hilger)

[6] Liggett T M 1985 *Interacting Particle Systems* (Heidelberg: Springer)

[7] Ódor G 2004 Universality classes in non-equilibrium lattice systems *Preprint* cond-mat/0205644 (*Rev. Mod. Phys.* **76** at press)

[8] Zhong D and ben Avraham D 1995 Universality class of two-offspring branching annihilating random walks *Phys. Lett.* A **209** 333

[9] Cardy J and Täuber U C 1996 Theory of branching and annihilating random walks *Phys. Rev. Lett.* **77** 4780

[10] Dornic I, Chaté H, Chave J and Hinrichsen H 2001 Critical coarsening without surface tension: the voter universality class *Phys. Rev. Lett.* **87** 5701

[11] Droz M, Ferreira A L and Lipowski A 2003 Splitting the voter criticality *Phys. Rev.* E **67** 056108

[12] Cardy J L and Grassberger P 1985 Epidemic models and percolation *J. Phys. A: Math. Gen.* **18** L267

[13] Janssen H K 1985 Renormalized field theory of dynamical percolation Z. *Phys.* B **58** 311

[14] Rossi M, Pastor-Satorras R and Vespignani A 2000 Universality class of absorbing phase transitions with a conserved field *Phys. Rev. Lett.* **85** 1803

[15] Lübeck S 2002 Scaling behaviour of the order parameter and its conjugated field in an absorbing phase transition around the upper critical dimension *Phys. Rev.* E **65** 046150

[16] Lübeck S and Heger PC 2003 Universal scaling behaviour at the upper critical dimension of non-equilibrium continuous phase transitions *Phys. Rev. Lett.* **90** 230601

[17] Jensen I 1993 Critical behaviour of the pair-contact process *Phys. Rev. Lett.* **70** 1465

[18] Jensen I and Dickman R 1993 Non-equilibrium phase transitions in systems with infinitely many absorbing states *Phys. Rev.* E **48** 1710

[19] Carlon E, Henkel M and Schollwöck U 2001 Critical properties of the reaction–diffusion model $2A \to 3A$, $2A \to \emptyset$ *Phys. Rev.* E **63** 036101

[20] Dickman R and Kamphorst Leal da Silva J 1998 Moment ratios for absorbing-state phase transitions *Phys. Rev.* E **58** 4266

[21] Kamphorst Leal da Silva J and Dickman R 1999 Pair-contact process in two dimensions *Phys. Rev.* E **60** 5126

[22] Lübeck S and Willmann R D 2002 Universal scaling behaviour of directed percolation and the pair-contact process in an external field *J. Phys. A: Math. Gen.* **35** 10205

[23] Grassberger P and de la Torre A 1979 Reggeon field theory (Schlögl's first model) on a lattice: Monte Carlo calculations of critical behaviour *Ann. Phys., NY* **122** 373–96

