

Classification of phase transitions in reaction-diffusion models

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Equilibrium phase transitions are associated with rearrangements of minima of a (Lagrangian) potential. Treatment of nonequilibrium systems requires doubling of degrees of freedom, which may be often interpreted as a transition from the “coordinate”- to the “phase”-space representation. As a result, one has to deal with the Hamiltonian formulation of the field theory instead of the Lagrangian one. We suggest a classification scheme of phase transitions in reaction-diffusion models based on the topology of the phase portraits of corresponding Hamiltonians. In models with an absorbing state such a topology is fully determined by intersecting curves of zero “energy.” We identify four families of topologically distinct classes of phase portraits stable upon renormalization group transformations.

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I. INTRODUCTION

The last decade witnessed the rapid growth of interest in reaction-diffusion models [1–15]. Such models are employed for a description of phenomena ranging from the kinetics of chemical reactions to the evolution of biological populations. The subject of particular interest is the description of dynamical phase transitions in reaction-diffusion kinetics. An important example is absorbing phase transitions. Upon such a transition the system goes from an active (“living”) phase to an absorbing (“dead”) state with no escape from it.

Grassberger and Janssen [16,17] realized that many of the absorbing-state transitions belong to the same universality class as the directed percolation (DP) model. Since then, the DP universality class was extensively studied both analytically and numerically (see Refs. [1,3,18–24]). The DP universality class is extremely robust. In fact, exceptions to the DP transitions are rare. However, if the microscopic dynamics possesses additional symmetries, the universality class of the transition may be different. For example, parity conservation (PC) is known to drive the transition to a new distinct universality class [1,3,5,25,26]. Recently other possible universality classes have been studied [1,27–40]. Among them is a pair contact process with diffusion (PCPD), the critical behavior of which has not yet been described analytically [8,41–56].

Despite extensive accumulated knowledge, it seems that a guiding principle, allowing one to distinguish between various types of the transitions, is still missing. The purpose of this paper is to suggest a simple scheme, providing, at least, an educated guess regarding the universality class of the reaction-diffusion model at hand. The scheme is based on the topology of the phase portraits of the system’s Hamiltonian. Before elaborating on it, let us briefly recall the corresponding strategy for equilibrium systems.

An equilibrium system may be characterized by an action (energy)

$$S = \int d^d x [D(\nabla q)^2 + V(q)], \quad (1)$$

written in terms of the order parameter $q(x)$ (for simplicity we restrict ourselves to the one-component order parameter).

The potential function $V(q)$ encompasses information about possible phase transitions. Specifically, one monitors the behavior of the *minima* of $V(q)$ as a function of the control parameter to infer the existence and type of transition. For example, a wide class of models may be described by a potential of the form

$$V(q) = hq + mq^2 + uq^4. \quad (2)$$

For $m < 0$ the system exhibits a first-order transition when h changes its sign (for $d > 1$) and the two minima interchange. In the symmetric case $h=0$, the system may undergo a second-order transition when the parameter m is swept through zero, so a single minimum is split in two. Below the critical dimension $d_c=4$ this second-order transition is characterized by non-mean-field critical exponents. To find the exponents one typically employs the renormalization group (RG) technique. The RG technique treats the coefficients m and u of the potential (2) as functions of the running spatial scale. For $\epsilon=d_c-d > 0$ the potential scales towards the non-trivial fixed point potential, $V^*(q) \neq 0$, with $m^* \sim \epsilon^2$ and $u^* \sim \epsilon$. Notice that the action (1) essentially specifies the Lagrangian field theory.

One may ask whether a similar strategy exists for non-equilibrium phase transitions in reaction-diffusion systems. To answer this question one has to recall that a description of nonequilibrium systems requires doubling of the degrees of freedom. There are various manifestations of this statement depending on the specific context. In quantum kinetics it is known as the Keldysh technique [57]. It employs time evolution along a closed contour, so one has to keep two copies of each field: one for the forward and another for the backward evolution. In a classical context the Martin-Siggia-Rose [58–62] method requires an additional set of fields to resolve the functional δ functions of Langevin equations. Most importantly for the present subject, in reaction-diffusion kinetics the Doi-Peliti [63,64] operator technique deals with the creation and annihilation operators for each reagent. Thus it employs two variables (or one complex field) for every *real* physical degree of freedom. (For a discussion of the connections between these techniques see, e.g., Refs. [65,66].)

An important observation is that in all these examples the two sets of fields (being properly transformed) may be considered as canonically conjugated variables. As a result, instead of the equilibrium order parameter $q(x)$, one has to deal with the canonical pair $q(x,t)$ and $p(x,t)$. Correspondingly a reaction-diffusion system may be described by the *Hamiltonian* action

$$S = \int dt \int d^d x [p \partial_t q + D \nabla p \nabla q - H_R(p,q)], \quad (3)$$

where the Hamiltonian $H_R(p,q)$ is determined by the set of reactions specific for a given model (see below).

Comparing Eqs. (3) and (1), one notices that the reaction Hamiltonian $H_R(p,q)$ plays a role similar to the effective potential $V(q)$ in equilibrium statistical mechanics. Thus it is plausible that $H_R(p,q)$ may encode information about possible nonequilibrium transitions in a way analogous to what $V(q)$ does. Specifically, one wants to know what is the Hamiltonian analog of the potential minima, given by $\partial_q V = 0$, in the Lagrangian formulation. The answer is that it is the *classical* equations of motion: $\partial_t q = \partial_p H_R$ and $\partial_t p = -\partial_q H_R$. One is looking, therefore, for a geometric way to picture the Hamiltonian equations of motion. We argue below that the way to do it (at least for the one-component models) is to consider the phase-space trajectories in the (p,q) plane. Indeed, the classical equations of motion conserve “energy.” Thus the phase-space trajectories are given by the curves $H_R(p,q) = \text{const}$. Moreover, for systems with absorbing states the only trajectories which may intersect correspond to zero energy. As a result, the set of curves

$$H_R(p,q) = 0 \quad (4)$$

determines entirely the topology of the phase space.

The main message of this paper is that the curves specified by Eq. (4) and the corresponding topology of the phase portrait classify possible phase transitions in reaction-diffusion models. It is the web of the zero-“energy” trajectories which plays the role of minima of the $V(q)$ potential in the equilibrium statistical mechanics. A topological rearrangement of this web as a function of the control parameter signals the existence of a phase transition. The corresponding topology is in one-to-one correspondence with the universality classes.

Below we show that the number of distinct generic phase-space topologies (for one-component systems) is rather limited, indicating that all possible universality classes may be exhausted. Some of the topologies correspond to first-order transitions, while others to continuous ones [much the way potential (2) contained both]. The latter class may develop nontrivial critical exponents below a certain critical dimension d_c . The way to find these exponents is to follow the RG flow of constants of the Hamiltonian $H_R(p,q)$ upon elimination of the small-scale fluctuations. While the Hamiltonian itself may be complicated, it is only the topology of the phase space that matters, not the specific shape of the curves. Any given topology may be modeled by a simple polynomial of q and p , again much the way the simple polynomial (2) suffices to describe many equilibrium systems. Thus one

must follow only changes of the topology of the phase portrait upon RG transformations. One should also verify that a given topology is stable upon RG transformations—i.e., that it cannot be reduced to a more generic one by decimation. The resulting fixed-point topologies and corresponding fixed-point Hamiltonians $H_R^*(q,p)$ provide information about the universality classes.

We found that the DP universality class (represented by the simplest triangular structure on the phase plane) serves as parent for a family of descending classes. Each subsequent class in the family is characterized by a minimal number k of particles needed to initiate reactions. We denote it as the k -particle contact process with diffusion (kCPD). Here 1CPD is DP, while 2CPD is the PCPD (for a review see Ref. [8] and references therein). According to scaling analysis, above the upper critical dimension $d_c = 4/k$ the kCPD’s are characterized by mean-field critical exponents—e.g., $\beta = 1$ and $\nu_{\perp} = k/2$. For $d \leq d_c$ and $k = 2, 3$ we found that RG flows to a strong-coupling fixed point that cannot be accessed in the ϵ expansion (see also Refs. [8,67]). We also discuss the possible nature of the strong-coupling fixed point for $k = 2$.

Similarly the PC universality class generates a family of classes, characterized by a minimal number k , of incoming particles required for *all* reactions. We call them k -particle parity conserving (kPC). Their upper critical dimension is $d_c = 2/k$. In addition to kCPD and kPC we identify two more families of universality classes. They both originate from reversible reactions which may go in both directions with different rates. We call them k -particle reversible (kR) and k -particle reversible parity conserving (kRPC). In both cases k stays for a minimal number of incoming particles. Their critical dimensions are $2/k$ and $2/(k+1)$ correspondingly.

These four families seem to exhaust all possible continuous transitions reachable by the tuning of a *single* control parameter and capable of exhibiting a *non-mean-field* behavior. This means that any phase portrait, topologically different from that of the four families, is unstable upon renormalization. In the large-scale limit it flows towards one of the stable topologies. The latter are protected by certain symmetries of the action against deformations introduced by the RG. The fluctuation-induced renormalization may be not effective if the space dimensionality is sufficiently high. As a result, other topologies may appear to be stable and lead to different universality classes. However, by virtue of the ineffectiveness of fluctuations, such universality classes are bound to exhibit trivial *mean-field* behavior.

The paper is organized as follows: in Sec. II we introduce reaction Hamiltonians and their phase portraits. Section III is devoted to models exhibiting the first-order transitions and discusses the topological structure of their phase portraits. In Sec. IV models of the DP universality class and its derivatives, kCPD’s, are considered. We demonstrate that the triangular topology of the phase portrait is the typical feature of all universality classes of this kind. In Sec. V we consider the parity conserving model and its generalizations, kPC’s. The rectangular phase portrait topology of the reversible reaction models, kR’s and kRPC’s, is discussed in Sec. VI. Finally some conclusions and outlook are drawn in Sec. VII.