[24] Janssen H K 1981 On the non-equilibrium phase transition in reaction–diffusion systems with an absorbing stationary state *Z. Phys.* B **42** 151
[25] López C and Muñoz M A 1997 Numerical analysis of a Langevin equation for systems with infinite absorbing states *Phys. Rev.* E **56** 4864
[26] Jimenez-Dalmaroni A and Hinrichsen H 2003 Epidemic processes with immunization *Phys. Rev.* E **68** 036103
[27] Muñoz M A, Grinstein G, Dickman R and Livi R 1996 Critical behaviour of systems with many absorbing states *Phys. Rev. Lett.* **76** 451
[28] van Wijland F 2002 Universality class of non-equilibrium phase transitions with infinitely many absorbing states *Phys. Rev. Lett.* **89** 190602
[29] Dickman R 1989 Universality and diffusion in non-equilibrium critical phenomena *Phys. Rev.* B **40** 7005
[30] Grassberger P 1982 On phase transitions in Schlögl's second model *Z. Phys.* B **47** 365
[31] Howard M J and Täuber U C 1997 'Real' versus 'imaginary' noise in diffusion-limited reactions *J. Phys. A: Math. Gen.* **30** 7721
[32] Henkel M and Mendes J F F 1996 unpublished
[33] White S R 1992 Density-matrix formulation for quantum renormalization groups *Phys. Rev. Lett.* **69** 2863
[34] White S R 1993 Density-matrix algorithms for quantum renormalization groups *Phys. Rev.* B **48** 10345
[35] Schollwöck U 2004 Density-matrix renormalization group *Rev. Mod. Phys.* at press
[36] Kaulke M and Peschel I 1998 A DMRG study of the q-symmetric Heisenberg chain *Eur. Phys. J.* B **5** 727
[37] Carlon E, Henkel M and Schollwöck U 1999 Density-matrix renormalization group and reaction–diffusion processes *Eur. Phys. J.* B **12** 99
[38] Hinrichsen H 2001 Pair-contact process with diffusion: a new type of non-equilibrium critical behaviour? *Phys. Rev.* E **63** 036102
[39] Ódor G 2000 Critical behaviour of the one-dimensional annihilation–fission process $2A \to \emptyset, 2A \to 3A$ *Phys. Rev.* E **62** R3027
[40] Hinrichsen H 2001 Cyclically coupled spreading and pair-annihilation *Physica* A **291** 275
[41] Ódor G 2001 Phase transition of the one-dimensional coagulation–production process *Phys. Rev.* E **63** 067104
[42] Park K, Hinrichsen H and Kim I-M 2001 Binary spreading process with parity conservation *Phys. Rev.* E **63** R065103
[43] Henkel M and Hinrichsen H 2001 Exact solution of a reaction–diffusion process with three-site interactions *J. Phys. A: Math. Gen.* **34** 1561
[44] Henkel M and Schollwöck U 2001 Universal finite-size scaling amplitudes in anisotropic scaling *J. Phys. A: Math. Gen.* **34** 3333
[45] Ódor G, Marques M C and Santos M A 2002 Phase transition of a two-dimensional binary spreading model *Phys. Rev.* E **65** 056113
[46] Ódor G 2002 Multicomponent binary spreading process *Phys. Rev.* E **66** 026121
[47] Noh J D and Park H 2004 Novel universality class of absorbing transitions with continuously varying exponents *Phys. Rev.* E **69** 016122
[48] Park K and Kim I-M 2002 Well-defined set of exponents for a pair-contact process with diffusion *Phys. Rev.* E **66** 027106
[49] Dickman R and de Menezes M A F 2002 Nonuniversality in the pair-contact process with diffusion *Phys. Rev.* E **66** 045101
[50] Hinrichsen H 2003 Stochastic cellular automaton for the coagulation–fission process $2A \to 3A, 2A \to A$ *Physica* A **320** 249
[51] Kockelkoren J and Chaté H 2003 Absorbing phase transition of branching-annihilating random walks *Phys. Rev. Lett.* **90** 125701
[52] Ódor G 2003 Critical behaviour of the one-dimensional diffusive pair-contact process *Phys. Rev.* E **67** 016111
[53] Paessens M and Schütz G M 2004 Phase transitions and correlations in the bosonic pair-contact process with diffusion: exact results *J. Phys. A: Math. Gen.* **37** 4709
[54] Barkema G T and Carlon E 2003 Universality in the pair-contact process with diffusion *Phys. Rev.* E **68** 036113
[55] Hinrichsen H 2003 The diffusive pair-contact process and non-equilibrium wetting, unpublished notes *Preprint* cond-mat/0302381
[56] Ódor G 2004 Private communication
[57] Toussaint D and Wilczek F 1983 Particle–antiparticle annihilation in diffusive motion *J. Chem. Phys.* **78** 2642
[58] Muñoz M, Grinstein G and Tu Y 1997 Survival probability and field theory in systems with absorbing states *Phys. Rev.* E **56** 5101
[59] Jensen I 1999 Low-density series expansions for directed percolation: I. A new efficient algorithm with applications to the square lattice *J. Phys. A: Math. Gen.* **32** 5233

[60] ben Avraham D and Köhler J 1992 Mean-field (n, m)-cluster approximation for lattice models *Phys. Rev.* A **45** 8358
[61] Gutowitz H A, Victor J D and Knight B W 1987 Local structure theory for cellular automata *Physica* D **28** 18
[62] Dickman R 1988 Mean-field theory of the driven diffusive lattice gas *Phys. Rev.* A **38** 2588
[63] Houchmandzadeh B 2002 Clustering of diffusing organisms *Phys. Rev.* E **66** 052902
[64] Henkel M 2003 On lower bounds of the solutions of some simple reaction–diffusion equations *Preprint* math-ph/0309027
[65] Grassberger P 1999 Private communication
[66] Marques M C, Santos M A and Mendes J F F 2001 Static critical behaviour in the inactive phase of the pair-contact process *Phys. Rev.* E **65** 066110
[67] Dickman R, Rabêlo W R M and Ódor G 2002 Pair-contact process with a particle source *Phys. Rev.* E **65** 016118
[68] Szolnoki A 2002 Dynamical mean-field approximation for a pair-contact process with a particle source *Phys. Rev.* E **66** 057102
[69] Schütz G M 2000 Exactly solvable models for many-body systems far from equilibrium *Phase Transitions and Critical Phenomena* vol 19, ed C Domb and J L Lebowitz (London: Academic)
[70] Henkel M 2003 Reaction–diffusion processes and their connection with integrable quantum spin chains *Classical and Quantum Nonlinear Integrable Systems: Theory and Applications* ed A Kundu (Bristol: Institute of Physics Publishing) p 256
[71] Privman V (ed) 1990 *Finite-Size Scaling and Numerical Simulation of Statistical Systems* (Singapore: World Scientific)
[72] Lauritsen K B, Fröjdh P and Howard M 1998 Surface critical behaviour in systems with absorbing states *Phys. Rev. Lett.* **81** 2104
[73] Fröjdh P, Howard M and Lauritsen K B 1998 Directed percolation with a wall or edge *J. Phys. A: Math. Gen.* **31** 2311
[74] Bulirsch R and Stoer J 1964 Fehlerabschätzungen und Extrapolation mit rationalen Funktionen bei Verfahren vom Richardson-Typus *Numer. Math.* **6** 413
[75] Henkel M and Schütz G 1988 Finite-lattice extrapolation algorithms *J. Phys. A: Math. Gen.* **21** 2617
[76] Hinrichsen H 2003 Roughening transition driven by a binary spreading process *Eur. Phys. J.* B **31** 365
[77] Mendes J F F 1996 Private communication
[78] van Wijland F, Oerding K and Hilhorst H J 1998 Wilson renormalization of a reaction–diffusion process *Physica* A **251** 179
[79] ben Avraham D, Burschka M and Doering C R 1990 Statics and dynamics of a diffusion-limited reaction: anomalous kinetics, non-equilibrium self-ordering and a dynamic transition *J. Stat. Phys.* **60** 695
[80] Privman V and Fisher M E 1984 Universal critical amplitudes in finite-size scaling *Phys. Rev.* B **30** 322
[81] Privman V, Hohenberg P C and Aharony A 1993 Universal critical-point amplitude relations *Phase Transitions and Critical Phenomena* vol 14, ed C Domb and J L Lebowitz (London: Academic)
[82] Barber M N and Hamer C J 1982 Extrapolation of sequences using a generalized epsilon algorithm *J. Aust. Math. Soc.* B **23** 229
[83] Fröjdh P, Howard M and Lauritsen K B 2001 Directed percolation and systems with absorbing states: impact of boundaries *Int. J. Mod. Phys.* B **15** 1761
[84] Essam J W, Guttmann A J, Jensen I and Tanlakishani D 1996 Directed percolation near a wall *J. Phys. A: Math. Gen.* **29** 1619
[85] Park K 2003 Private communication
[86] Alon U, Evans M R, Hinrichsen H and Mukamel D 1998 Roughening transition in a one-dimensional growth process *Phys. Rev. Lett.* **76** 2746
[87] Alon U, Evans M R, Hinrichsen H and Mukamel D 1998 Smooth phases, roughening transitions and novel exponents in one-dimensional growth models *Phys. Rev.* E **57** 4997
[88] Hinrichsen H and Ódor G 1999 Roughening transition in a model for dimer adsorption and desorption *Phys. Rev. Lett.* **82** 1205
[89] Hinrichsen H and Ódor G 1999 Critical behaviour of roughening transitions in parity-conserving growth processes *Phys. Rev.* E **60** 3842
[90] Goldschmidt Y Y, Hinrichsen H, Howard M J and Täuber U C 1999 Novel non-equilibrium critical behaviour induced by unidirectional coupling of stochastic processes *Phys. Rev.* E **59** 6381
[91] Deloubrière O, Janssen H K, Täuber U C and Wijland F 2004 Private communication
[92] Lee B P 1994 Renormalization group calculation for the reaction $kA \to \emptyset$ *J. Phys. A: Math. Gen.* **27** 2633
[93] Janssen H K and Täuber U C 2004 Private communication

[94] van Wijland F 2001 Field theory for reaction–diffusion processes with hard-core particles *Phys. Rev.* E **63** 022101
[95] Park K, Hinrichsen H and Kim I-M 2002 Phase transition in a triplet process *Phys. Rev.* E **65** R025101
[96] Young R W, Roberts A J and Stuhne G 2001 Reproductive pair correlations and the clustering of organisms *Nature* **412** 328
[97] Godrèche C and Luck J-M 2001 Response of non-equilibrium systems at criticality: ferromagnetic models in dimension two and above *J. Phys. A: Math. Gen.* **33** 9141
[98] Picone A and Henkel M 2002 Response of non-equilibrium systems with long-range initial correlations *J. Phys. A: Math. Gen.* **35** 5572
[99] Paessens M and Henkel M 2003 The kinetic spherical model in a magnetic field *J. Phys. A: Math. Gen.* **36** 8983
[100] Ódor G 2003 Phase transition classes in triplet and quadruplet reaction–diffusion models *Phys. Rev.* E **67** 056114
[101] Ódor G 2004 Phase transitions of the binary production $2A \to 3A$, $4A \to \emptyset$ model *Phys. Rev.* E **69** 036112
[102] Chaté H 2003 Private communication
[103] Graham R L, Knuth D E and Patashnik O 1994 *Concrete Mathematics* (New York: Addison-Wesley)
[104] Janssen H K, Schaub B and Schmittmann B 1989 New universal short-time scaling behaviour of critical relaxation processes *Z. Phys.* B **73** 539