II. REACTION HAMILTONIANS AND PHASE PORTRAITS

The standard way to introduce the “quantum” reaction Hamiltonian is by employing the creation and annihilation operator technique of Doi and Peliti [10,11,63,64,68]. Here we choose to follow a different, though completely equivalent, strategy [69]. Consider a generic reaction that transforms k particles into m equivalent ones with the probability λ :



The corresponding master equation for the temporal evolution of the probability $\mathcal{P}_n(t)$ of a configuration with n particles has the form

$$\partial_t \mathcal{P}_n(t) = \lambda \left[\binom{n+k-m}{k} \mathcal{P}_{n+k-m}(t) - \binom{n}{k} \mathcal{P}_n(t) \right]. \quad (6)$$

The two terms on the right-hand side (RHS) represent the probabilities of “in” and “out” processes correspondingly. The master equation (6) is to be supplemented with an initial distribution—e.g., $\mathcal{P}_n(0) = e^{-n_0} n_0^n / n!$, the Poisson distribution with the mean value n_0 , or $\mathcal{P}_n(0) = \delta_{n,n_0}$, the fixed initial particle number.

Let us define now a *generating function* as

$$G(p,t) \equiv \sum_{n=0}^{\infty} p^n \mathcal{P}_n(t). \quad (7)$$

The parameter p will play the role of the canonical momentum; so far, it has been introduced purely formally. The value $p=1$ plays a special role. First, the conservation of probability implies the normalization condition

$$G(1,t) \equiv 1. \quad (8)$$

Second, the moments of $\mathcal{P}_n(t)$ may be expressed through derivatives of the generating function at $p=1$ —e.g., $\langle n(t) \rangle \equiv \sum_n n \mathcal{P}_n(t) = \partial_p G(p,t)|_{p=1}$. Knowing the generating function, one may find the probability of having (integer) n particles at time t as $\mathcal{P}_n(t) = \partial_p^n G(p,t)|_{p=0} / n!$.

In terms of the generating function the master equation (6) may be *identically* rewritten as

$$\partial_t G = \hat{H}_R(p, \hat{q}) G, \quad (9)$$

where the non-Hermitian normally ordered operator \hat{H}_R stays for

$$\hat{H}_R(p, \hat{q}) = \frac{\lambda}{k!} (p^m - p^k) \hat{q}^k. \quad (10)$$

Here we have introduced the “coordinate” operator

$$\hat{q} \equiv \frac{\partial}{\partial p}, \quad (11)$$

obeying the canonical commutation relation $[\hat{q}, p] = 1$. Because of the obvious analogy with the Schrödinger equation, we shall refer to the operator \hat{H}_R as the Hamilton operator in the p representation. From the normalization condition, Eq. (8), it follows that

$$\hat{H}_R(p, \hat{q})|_{p=1} = 0. \quad (12)$$

Any Hamiltonian derived from a probability conserving master equation necessarily satisfies this property.

One can easily generalize this construction for the case where many reactions with rates λ_{km} take place at the same time. To this end one can simply algebraically add the corresponding partial Hamiltonians to obtain the full reaction Hamiltonian. If there is no particle production from the vacuum—i.e., $k \neq 0$ for any m —the empty state with $n=0$ is an absorbing state in the sense that the system can never leave it. According to Eq. (10) any Hamiltonian function describing a system with empty absorbing state must satisfy

$$H_R(p, q)|_{q=0} = 0 \quad (13)$$

in addition to Eq. (12).

Before considering the full “quantum” problem, Eq. (9), let us analyze the corresponding classical dynamics. The classical equations of the motion are

$$\partial_t q = \frac{\partial}{\partial p} H_R(p, q), \quad (14)$$

$$\partial_t p = - \frac{\partial}{\partial q} H_R(p, q). \quad (15)$$

Due to Eqs. (10) and (12), $p=1$ is always one of the solutions of Eq. (15). Substituting $p=1$ into Eq. (14), one obtains [for the Hamiltonian (10)]

$$\partial_t q = \frac{\lambda}{k!} (m-k) q^k. \quad (16)$$

This is nothing but the mean-field rate equation for the average particle number $\langle n(t) \rangle$, neglecting all fluctuation effects. Therefore one may identify the variable q as the reaction “coordinate” (in fact this notation is not precise, since it is true only along the line $p=1$).

In order to proceed with the classical problem, Eqs. (14) and (15), beyond the reaction rate approximation ($p=1$), it is convenient to consider the phase space of the system. The classical equations of motion (14) and (15) conserve energy. As a result, the phase-space (p, q) evolution of the system takes place along the trajectories given by $H_R(p, q) = \text{const}$, where the constant energy is determined from the initial conditions. Among all possible trajectories the ones with $H_R=0$ play a special role. For one thing, the evolution prescribed by the rate equation ($p=1$) takes place along one of such lines [cf. Eq. (12)]. More importantly, the trajectories with $H_R=0$ may intersect each other. Indeed, the two zero-energy lines, guaranteed by Eqs. (12) and (13)—i.e., $p=1$ and $q=0$ —intersect in the point $(1, 0)$. Therefore the set of intersecting zero-energy curves plays the role of separatrix; i.e., it divides the entire phase space on the isolated sectors. All other trajectories cannot intersect the zero-energy ones and are confined to one of the sectors. The web of the zero-energy curves uniquely determines the topology of the phase portrait. An example of such a construction is given in Fig. 1.

Going back to the full “quantum” problem, one may write a formal solution of Eq. (9) as

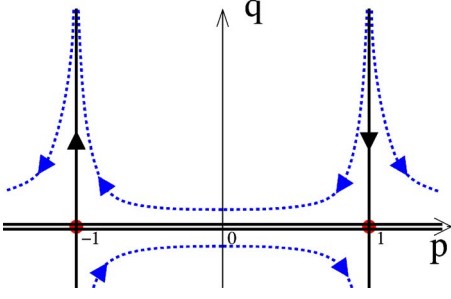


FIG. 1. (Color online) Phase portrait of the binary annihilation system, $2A \rightarrow 0$. The corresponding classical Hamiltonian is given by $H_R(p, q) = \frac{\lambda}{2}(1-p^2)q^2$. Solid black lines show zero-energy trajectories: generic lines $p=1$ and double degenerate $q=0$ and the “accidental” line $p=-1$. Dashed colored curves indicate trajectories with nonzero energy. The arrows show the evolution direction.

$$G(p_f, t_f) = \int U(p_f, t_f; p_0, t_0) G_0(p_0) dp_0, \quad (17)$$

where the Green function $U(p_f, t_f; p_0, t_0)$ is given by the T exponent: $T \exp\{\hat{H}_R t\}$. Dividing the time interval $[t_0, t_f]$ into $N \rightarrow \infty$ steps and introducing the resolution of unity at each one of them, one obtains the Feynman representation

$$U(p_f, t_f; p_0, t_0) = \int \mathcal{D}p(t) \mathcal{D}q(t) e^{-S[p, q]}, \quad (18)$$

with the Hamiltonian action

$$S[p, q] = \int_{t_0}^{t_f} dt [p \partial_t q - H_R(p, q)]. \quad (19)$$

To combine reaction kinetics with the random walk on a lattice, one needs to modify the master equation. The corresponding generating function becomes a function of many variables p_i , where the index i enumerates the lattice sites. One may also introduce the conjugated variables $\hat{q}_i = \partial / \partial p_i$. The resulting Hamiltonian takes the form

$$\hat{H} = -\tilde{D} \sum_{\langle i, j \rangle} (p_i - p_j)(\hat{q}_i - \hat{q}_j) + \sum_i \hat{H}_R(p_i, \hat{q}_i), \quad (20)$$

where \tilde{D} is a hopping probability per unit time and the sum in the first term on the RHS runs over nearest neighbors i, j . Taking the continuum limit [63,64] and introducing the pair of canonically conjugated fields $p(x, t)$ and $q(x, t)$, one arrives at the quantum field theory with the Hamiltonian action (3). The diffusion constant in Eq. (3) is given by $D = \tilde{D} a^2$, where a is the lattice constant.

Unless the system is very close to extinction, the functional integral in Eq. (18) may be evaluated in the saddle point approximation. In such a case the Green function is given by the exponentiated action of a classical trajectory, satisfying the proper boundary conditions [69] [much the same way as the minima of the potential $V(q)$, Eq. (2), dominate the partition function away from an equilibrium phase transition]. A possible phase transition may be associated with a qualitative change in the behavior of the phase-space

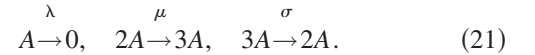
trajectories (cf. the rearrangement of minima of the potential upon an equilibrium transition). In other words, phase transitions lead to a change of topology of the phase-space portrait. Since the latter is determined by the set of the zero-energy lines, it is the rearrangement of this set, upon variation of a control parameter, which must be associated with the phase transition.

If a system is close enough to a phase transition (or extinction), the saddle point approximation may lose its validity (below critical dimensionality d_c). One can then employ the RG technique to progressively integrate out the small-scale fluctuations. Upon such a procedure the constants and even the functional form of the reaction Hamiltonian flow. However, one needs to follow the topology of the phase space, rather than a specific form of the trajectories. Around the transition the topology may be fully encoded in a relatively simple polynomial, which in turn provides a full characterization of the transition (at least for small $\epsilon = d_c - d$). Considering all distinct topologies, stable upon RG transformations, one may classify the possible phase transitions.

We turn now to an illustration of these ideas with specific examples.

III. MODELS WITH FIRST-ORDER TRANSITIONS

Consider a set of reactions, given by

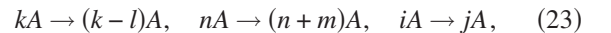


The corresponding reaction Hamiltonian, according to Eq. (10), may be written as

$$H_R = \left(\lambda - \frac{\mu}{2} p^2 q + \frac{\sigma}{6} p^2 q^2 \right) (1-p) q. \quad (22)$$

There are three zero-energy curves: the two generic lines $p=1$ and $q=0$, following from Eqs. (12) and (13), and the additional “accidental” curve $p^2 = 2\lambda / (\mu q - \sigma q^2 / 3)$. The phase portrait of the system is depicted in Figs. 2(a)–2(c). Its topology is qualitatively different for $\mu < \mu_c = \sqrt{8\lambda\sigma}/3$ and $\mu > \mu_c$. In the former case, Fig. 2(a), the “accidental” curve does not intersect the mean-field line $p=1$ and the flow along the latter is directed towards $q=0$ (extinction). For $\mu = \mu_c$ the two curves touch each other, Fig. 2(b), creating a stationary point with a finite concentration $q = 3\mu / (2\sigma)$. At a larger creation rate $\mu > \mu_c$, there is a stable point with concentration $\langle n \rangle$, Fig. 2(c).

This is the first-order transition scenario. Indeed, the stable concentration experiences a discontinuous jump from zero at $\mu < \mu_c$ to some finite value at $\mu \geq \mu_c$. It may be generalized to any reaction set of the form



where the first two reactions satisfy the condition $k < n$ and the last reaction is necessary to ensure a finite particle density by having $i > n, j$ (for hard-core “fermionic” models this restriction is intrinsic and the last reaction may be omitted). The corresponding reaction Hamiltonian may be written as

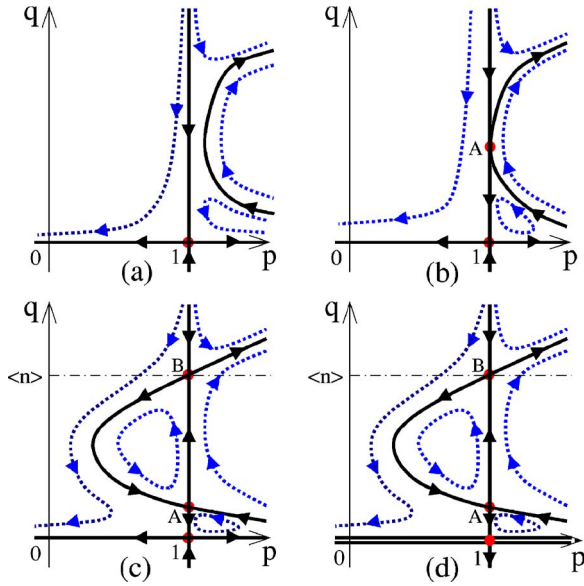


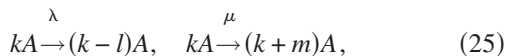
FIG. 2. (Color online) Phase portraits of the system exhibiting the first-order phase transition. Thick solid lines represent the zero-energy trajectories. (a)–(c) The set, Eq. (21): (a) extinction phase, (b) transition point, and (c) active phase. (d) Reaction set of the type of Eq. (23) with $k=2$, $n=3$, and $i=4$ in the active phase.

$$H_R = [h_1(p) - h_2(p)q^{n-k} + h_3(p)q^{i-k}](1-p)q^k, \quad (24)$$

where the functions h_1 , h_2 , and h_3 are positive in the interval $p \in [0, 1]$. An example of the phase portrait in the active phase and $k=2$ is depicted in Fig. 2(d).

Strictly speaking, the condition $\mu = \mu_c$ [Fig. 2(b)] signifies the appearance of the *metastable* state (unless $D \rightarrow \infty$). Such a metastable state becomes stable at some larger creation rate $\tilde{\mu}_c(D) > \mu_c$. Therefore, in terms of the bare system's parameters the actual first-order transition takes place when the phase portrait has a form of Fig. 2(c). Alternatively, one may imagine integrating out spatial fluctuations (governed by the diffusion constant D) and plotting the phase portrait of the effective zero-dimensional ($d=0$) system in terms of the *renormalized* parameters. It is in this latter sense that the transition point is depicted by Fig. 2(b).

An interesting limiting case [51,52] of the first-order transition is the reaction set



described by the Hamiltonian

$$H_R = h(p)(1-p)q^k, \quad (26)$$

where $h(p)$ is a polynomial the degree $k+m-1$. The zero-energy lines are given by $p=1$, the k times degenerate line $q=0$ along with the lines $p=p_i$, where p_i are roots of the polynomial $h(p_i)=0$, Fig. 3. It is easy to check that for $\mu_c = \frac{\lambda}{m}$ one of the roots of the polynomial is $p_1=1$. In this situation the $p=1$ zero-energy line is doubly degenerate, corresponding to the first-order transition. Upon such a transition the $p=1$ and $p=p_1$ lines interchange their relative posi-

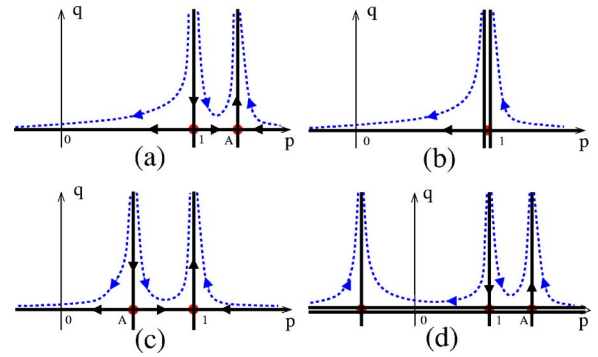


FIG. 3. (Color online) Phase portraits of the system, Eq. (25), exhibiting the first-order phase transition. Thick solid lines represent the zero-energy trajectories. (a)–(c) Reaction set with $k=l=m=1$: (a) extinction phase, (b) transition point, and (c) unlimited proliferation phase. (d) Reaction set with $k=l=2$ and $m=1$ in the extinction phase.

tions and the extinction behavior turns into the unlimited proliferation one.

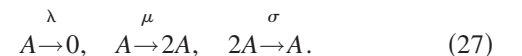
Notice that adding a proliferation-restricting reaction $iA \rightarrow jA$, with $i > k$, to the set (25) qualitatively changes its phase portrait. In general, such a modification leads to a continuous phase transition [see, e.g., Eqs. (27) and (37) below]. An analogous transformation of the first-order to the continuous transition takes place for restricted (“fermionic”) reaction rules [32,70]. This is consistent with the conjecture that the “fermionic” condition implies an effective annihilation process of the order of $k+1$; see, e.g., Refs. [1,3] and references therein.

The phase portrait description given above has the status of the mean-field consideration only (much the same way as the finding of minima of the effective potential, Eq. (2), in the equilibrium theory). It does *not* exclude the possibility that below some lower critical dimension d'_c the fluctuations may drastically change the system's behavior. In particular, a transition, being first order in the mean-field scenario, may be turned to a continuous one by fluctuation effects. This may explain the apparent continuous transition seen in $d=1$ systems, similar to those given by Eq. (23) [49,71,72]. It was also observed in some fermionic reaction schemes that the first-order transition observed at large D turns out to be continuous for $D < D_c$ [73,74]. The subject definitely needs more investigation both analytical and numerical.

IV. DIRECTED PERCOLATION AND ITS GENERALIZATIONS

A. DP models

Consider a reaction set which includes death, branching, and coalescence reactions:



The corresponding reaction Hamiltonian takes the form

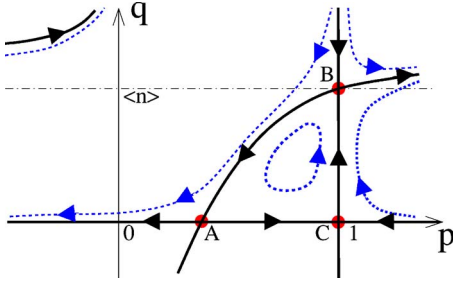


FIG. 4. (Color online) Phase portrait of the DP system in the active phase. Thick solid lines represent zero-energy trajectories which divide the phase space into a number of disconnected regions. Point $B=(1, 2(\mu-\lambda)/\sigma)$ represents the active mean-field point. The system is brought to the phase transitions if points A , B , and C coalesce.

$$H_R = \lambda(1-p)q + \mu(p^2-p)q + \frac{\sigma}{2}(p-p^2)q^2$$

$$= \left(\lambda - \mu p + \frac{\sigma}{2} p q \right) (1-p)q. \quad (28)$$

The phase portrait of the DP system is depicted in Fig. 4. The lines of zero energy are generic $p=1$ and $q=0$ trajectories along with the “accidental” trajectory $q=2(\mu p-\lambda)/\sigma p$. According to the mean-field analysis [classical equations (14) and (15) with $p=1$], there is an active phase with the average density

$$\langle n \rangle = 2 \frac{\mu - \lambda}{\sigma} \quad (29)$$

for $\mu > \lambda$. The active phase corresponds to point B in Fig. 4. The system may be brought to extinction by driving the control parameter $m = \mu - \lambda$ through zero. Therefore the $\mu = \lambda$ point corresponds to the continuous phase transition. The transition is represented by the phase portrait with the three zero-energy trajectories intersecting at the *single* point $(1, 0)$. According to Eq. (29) the mean-field order-parameter exponent is $\beta=1$. The other mean-field exponents [1] are $\nu_{\perp} = 1/2$, $\nu_{\parallel} = 1$.

To go beyond the mean-field picture one needs to investigate the immediate vicinity of the phase transition. To focus on this regime it is convenient to shift the momentum variable

$$p - 1 \rightarrow p. \quad (30)$$

Moreover, close to the transition the phase portrait and thus the Hamiltonian may be modeled by the three intersecting *straight* lines, Fig. 5(a)–5(c). This way one arrives at the model Hamiltonian, applicable close to the DP transition:

$$H_R = (m + up - vq)pq. \quad (31)$$

The bare values of the constants are given by $m = \mu - \lambda$, $u = \mu$, and $v = \sigma/2$. The corresponding action, Eq. (3), acquires the form [1,6,7]

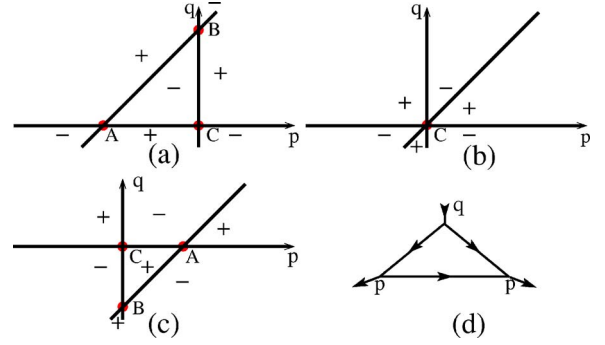


FIG. 5. (Color online) Generic phase portrait of DP models in the vicinity of the phase transition [after the shift, Eq. (30)]. (a) Active phase, $m > 0$; (b) transition point, $m = 0$; (c) extinction phase, $m < 0$. The plus and minus signs show the sign of the Hamiltonian in each sector. (d) The one-loop diagram renormalizing u vertex (vertices m and v are renormalized in a similar way).

$$S = \int dt d^d x [p(\partial_t - D\nabla^2)q - mpq - up^2q + vpq^2], \quad (32)$$

which may be recognized as a Reggeon field theory action [75,76].

There are many other reaction sets, in addition to Eq. (27), with the same “triangular” topology of the phase portrait. Some of the examples are $A \rightarrow 0$; $A \rightarrow (m+1)A$; $2A \rightarrow A$, $m > 1$, or $A \rightarrow 2A$; $2A \rightarrow 0$ (see also Sec. IV C); etc. In the vicinity of the phase transition they all exhibit the topology of the phase portrait depicted in Figs. 5(a)–5(c). Therefore they all may be described by the model Hamiltonian (31). Accordingly they all belong to the same DP universality class.

Naive scaling dimensions of the action (32) are $z=2$, while $[p]+[q]=d$. Since one expects [77] both vertices u and v to have the same scaling dimensions, one finds $[p]=[q]=d/2$. As a result, the bare scaling dimensions of the vertices are $[m]=2$, while $[u]=[v]=2-d/2$. Therefore below the critical dimension $d_c=4$ the nonlinear vertices u and v are relevant and the mean-field treatment is expected to fail.

The one-loop corrections to the naive scaling are given by the triangular diagrams, like the one depicted in Fig. 5(d). Such diagrams are logarithmically divergent in $d=4$, as expected. Straightforward calculations [1,7] (see Ref. [17] for the two-loop approximation) lead to the following set of RG equations:

$$\partial_t m = (2 - Suv)m, \quad (33)$$

$$\partial_t u = (\epsilon/2 - 2Suv)u, \quad (34)$$

$$\partial_t v = (\epsilon/2 - 2Suv)v, \quad (35)$$

where $\epsilon=4-d$ and the differentiation is over the logarithm of the scaling factor. We have introduced the factor

$$S = \partial_l \frac{1}{4} \int_{\Lambda e^{-l}}^{\Lambda} \frac{d^d k}{D^2 k^4} = \frac{\Lambda^{d-4}}{32\pi^2 D^2}, \quad (36)$$

which may be absorbed in the proper redefinition of the running constants.

According to Eqs. (34) and (35), $\partial_l(u/v)=0$, meaning that the slope of the “accidental” zero-energy line, $q=(m+up)/v$, remains intact upon the renormalization procedure. In fact, this statement is exact because of the symmetry [78]. As a result, the overall topology of the phase portrait is preserved by the RG. For $d < 4$ the RG equations (33)–(35) predict a nontrivial fixed point given by $m^*=0$, $u^*=\sqrt{\epsilon\mu/(4S\sigma)}$, and $v^*=\sqrt{\epsilon\sigma/(4S\mu)}$. Substituting these values into Eq. (31), one finds the fixed-point reaction Hamiltonian $H_R^*(p, q)$ corresponding to the DP universality class phase transitions. Its phase portrait is depicted in Fig. 5(b). Linearizing the RG equations (33)–(35) near the fixed point, one finds $\partial_l m = \nu_{\perp}^{-1} m$ with the critical exponent $\nu_{\perp}=(2-\epsilon/4)^{-1} \approx 1/2 + \epsilon/16$. The other critical exponents may be deduced in the standard way [1,7]—e.g., $\beta \approx 1 - \epsilon/6$.

B. k -particle contact processes

As mentioned in the Introduction, the DP universality class is extremely robust. This fact is due to the stability of the “triangular” topology of the phase portrait near the transition. One may try to change this topology by, say, requiring four or more zero-energy trajectories to intersect in the same point. It is clear, however, that in general one must fine-tune more than one parameter to reach such a scenario. Even if bare reaction rates are specially chosen to let it happen, the tuning is not expected to survive upon RG integration of fluctuations. Therefore crossing of more than three lines is possible only at a multicritical transition point. The only way to go beyond the DP is if a different topology of the phase portrait is imposed by an additional *symmetry*.

In this section we discuss a class of models where the *minimum* number of particles needed to initiate *any* reaction is restricted to be $k > 1$. According to Eq. (10) *all* terms in the corresponding reaction Hamiltonian must contain \hat{q}^k or higher power. In terms of the phase portrait it means that the generic $q=0$ zero-energy trajectory is k times degenerate. To emphasize the difference with nondegenerate lines, we denote such k -degenerate trajectories by k closely spaced parallel lines. An important fact is that the degeneracy is preserved by the RG transformations. Indeed, the fluctuations cannot initiate a reaction with fewer than k incoming particles, if it is not in the original reaction set. We denote such models as k -particle contact processes with diffusion (kCPD).

To be specific, let us consider the case of $k=2$, which is represented by, e.g., the following set of reactions:



The corresponding reaction Hamiltonian takes the form

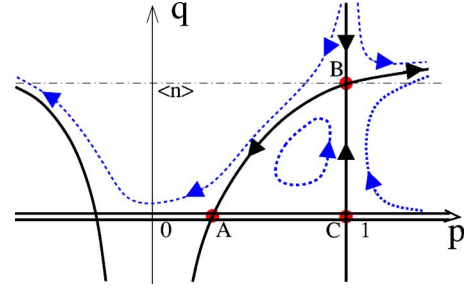


FIG. 6. (Color online) Phase portrait of the 2CPD system in the active phase (cf. DP, Fig. 4). The zero-energy line $q=0$ is doubly degenerate and is depicted by the double line. At the transition points A, B, and C coalesces.

$$\begin{aligned} H_R &= \frac{\lambda}{2}(1-p^2)q^2 + \frac{\mu}{2}(p^3-p^2)q^2 + \frac{\sigma}{6}(p^2-p^3)q^3 \\ &= \frac{1}{2} \left(\lambda(1+p) - \mu p^2 + \frac{\sigma}{3} p^2 q \right) (1-p)q^2. \end{aligned} \quad (38)$$

The phase portrait of the 2CPD system is depicted in Fig. 6. The lines of zero energy are generic $p=1$ and *doubly-degenerate* $q=0$ trajectories. The “accidental” trajectory is given by $q=3[\mu p^2 - \lambda(1+p)]/(\sigma p^2)$. There is an active phase with average density $\langle n \rangle = (3\mu - 6\lambda)/\sigma$ for $\mu > 2\lambda$. It corresponds to point B in Fig. 6. The system may be driven to extinction by tuning the control parameter $m = \mu/2 - \lambda$ to zero. Therefore the $\mu/2 = \lambda$ point corresponds to the continuous phase transition. At the transition point the *four* (we count the $q=0$ line twice) zero-energy lines are intersecting in the single point $(1, 0)$.

Focusing on the transition region, one may shift the momentum variable $p-1 \rightarrow p$ and model the zero-energy trajectories by straight lines, Fig. 7(a). The resulting model Hamiltonian, applicable close to the transition, is

$$H_R = (m + up - vq)pq^2. \quad (39)$$

The bare values of the constants are given by $m = \mu/2 - \lambda$, $u = \mu - \lambda/2$, and $v = \sigma/6$. Since near the transition $m \approx 0$ and thus $\mu \approx 2\lambda > 0$, one finds for the bare value $u \approx 3\lambda/2 > 0$. Apart from Eq. (37), there are infinitely many other reaction sets, which have the same topology as the phase portraits. Therefore the phase transition of these other models is described by the same model Hamiltonian (39). Examples include $2A \rightarrow A$, $2A \rightarrow 4A$, $4A \rightarrow 0$, etc.

In an analogous way, one may show that the phase portrait of a generic kCPD process, such as, e.g., $kA \rightarrow 0$, $kA \rightarrow (k+1)A$, $(k+1)A \rightarrow kA$, contains a triangle of

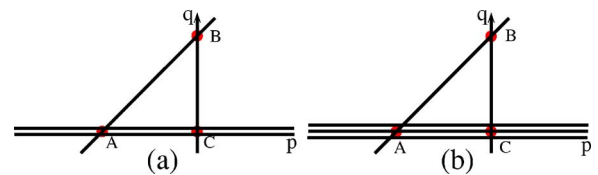


FIG. 7. (Color online) Generic phase portraits of (a) 2CPD models and (b) 3CPD models in the active phase.

k -times-degenerate $q=0$ line, $p=0$ line [after the shift, Eq. (30)], and “accidental” $q=(m+up)/v$ diagonal line; see Fig. 7(b). Thus it may be described by a model Hamiltonian of the form

$$H_R = (m + up - vq)pq^k, \quad (40)$$

where m is the control parameter of the transition and u and v are positive constants.

To find scaling exponents near the transition one assigns bare dimensions $z=2$ and $[p]+[q]=d$. There are no perturbative corrections to the propagator (for $k \geq 2$), and thus one does not expect these exponents to be changed in the ϵ expansion. Since both u and v vertices have to be equally (ir)relevant on the mean-field level, one has to choose the bare dimensions as $[p]=[q]=d/2$. As a result, the bare scaling dimensions of the vertices are $[m]=2-(k-1)d/2$ and $[u]=[v]=2-kd/2$. According to this scaling analysis the critical dimension is expected to be $d_c=4/k$. The corresponding mean-field exponents of the kCPD transitions at $d > d_c$ are $\beta=1$ and $\nu_{\perp}=k/2$. Only the $k=2$ and $k=3$ processes are expected to exhibit nontrivial behavior in the physically relevant dimensions [79,80]. We shall analyze these two cases below.

The 2CPD transition is described by the action (3) with the reaction Hamiltonian (39) (see, e.g., Ref. [8]). Its critical dimension is $d_c=2$. The one-loop renormalization is given by two-vertex loops, which are logarithmically divergent in $d=2$. One arrives [67] at the following set of RG equations:

$$\partial_l m = (1 + \epsilon/2 + \tilde{S}u)m, \quad (41)$$

$$\partial_l u = (\epsilon + \tilde{S}u)u, \quad (42)$$

$$\partial_l v = (\epsilon + 3\tilde{S}u)v, \quad (43)$$

where $\epsilon=2-d$ and

$$\tilde{S} = \partial_l \frac{1}{2} \int_{\Lambda e^{-l}}^{\Lambda} \frac{d^d k}{Dk^2} = \frac{\Lambda^{d-2}}{4\pi D}. \quad (44)$$

Notice that the sign of the perturbative corrections in Eqs. (41)–(43) is *opposite* to that in the corresponding DP RG equations (33)–(35). As a result, the weak-coupling fixed point appears to be absolutely unstable for $d \leq d_c$ (for positive initial u). Its region of stability for $d > d_c$ is finite and shrinking as $d \rightarrow d_c$ from above [81]. Solving Eq. (42), one finds that the coupling constant u diverges once the RG reaches a certain spatial scale $\xi^{-1} = \Lambda e^{-l}$, where, in $d < 2$,

$$\xi = \left(\frac{\epsilon D}{u_0} \right)^{1/(2-d)} \quad (45)$$

(here u_0 is an initial value of u). In $d=2$ one finds that $\xi = \Lambda^{-1} \exp(4\pi D/u_0)$. This indicates that some new physics shows up at the scale ξ . In Appendix A we suggest that the system may develop anomalous averages, similar to those in BCS theory. The corresponding “coherence length” appears to be exactly ξ . (See also Refs. [8,67] for further discussion.)

A similar situation is encountered for $k=3$. The critical dimension is $d_c=4/3$. The RG analysis of Eq. (40) with

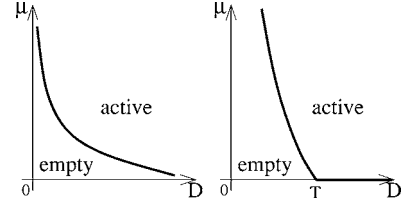


FIG. 8. Schematic phase boundary in the parameter space (D, μ) of the $\lambda=0$ reaction set (49). (a) $d \leq d'_c$, the transition along the entire line is of kCPD class. (b) $d > d'_c$, to the left of the tricritical point T the transition is of kCPD class, while to the right it is $\mu=0$ mean-field transition.

$k=3$ shows that the only vertex which acquires perturbative corrections is v . The corresponding RG equations are

$$\partial_l m = (2 - d)m, \quad (46)$$

$$\partial_l u = (2 - 3d/2)u, \quad (47)$$

$$\partial_l v = (2 - 3d/2)v - 3\tilde{S}mu. \quad (48)$$

Once again, the coupling constant u grows indefinitely and the ϵ expansion fails to predict critical exponents.

C. Critical point and mean-field transitions

In the discussions above we have avoided considering an exact location of the critical point in the parameter space of the problem. Instead, we have concentrated on the universal properties of the transition itself. The only thing we had to assume is that the three intersection points A , B , and C in Figs. 5 and 7 can be made to collapse. In other words, the parameter m in Eqs. (31) or (40) can be made to be zero. In terms of the bare parameters of the model [e.g., Eq. (27)] this corresponds to $\mu=k\lambda$. However, the actual transition may take place away from the $\mu=k\lambda$ point. Indeed, it is the *renormalized* parameter m that vanishes at criticality, *not* the bare one.

The particular case of bare $\lambda=0$, e.g.,

$$kA \xrightarrow{\mu} (k+1)A, \quad (k+1)A \xrightarrow{\sigma} 0, \quad (49)$$

has attracted a lot of attention [5,15,77]. The naive mean-field expectation is that such a system is always in its active phase, unless $\mu=0$. Yet it is clear that any finite-size system is bound to end up in its empty absorbing state after long enough time. [The latter may be estimated as an exponentiated classical action accumulated along the trajectory leading from the active mean-field state (point B in Figs. 4 and 6) to the empty absorbing state (point A) [69].] Therefore, if the diffusion time between the sites is longer than the respective extinction time, the system evolves towards extinction even at $\mu > 0$. As a result, there is a nontrivial phase separation boundary in the parameter space (D, μ) of the $\lambda=0$ system [15], Fig. 8. One may interpret the appearance of this nontrivial line as the generation of the effective annihilation rate $\lambda_{eff}(D, \mu) > 0$. For example, two successive processes $A \rightarrow 2A$ and $2A \rightarrow 0$ result in an $A \rightarrow 0$ effective rate. Conse-

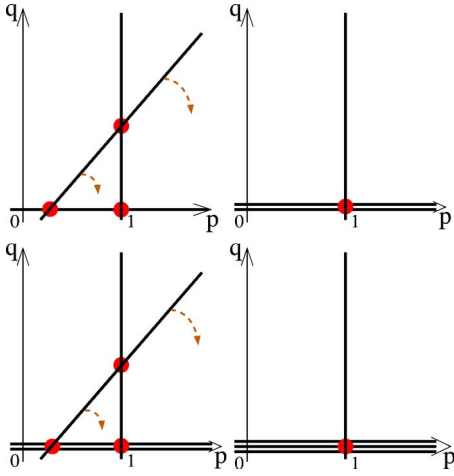
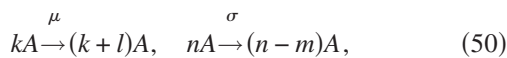


FIG. 9. (Color online) Phase portrait evolution upon $\mu=0$ mean-field transitions: (a) $k=1$ and $\mu>0$, decreasing the branching rate μ is schematically shown by the dashed arrows. (b) $k=1$ and $\mu=0$, the “accidental” line becomes horizontal and the local topology of the phase portrait is that of the binary annihilation reaction; cf. Fig. 1. (c) $k=2$ and $\mu>0$. (d) $k=2$ and $\mu=0$, the topology is that of the 3-plet annihilation reaction, $3A \rightarrow 0$.

quently the phase transition along the nontrivial critical line is represented by the evolution of the phase portraits depicted in Figs. 5 and 7 and belongs to the kCPD universality classes.

The crucial observation made by Cardy and Täuber [5] is that at and below a certain lower critical dimension d'_c the separation boundary extends to an arbitrarily large diffusion constant D , Fig. 8(a). This fact may be associated with a divergent perturbative correction to the coupling constant m . In the two most interesting cases DP and 2CPD such a correction is given by the two-vertex loop, Eq. (44). As a result, the corresponding lower critical dimension is $d'_c=2$. Above the lower critical dimension, $d>d'_c$, there is a tricritical point $T=(D_c, 0)$, such that for $D>D_c$ the transition occur only at $\mu=0$ [15], Fig. 8(b).

The evolution of the phase portrait corresponding to such a $\mu=0$ transition is depicted in Fig. 9 (cf. Figs. 5 or 7). At $\mu=0$ the only remaining reaction is $n \geq 2$ particle annihilation, $(k+1)A \rightarrow 0$, with the critical dimensionality $d_c=2/(k-1) \leq 2$. Thus, the critical dimensionality of the $\mu=0$ transitions is smaller than d'_c —the minimum dimensionality above which the $\mu=0$ transitions may take place. As a result, all such transitions occur *above* their respective critical dimensionality and therefore exhibit mean-field behavior. The generic scheme for a mean-field $\mu=0$ transition may be written as [70]



where $k < n$. The corresponding rate equation is

$$\partial_t q = \mu \frac{l}{k!} q^k - \sigma \frac{m}{n!} q^n. \quad (51)$$

The stationary density is proportional $\langle n \rangle \propto (\mu/\sigma)^{1/(n-k)}$, leading to the mean-field critical exponent $\beta=1/(n-k)$. The

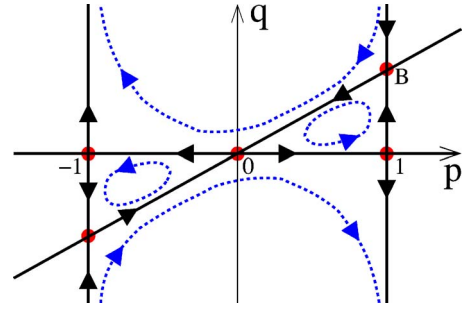


FIG. 10. (Color online) Phase portrait of the parity conserving model, Eq. (52). Notice the reflection symmetry around the origin.

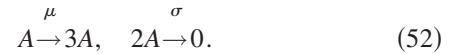
other mean-field exponents can be also deduced in a straightforward way [70].

There are two important exceptions where the $\mu=0$ transitions in the reaction set Eq. (50) may exhibit non-mean-field behavior. These are the cases where generation of the effective $\lambda_{eff}(D, \mu)$ is prohibited by certain symmetries. This may lead to a scenario with $d'_c < d_c$, thus leaving a window $d'_c < d \leq d_c$ for non-mean-field $\mu=0$ transitions. There are two such symmetries: (i) parity conservation (both l and m are even), discussed in Sec. V, and (ii) reversal symmetry ($k+l=n$ and $n-m=k$), discussed in Sec. VI.

V. PARITY CONSERVING MODELS

A. PC model

As was mentioned above the parity conservation may lead to a new nontrivial universality class. Consider the simplest PC reaction set



The corresponding reaction Hamiltonian takes the form

$$H_R = (up - vq)(p^2 - 1)q, \quad (53)$$

where the bare values of the constants are given by $u=\mu$ and $v=\sigma/2$. The corresponding action is invariant under the following transformations [5]:

$$p \rightarrow -p, \quad q \rightarrow -q, \quad (54)$$

which may be traced back to the conservation of parity. As a result, the phase portrait, Fig. 10, possesses the reflection point at the origin. This symmetry is preserved upon RG transformations. Therefore the “accidental” zero-energy line $[q=up/v$, according to Eq. (53)] is bound to be an odd function and thus pass through the origin. Its shape, however, may change in the process of renormalization. Consequently the phase transition cannot be described by the coalescence of three points A , B , and C and its nature is different from the DP class.

According to the mean-field equation $\partial_t q = 2\mu q - \sigma q^2$, the model is always in the active phase with the number of particles $\langle n \rangle = 2\mu/\sigma = u/v$. The only way to drive the mean-field dynamics towards extinction is to send $u=\mu \rightarrow 0$. In other words, the critical point is $u_c=0$. One may discuss, though,

the scaling of particle density with $u - u_c = u$ and this way define the “magnetization” exponent β :

$$\langle n \rangle \sim u^\beta, \quad (55)$$

where the mean-field value of the exponent is $\beta = 1$.

Turning to the fluctuations, one notices that it is not possible to perform the shift of momentum, Eq. (30), and focus on the immediate vicinity of the (1, 0) point on the phase plane. Because of the symmetry (54), one has to keep the entire interval $p \in [-1, 1]$ under consideration; see Fig. 10. Therefore one must choose the scaling dimension $[p] = 0$. Since the bare scaling requires $[p] + [q] = d$, the naive scaling dimension of q is $[q] = d$. As a result, one finds (since $z = 2$) $[u] = 2$ and $[v] = 2 - d$ and the critical dimension is $d_c = 2$. One may worry that since $[p] = 0$, it is not possible to restrict the consideration to the low-order polynomial in p . Instead, one has to keep all the powers of p , resorting to the functional RG. We perform such a procedure in Appendix B and show that it actually justifies the use of the truncated reaction Hamiltonian (53).

The one-loop RG calculation, utilizing the two-vertex loop (which is logarithmically divergent in $d = 2$), yields the following RG equations [5,7]:

$$\partial_t u = (2 - 3\tilde{S}v)u, \quad (56)$$

$$\partial_t v = (\epsilon - \tilde{S}v)v, \quad (57)$$

where $\epsilon = 2 - d$ and \tilde{S} is given by Eq. (44). For $\epsilon > 0$ there is a nontrivial stable fixed point $v^* = \epsilon/\tilde{S}$. In the vicinity of this fixed point the relevant parameter u scales as $\partial_t u = (2 - 3\epsilon)u$ and thus its new scaling dimension is

$$[u] = 2 - 3\epsilon = 3d - 4. \quad (58)$$

This leads to the non-mean-field exponent β given by

$$\beta = d/[u] \approx 1 + \epsilon. \quad (59)$$

The fact that $\beta > \beta^{MF} = 1$ means that the actual density in $d < 2$ is less than the mean-field prediction. The fluctuations drive the system closer to extinction. Cardy and Täuber [5] suggested that for $d < d'_c \approx 4/3$ there is an extinct phase at finite μ and the transition to the active phase takes place at some $\mu_c > 0$ and estimated the corresponding critical exponents. Recently, the PC model was reexamined employing the so-called nonperturbative renormalization group method by Canet *et al.* [26,82]. They confirmed the existence of the $\mu > 0$ transition for the PC model below $d'_c = 4/3$ and estimated the exponents with fair accuracy for $d = 1$.

B. Generalized PC models

One may invent other models conserving parity. For example, Cardy and Täuber [5] considered the class of parity conserving models $2A \rightarrow 0$, and $A \rightarrow (m+1)A$ with even m . The corresponding reaction Hamiltonian is $H_R = [uph_m(p) - vq](p^2 - 1)q$, where $h_m(p) = (p^m - 1)/(p^2 - 1)$ is an even polynomial. Its phase portrait is topologically identical to Fig. 10. Thus one expects this reaction set to belong to the

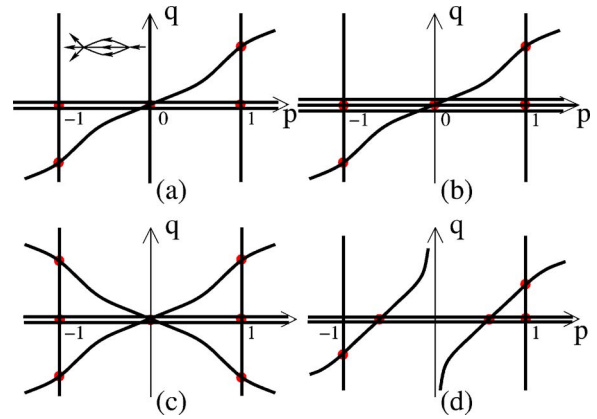
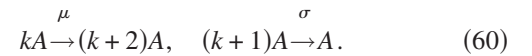


FIG. 11. (Color online) Phase diagrams of kPC models. (a) 2PC model, the inset shows the diagram leading to the logarithmic corrections in $d = 1$. (b) 3PC model. (c) 2PC model with all reactions including only an even number of particles. This topology is not stable and evolves towards (a). (d) 2PC with $2A \rightarrow 0$, the corresponding topology is essentially equivalent to the 2CPD model, Fig. 6.

same universality class as the PC model. This was indeed the conclusion of Ref. [5].

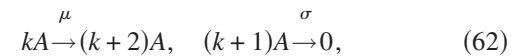
To find a different topology of the phase portrait and therefore a new universality class one needs to impose an additional symmetry. Following Sec. IV B, we shall consider parity conserving reactions with minimal number $k > 1$ needed to initiate all reactions. For example, consider a parity conserving set of reactions with even k :



The reaction Hamiltonian is

$$H_R = [up^{k-1} - v h_k(p)q]p(p^2 - 1)q^k, \quad (61)$$

where $h_k(p)$ is an even polynomial of the degree $k-2$, $u = \mu/k!$, and $v = \sigma/(k+1)!$. The corresponding phase portrait is depicted in Fig. 11(a). For an odd k a representative set of reactions is



with the reaction Hamiltonian

$$H_R = [up^k - v h_{k+1}(p)q](p^2 - 1)q^k, \quad (63)$$

where $h_{k+1}(p)$ is an even polynomial of degree $k-1$. The corresponding phase portrait is depicted in Fig. 11(b). These phase portraits are topologically stable upon RG transformations and thus represent a set of distinct universality classes. We call them k -particle parity conserving (kPC) classes.

Assigning the scaling dimensions as in the PC model, $[p] = 0$, $[q] = d$, and $z = 2$, one finds $[u] = 2 - (k-1)d$ and $[v] = 2 - kd$. At the critical dimension v turns out to be relevant and thus $d_c = 2/k$. Therefore at any physical dimension the kPC behavior is described by the mean field. The only exception is the 2PC model, Fig. 11(a), which acquires logarithmic corrections to the mean-field scaling at $d = 1$. The renormalization is due to the two-loop diagrams built with

the help of the p^3q^3 vertex; see the inset in Fig. 11(a).

Other attempts to generalize the PC universality class appear to be unstable against RG transformations. For example, consider a parity conserving set which contains only an *even* number of reagents: $2A \rightarrow 4A$ and $4A \rightarrow 0$. The corresponding reaction Hamiltonian is given by $H_R = [up^2 - v(1+p^2)q^2](p^2 - 1)q^2$. Its phase portrait is depicted in Fig. 11(c). In addition to the PC symmetry, Eq. (54), the Hamiltonian and the phase portrait possess

$$q \rightarrow -q \quad (64)$$

symmetry. However, this is *not* the symmetry of the full action, Eq. (3). Therefore this symmetry is not stable against the RG transformations. Indeed, e.g., using three vertexes p^2q^2 , one may generate a p^3q^3 vertex which violates the symmetry (64). As a result the system belongs to the 2PC class and its phase portrait drifts towards Fig. 11(a).

One may add a competing annihilation reaction to the $kA \rightarrow (k+2)A$ process of kPC for $k \geq 2$, such as $kA \rightarrow (k-2)A$. For example,



Because of the competition, one expects the absorbing-state transition to happen at $m=2\mu-\lambda=0$. The Hamiltonian is $H_R = (m-u+up^2-vpq)(p^2-1)q^2$; it obeys the PC symmetry (54). The phase portrait is plotted in Fig. 11(d). One notices that in the vicinity of the transition the *local* topology is indistinguishable from Figs. 6 and 7(a). Therefore the transition belongs to the same universality class as 2CPD (see Sec. IV B). This fact was already noticed in numerical simulations [44,47], but, to the best of our knowledge, remained unexplained. The identity of the phase portrait's topologies in the vicinity of transition immediately explains the universality. One can show that the other kPC processes with competition in the k -particle channel belong to the same universality classes as the corresponding kCPD models. The example of the model, Eq. (65), shows that parity conservation is not a crucial feature to discriminate the PC class (see also Refs. [1,83]). It is rather the topology of the phase portrait in the vicinity of the transition that discriminates various universality classes.

VI. REVERSIBLE REACTIONS

All the phase transitions, discussed above, are associated with a deformation and rearrangement of a characteristic *triangular* structure (possibly with one degenerate side) on the phase plane. There is one more possibility for a stable transition topology which is a *rectangular* structure. All models exhibiting rectangular topology consist of a *single* reaction which is allowed to go in both directions with different rates.

Consider, for example, the reversible reaction [same as DP, Eq. (27), but without $A \rightarrow 0$]



The corresponding reaction Hamiltonian is

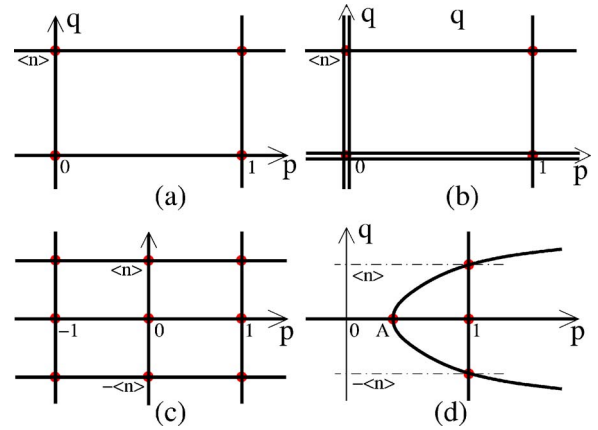


FIG. 12. (Color online) (a)–(c) Phase portraits of reversible reactions. (a) $A \leftrightarrow 2A$ and (b) $2A \leftrightarrow 3A$. (c) Parity conserving $A \leftrightarrow 3A$. (d) A topology with $q \rightarrow -q$ symmetry unstable against RG transformations; see Sec. VII.

$$H_R = \mu(p^2 - p)q + \frac{\sigma}{2}(p - p^2)q^2 = (p^2 - p)(uq - vq^2), \quad (67)$$

where $u = \mu$ and $v = \sigma/2$. The phase portrait is depicted in Fig. 12(a) and has characteristic rectangular shape comprised by the generic lines $p=1$ and $q=0$ along with the *two* “accidental” ones $p=0$ and $q=u/v$. The mean field predicts the average density to be $\langle n \rangle = u/v$. The control parameter is $u = \mu$ with the critical value $u_c = 0$. Consequently the mean-field “magnetization” exponent is $\beta = 1$, in agreement with the general scheme [70]; cf. Eqs. (50) and (51). One may ask if the mean-field behavior can be modified by the fluctuations.

To answer this question, one notices that the phase portrait topology is stable against renormalization. I.e., no terms violating the rectangular structure are generated. It may be checked either by considering possible diagrams or realizing that the action possesses the symmetry

$$p \rightarrow \frac{v}{u}q, \quad q \rightarrow \frac{u}{v}p, \quad t \rightarrow -t. \quad (68)$$

To keep the entire interval $p \in [0, 1]$ unchanged upon rescaling [84], one has to choose the scaling dimensions as $[p] = 0$ and $[q] = d$, then $[u] = 2$ and $[v] = 2 - d$. From here one concludes that the critical dimension is $d_c = 2$. The RG equations are

$$\partial_t u = (2 - \tilde{S}v)u, \quad (69)$$

$$\partial_t v = (\epsilon - \tilde{S}v)v, \quad (70)$$

where $\epsilon = 2 - d$ and \tilde{S} is given by Eq. (44). For $\epsilon > 0$ there is a stable fixed point at $v^* = \epsilon/\tilde{S}$. In its vicinity u scales as $\partial_t u = (2 - \epsilon)u$; thus its new scaling dimension is $[u] = 2 - \epsilon = d$ (see also Appendix B). As a result, the exponent is given by $\beta = d/[u] = 1 + O(\epsilon^2)$. At least in this order, it is not affected by the fluctuations. In fact, $\beta = 1$ is proven to be exact in d

$\beta=1$, Ref. [12]. Using detailed balance, Ref. [84] argues that $\beta=1$ is exact in any dimension.

A generic reversible reaction $kA \leftrightarrow mA$, with $m > k$, is described by $H_R = (p^m - p^k)(uq^k - vq^m)$. Its zero-energy lines are $q=0$ and $p=0$, both k times degenerate, along with nondegenerate $p=1$ and $q=\langle n \rangle = (u/v)^{1/(m-k)}$. For the parity conserving case ($m-k$ even) also $p=-1$ and $q=-\langle n \rangle$, Fig. 12(c). By a proper rescaling of p and q the Hamiltonian may be brought to the symmetric separable form $H_R = -f(p)f(q)$. The corresponding action is symmetric against $p \leftrightarrow q$ and $t \rightarrow -t$. Therefore the rectangular structure is stable in the course of renormalization. The topological structure is fully determined by the index k and the parity.

Therefore, one may identify two more families of universality classes. One is parity nonconserving, represented by the reversible reaction



(a higher number of offsprings, $k+1+2n$, does not change the universality class) with the reaction Hamiltonian

$$H_R = (p-1)(u-vq)p^k q^k. \quad (72)$$

We denote it as k -particle reversible (kR). The action possesses the symmetry (68), rendering stability of the rectangular topology. The upper critical dimension is $d_c = 2/k$. An example is $2A \leftrightarrow 3A$ [see Fig. 12(b)], with $d_c = 1$.

The parity conserving reversible reactions



(a higher number of offsprings, $k+2n$, does not alter the universality class) with the reaction Hamiltonian

$$H_R = (p^2-1)(u-vq^2)p^k q^k. \quad (74)$$

We denote it as kRPC. The corresponding action is symmetric against two symmetries, Eqs. (54) and (68). They impose stability of the rectangular topology symmetric with respect to reflection around the origin. The critical dimension of the kRPC family is $d_c = 2/(k+1)$. An example is $A \leftrightarrow 3A$ [see Fig. 12(c)] with $d_c = 1$. All other reactions of this type have $d_c < 1$ and thus are fully described by the mean-field treatment (see, however, Ref. [70]).

VII. CONCLUSIONS

We have argued that the universality classes of phase transitions in reaction-diffusion models may be classified according to the topological structures of the corresponding phase spaces. This structure is fully encoded in the web of the zero-energy trajectories. The simplest and most stable structure is given by three mutually intersecting lines. By changing a single control parameter the three intersection points may be made to coalesce; see Fig. 5. At such a value of the control parameter the system undergoes a phase transition into the absorbing phase. The corresponding universality class is known as directed percolation.

There are only a limited number of ways to organize a *continuous* phase transition, governed by a *single* control parameter, which utilizes topology different from the DP. We

have identified *four* families of such transitions, which are stabilized by an additional symmetry or symmetries.

(i) A generic reaction set constrained by the requirement that *all* reactions need at least k incoming particles. The corresponding phase portrait is bound to have the $q=0$ line to be k times degenerate, Fig. 7. This property is robust against RG transformations. Indeed, no vertices with fewer than k external q “legs” can be generated. The triangular topology with one k -degenerate line, Fig. 7, defines a family of universality classes. We call them kCPD’s ($k=1$ is DP). The scaling considerations suggest that their upper critical dimension is $d_c = 4/k$ [81].

(ii) A set of reactions which conserve parity. In this case the Hamiltonian and the action are invariant under the transformation (54). It dictates the reflection symmetry of the corresponding phase portraits, Figs. 10 and 11. The symmetry is preserved upon renormalization. In addition to parity conservation one may require a minimal number k of incoming particles for every reaction. This generates the phase portraits depicted in Fig. 11. There is one universality class for every k , termed kPC, Figs. 11(a) and 11(b) ($k=1$ is PC). Their upper critical dimension is $d_c = 2/k$. To realize a kPC transition, the reaction starting from the minimal number k of particles must go only up—e.g., $kA \rightarrow (k+2)A$. By adding a downgoing reaction—e.g., $kA \rightarrow (k-2)A$ (for $k \geq 2$)—the model is transformed into the kCPD class (despite the parity conservation).

(iii) A single reaction which is allowed to go both directions, with different rates: $kA \leftrightarrow (k+1+2n)A$. The corresponding reaction Hamiltonian and the action are symmetric under the exchange transformation, Eq. (68). The phase portrait has the stable rectangular structure with k -degenerate $p=0$ and $q=0$ lines, Figs. 12(a) and 12(b). Upon decreasing the creation rate the rectangle collapses onto the interval $p \in [0, 1]$. We call such transitions kR. Their critical dimension is $d_c = 2/k$ (same as kPC, but exponents are different in $d < d_c$).

(iv) A single reaction which is allowed to go both directions and conserves parity: $kA \leftrightarrow (k+2n)A$. The corresponding reaction Hamiltonian and the action are symmetric under the *two* symmetry transformations, Eqs. (54) and (68). The corresponding phase portrait has the stable “checked” structure, Fig. 12(c), which collapses when sending the creation rate to zero. We denote such transitions as kRPC. Their critical dimension is $d_c = 2/(k+1)$.

Altogether we identify five nontrivial universality classes with $d_c > 1$: DP, PCPD, 3CPD, PC, and 1R. In addition there are four marginal classes with $d_c = 1$: 4CPD, 2PC, 2R, and 1RPC. In sufficiently high dimensions there are other universality classes not belonging to the four families described above. However, they are bound to be of the *mean-field* type and do not have nontrivial representatives.

We have not found any other stable, topologically distinct structures in the phase space. Consider, for example, the topology depicted in Fig. 12(d). The phase portrait is symmetric under the transformation $q \rightarrow -q$. A corresponding reaction set consists of reactions *all* starting from *odd* number of particles: e.g., $A \rightarrow 0$, $A \rightarrow 2A$, and $3A \rightarrow 0$. The corresponding Hamiltonian [after the shift (30) and neglecting irrelevant

terms] is $H_R=(m+up-vq^2)pq$. By changing the parameter m —e.g., by increasing the rate of annihilation $A \rightarrow 0$ —one may bring the system to the phase transition into the extinction phase. Naively, such a transition is associated with the vertex of the parabola crossing the point $(1,0)$; see Fig. 12(d). Such a topology is different from all those considered above and could represent a new universality class.

However, the $q \rightarrow -q$ symmetric phase portrait, Fig. 12(d), is *unstable* upon renormalization. Indeed, combining two vertices pq^3 and p^2q in the loop, one generates the pq^2 term, which violates the symmetry. This term represents the induced reaction $2A \rightarrow A$, originating from two reactions $A \rightarrow 2A$ followed by $3A \rightarrow 0$. In other words, $q \rightarrow -q$ is *not* a symmetry of the action and therefore it is not preserved by the RG. As a result, the initially symmetric zero-energy line $p=(vq^2-m)/u$ is shifted and deformed upon renormalization. The topology drifts either towards the first order scenario, Fig. 2, or towards the DP, Fig. 5. To keep the vertex of the parabola right at the $q=0$ line, one has to fine-tune at least one additional control parameter, besides m . This is the case of a tricritical transition point [35–39].

In the present work we have restricted ourselves to the one-component reactions. It is desirable to extend the strategy to reaction-diffusion models with several reagents. Each new reagent brings an additional reaction coordinate and corresponding momentum. E.g., a two-component model requires four-dimensional phase space with 3D surfaces of constant energy. The corresponding classical dynamics may be not integrable, making the phase-space topology rather complicated. The situation may be simplified by the presence of conservation laws. For example, reaction $A+B \rightarrow 2B$ conserves the number of particles. This leads to a classical dynamics with an additional integral of motion, besides energy. It is most clearly seen after a canonical transformation [87] $p=e^P$, $q=Qe^{-P}$, which leads to the integral of motion $Q_A+Q_B=\text{const}$. Even with such simplifications understanding the full phase-space dynamics of multicomponent systems remains a challenge.

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APPENDIX A: 2CPD MODEL

Here we consider the 2CPD model (same as PCPD) which was shown to exhibit runaway RG flow for $d \leq 2$; see Sec. IV B. We shall argue that this behavior of the RG indicates a rearrangement of the ground state, such that the vacuum supports the anomalous averages of the type $\langle q^2 \rangle$, similar to the BCS theory.

In a vicinity of the phase transition the action of the model is given by Eq. (3) with the reaction Hamiltonian (39). To ensure convergence of the functional integral, it is conve-

nient to perform rotation of the integration contour in the complex p plane: $p \rightarrow ip$. This way one arrives at an action of the form

$$S = \int dt d^d x [ip(\partial_t q - D\nabla^2 q - mq^2 + vq^3) + up^2 q^2]. \quad (\text{A1})$$

We note, in parentheses, that this is the Martin-Siggia-Rose action of the following Langevin process with the multiplicative noise η :

$$\partial_t q = D\nabla^2 q + mq^2 - vq^3 + q\eta(x,t), \quad (\text{A2})$$

where $\langle \eta(x,t)\eta(x',t') \rangle = 2u\delta(x-x')\delta(t-t')$.

We shall assume now that the vacuum of the theory supports the anomalous average value

$$\langle q^2(x,t) \rangle = \Delta, \quad (\text{A3})$$

which is to be determined from the self-consistency condition. Neglecting the nonlinear fluctuation terms, the action acquires the form

$$S = \int dt d^d x [ip(\partial_t - D\nabla^2 + v\Delta)q + u\Delta p^2 - im\Delta p]. \quad (\text{A4})$$

With this Gaussian action one can evaluate $\langle q^2(x,t) \rangle$ and impose the condition (A3). This leads to the self-consistency equation

$$\Delta = u\Delta \int \frac{d^d k}{Dk^2 + v\Delta} + \frac{m^2}{v^2}. \quad (\text{A5})$$

Without the first term on the RHS, $\Delta=(m/v)^2$, this is simply the mean-field prediction for $\langle q^2(x,t) \rangle$. In $d \leq 2$ this equation has a nontrivial solution even at $m=0$. In particular at $d=2$ one finds

$$\Delta^{(d=2)} = \frac{\Lambda^2 D}{v} e^{-4\pi D/u}, \quad (\text{A6})$$

where $\Lambda \sim 1/a$ is the momentum cutoff. In $d < 2$ one obtains

$$\Delta^{(d<2)} \sim \frac{D}{v} \left(\frac{u}{(2-d)D} \right)^{2/(2-d)}. \quad (\text{A7})$$

As a result, one finds that the “order parameter” Δ is associated with the “coherence length” ξ , given by

$$v\Delta = D\xi^{-2}. \quad (\text{A8})$$

Notice that ξ is exactly the characteristic spatial scale for the breakdown of the RG treatment of Sec. IV B; see Eq. (45). This consideration suggests that the divergence of the RG flow is associated with the development of the anomalous average, Eq. (A3).

Let us mention a two-field coupled Langevin description that has been proposed for the related pair contact process without diffusion [85] and for 2CPD model as well [86]. In both cases a pair field and a singlet field were introduced in

order to show a phase transition and estimate the critical exponents (in fair agreement with those reported for microscopic models). More work is needed to appreciate the connections (if any) with our anomalous average microscopic approach.

APPENDIX B: FUNCTIONAL RENORMALIZATION GROUP

In some problems one cannot focus on the immediate vicinity of the $(1, 0)$ point in the phase plane (p, q) . Instead, one has to keep under consideration the entire interval $p \in [0, 1]$, or even $p \in [-1, 1]$. This happens, e.g., in parity conserving models, because of the $p \rightarrow -p$, $q \rightarrow -q$ symmetry. To keep the p interval intact upon renormalization, one must choose the scaling dimension $[p]=0$. Since the bare scaling requires $[p]+[q]=d$, one is left with the naive scaling dimension $[q]=d$. With such scaling dimensions one may restrict the reaction Hamiltonian to the lowest powers in q (typically the first and second), but one must keep *all* powers of p . As a result, one has to employ the functional RG treatment (cf. Ref. [67]).

The generic reaction Hamiltonian for the absorbing-state models, mentioned above, is

$$H_R = f(p)q - g(p)q^2, \quad (\text{B1})$$

where $f(p) = \sum_n f_n p^n$ and $g(p) = \sum_n g_n p^n$ are polynomials of p . From the normalization condition (12) it follows that

$$f(1) = g(1) = 0. \quad (\text{B2})$$

Specific models may possess additional symmetries which dictate further restrictions on the polynomials $f(p)$ and $g(p)$; e.g., for PC models $f(p)$ is odd, while $g(p)$ is even; due to parity conservation: $p \rightarrow -p$, $q \rightarrow -q$. We shall keep the presentation general, imposing these additional symmetries at a latter stage. Because of the assigned bare scaling dimensions $[p]=0$, $[q]=d$, and $z=2$, one finds $[f_n]=2$ and $[g_n]=2-d$. Thus the formal critical dimension is $d_c=2$.

The one-loop renormalization is given by the two-vertex loops and leads to the following set of the RG equations:

$$\partial_l f_n = 2f_n - \frac{1}{2} \tilde{S} \sum_{m,k} m(m-1) \delta_{n,m+k-2} f_m g_k, \quad (\text{B3})$$

$$\partial_l g_n = \epsilon g_n - \frac{1}{2} \tilde{S} \sum_{m,k} m(m-1) \delta_{n,m+k-2} g_m g_k, \quad (\text{B4})$$

where $\epsilon=2-d$ and \tilde{S} is given by Eq. (44). The factors $\frac{1}{2}m(m-1)$ describe the combinatorial number of pairs which may form the loop. The δ symbols enforce the proper number of the external (slow) ‘‘legs.’’ Equations (B3) and (B4) may be written as coupled partial differential equations for the functions $f(p, l) = \sum_n f_n(l) p^n$ and $g(p, l) = \sum_n g_n(l) p^n$:

$$\partial_l f = 2f - \frac{1}{2} \tilde{S} g \partial_p^2 f, \quad (\text{B5})$$

$$\partial_l g = \epsilon g - \frac{1}{2} \tilde{S} g \partial_p^2 g. \quad (\text{B6})$$

For $\epsilon > 0$, Eq. (B6) predicts the nontrivial stable fixed-point polynomial $g^*(p)$, satisfying $\partial_p^2 g^* = 2\epsilon/\tilde{S}$. In view of Eq. (B2) the proper solution is

$$g^*(p) = \frac{\epsilon}{\tilde{S}} (p-1)(p+\kappa), \quad (\text{B7})$$

where the parameter κ is not specified at this stage. Substituting this in to Eq. (B5) one finds

$$\partial_l f = 2f - \frac{\epsilon}{2} (p-1)(p+\kappa) \partial_p^2 f. \quad (\text{B8})$$

Since this is a linear equation, one may look for its solution in the form

$$f(p, l) = \sum_n e^{(2-E_n)l} \phi_n(p), \quad (\text{B9})$$

where the eigenfunctions $\phi_n(p)$ are solutions of the stationary equation

$$E_n \phi_n(p) = \frac{\epsilon}{2} (p-1)(p+\kappa) \partial_p^2 \phi_n(p). \quad (\text{B10})$$

Notice that if one chooses $\phi_n(j)$ to be a n th-degree polynomial, the RHS of Eq. (B10) is also a polynomial of the same degree. It is clear then that one may always find a solution $\phi_n(p)$ as a polynomial of the degree n . This means that if one started from a polynomial of some degree N , higher powers will not be generated by the RG. That is, the sum in Eq. (B9) is always confined to $1 \leq n \leq N$.

To find the eigenenergies E_n one needs to compare the coefficients of the leading power of p on both sides of Eq. (B10). This leads to $E_n = n(n-1)\epsilon/2$. From here and Eq. (B9) one finds that the scaling dimensions of the coefficients of the $f(p)$ polynomial at the nontrivial fixed point, Eq. (B7), are

$$[f_n] = 2 - E_n = 2 - n(n-1)\epsilon/2. \quad (\text{B11})$$

The conclusion is that it is sufficient to keep the polynomials $g(p)$ to be of the second degree [cf. Eq. (B7)] while $f(p)$ to be of the lowest possible degree consistent with the symmetries of the model.

In the PC model of Sec. V A, $g(p)$ must be even and thus $\kappa=1$, leading to $g(p) = g_2(p^2-1)$. On the other hand, $f(p)$ must be odd and at least of degree $n=3$ [$n=1$ odd polynomial cannot satisfy Eq. (B2)]. Therefore it can be chosen to be $f(p) = f_3(p^3-p)$. At the fixed point $g_2^* = \epsilon/\tilde{S}$ and $[f_3]=2-3\epsilon$. This justifies treatment of Sec. V A with the identifica-

tion $v=g_2$, and $u=f_3$.

In the reversible model $A \leftrightarrow 2A$ of Sec. VI, $g(p)=v(p^2-p)$ and thus $\kappa=0$. On the other hand, $f(p)=u(p^2-p)$ which is the proper stationary eigenfunction of Eq. (B10): $\phi_2(p)$. As

a result, no other terms in $f(p)$ polynomial are generated upon renormalization. This is consistent with the robustness of the rectangular structure. Since $u=f_2$, its scaling dimension according to Eq. (B11) is $[u]=2-\epsilon$.

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- [78] In fact the action, Eq. (32), after a proper rescaling possesses the rapidity symmetry $p \rightarrow -q$, $q \rightarrow -p$, and $t \rightarrow -t$, which shows the equivalence of u and v vertices. This “rapidity reversal” symmetry of the DP action implies the asymptotic equivalence of the survival probability and the order parameter decay at criticality. Due to this symmetry, the number of independent critical exponents for directed percolation is reduced compared to general absorbing phase transitions (see Refs. [3,4] and references therein).
- [79] In principle, $k=4$ may exhibit a marginally non-mean-field behavior in $d=1$, but we shall not try to investigate it here.
- [80] The restricted “fermionic” models may exhibit a different critical behavior in low-dimensional systems, than unrestricted models. The most striking example is a restricted analogy of the 2CPD model *without* diffusion (so-called pair contact process PCP). The PCP model belongs to DP universality class (even though there exist an infinitely many absorbing states [88,89]).
- [81] This leaves the possibility that even for $d>2$ the RG flows towards a strong-coupling fixed point, if the bare nonlinearity is sufficiently strong. As a result one may expect to observe a non-mean-field behavior for $d>2$.
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