Effective Langevin equations for the pair contact process with diffusion

Ivan Dornic,1 Hugues Chaté,1 and Miguel A. Muñoz2

1CEA – Service de Physique de l’État Condensé, Centre d’Études de Saclay, 91191 Gif-sur-Yvette, France
2Instituto de Física Teórica y Computacional Carlos I, Universidad de Granada, 18071 Granada, Spain

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We propose a system of coupled, real-valued, effective Langevin equations for the nonequilibrium phase transition exhibited by the pair contact process with diffusion (and similar triplet and quadruplet, n- uplet, processes). A combination of analytical and numerical results demonstrate that these equations account for all known phenomenology in all physical dimensions, including estimates of critical exponents in agreement with those reported for the best-behaved microscopic models. We show in particular that the upper critical dimension of these n-uplet transitions is \( \frac{d_n}{2} \), and \( d_n-1 \) for their anisotropic (biased) versions.

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Whereas there exists ample evidence of universality among out-of-equilibrium phase transitions, their full classification is by no means achieved. At equilibrium, coarse-grained descriptions in terms of Ginzburg-Landau-Wilson free-energy functionals and their associated Langevin equations encode in a systematic way the symmetries, conservation laws, and dimensionalities determining universality classes. Out of equilibrium, even the relevant ingredients are still debated, and continuous stochastic descriptions are often missing, so that the non-stochastic counterpart of the celebrated taxonomy by Hohenberg and Halperin [1] remains a distant achievement. Here we are interested in irreversible phase transitions into fluctuation-less absorbing states. Such transitions abound in non-equilibrium physical phenomena such as epidemics, catalysis, synchronization, or self-organized criticality [2]. The prominent directed percolation (DP) class, which encompasses all phase transitions into a single absorbing state (without additional symmetries, conservation laws, or disorder), well-established both theoretically and numerically, can be characterized by the following Langevin equation for a single coarse-grained, real density field \( \rho = \rho(x,t) \):

\[
\partial_t \rho = D \nabla^2 \rho + a \rho - b \rho^2 + \sigma \rho^4 \eta(t)
\]

(1)

where \( \eta = \eta(x,t) \) is a Gaussian white noise whose influence vanishes in the absorbing state \( \rho = 0 \). In spite of some recent progress in the search for Langevin descriptions of other classes of absorbing phase transitions, the situation of the DP class remains exceptional. Indeed, even if Eq. (1) can be derived rigorously for some reaction-diffusion models in this class, such Langevin equations sometimes simply do not exist. For example, for the simple annihilation process \( 2A \rightarrow 0 \) it is well-known that one obtains “imaginary noise” (see below), which precludes a well-behaved Langevin equation [3].

Reaction-diffusion systems where creation and annihilation processes require pairs of particles (while isolated ones can diffuse but not react) are usually considered to represent the pair-contact process with diffusion (PCPD) class. Studies of various models in this (putative) class have produced a series of conflicting results and opinions (see [4] for a review and references therein). From the numerical side it is still debated whether in \( d = 1 \) the PCPD behaves as DP or not, as numerics are often plagued with long transients [4, 5, 6, 7, 8, 9, 10, 11]. What seems to be widely accepted is that the upper critical dimension \( d_c \) is not 4 as in DP, but \( d_c = 2 \) [6, 12, 13]. It has also been shown numerically that when a bias (anisotropy) is introduced in the diffusion of isolated particles, the critical dimension is reduced to \( d_c = 1 \) (at odds with what happens for DP where biased diffusion plays no significant role) [14]. At the analytical level Janssen et al. [15] recently showed that a perturbative renormalization group analysis of the field theory derived from the microscopic reactions \( 2A \rightarrow 3A, 2A \rightarrow 0/A \) (together with diffusion of isolated \( A \) particles) yields only unphysical fixed points and runaway trajectories. Generalizations of the PCPD requiring triplets or quadruplets of particles for the reactions (respectively called TCPD and QCPD for “triplet and quadruplet contact process with diffusion”; \( n \)-CDP in general) have also been studied, with results at least as controversial as those for the PCPD [4, 16, 17].

What makes these problems interesting beyond the usual skirmishes between specialists is that the ingredient which seems to lead out of the DP class is the fact that 2 (\( n \), in general) particles are needed for reactions to occur. That such a microscopic constraint, not related to any new symmetry nor conservation law, should determine universal properties may indeed appear unacceptable, hence the opinion, held by some authors [9, 10, 11], that the observed critical behavior will eventually turn up to be in the DP class. Elucidating the critical behavior of the PCPD has thus become a milestone in the ongoing debate about universality out-of-equilibrium.

In this Letter, we propose a system of coupled, real-valued, effective Langevin equations for the nonequilibrium phase transition exhibited by the PCPD (and of the allied \( n \)-CDP models). Analyses of these equations allow us: i) to show that \( d_c = \frac{d_n}{2} \) with a reduction by unity...
when a biased diffusion is switched on, ii) to reproduce the correct (mean-field) critical exponents above $d_c$ in all cases, and iii) to estimate by direct numerical integration of these equations critical exponents in agreement with those of the best microscopic models in any dimension.

A continuous description of the PCPD problem, if possible at all, should be in terms of at least two fields as converging conclusions signal 14 15. Indeed, a two-field Langevin description has been successfully proposed for the related pair contact process without diffusion, the prototypical model with infinitely-many-absorbing states 3. As for that case, here a “pair-field” and a “singlet field” is the most natural choice. To build up a set of Langevin equations, we start from the following microscopic two-species reaction-diffusion model in the PCPD family 7: pair-activity is represented by usual DP-like reactions $B \rightarrow 2B$, $B \rightarrow 0$ while isolated particles diffuse and undergo pair annihilation $2A \rightarrow 0$. The two species are coupled cyclically: $B \rightarrow 2A$ (a “pair” separates into 2 particles) and $2A \rightarrow B$ (2 particles recombine into a “pair”). Using well-trodden techniques (see, e.g., 12), one arrives at the following coupled equations:

$$\begin{align*}
\partial_t \psi_B &= D_B \nabla^2 \psi_B + a_B \psi_B - b_B \psi_A^2 + c_B \psi_A^2 + \sigma_B \psi_B \eta_B \\
\partial_t \psi_A &= D_A \nabla^2 \psi_A - b_A \psi_A^2 + c_A \psi_B + i \sigma_A \psi_A \eta_B,
\end{align*}$$

(2)

where all coefficients depend on microscopic reaction rates and diffusion constants, and $\eta_A$ and $\eta_B$ are Gaussian white noises (including some cross correlations not specified here). The mapping through the two-species model disentangles the competition between the real, DP-like component of the noise, and the imaginary one (arising from the annihilation reaction $2A \rightarrow 0$) 20. But now both fields $\psi_A$ and $\psi_B$ are complex, and even though their noise-averages do correspond to the local densities $\rho_A$ and $\rho_B$ of $A$ and $B$ particles, the same is not true for higher-order moments, impeding physical intuition.

However, perusal of simulation results of PCPD-like models suggests that annihilation is only predominant deep inside the absorbing phase, and not in the active one nor around the critical point. Indeed, slightly subcritical quenches reveal a quasi-exponential departure from the critical power-law scaling, with the typical annihilation decay is $\ln t/t$ for pure annihilation, while for $d > 2$ the mean-field pure-annihilation decay $1/t$ imposes $\alpha = 2$. In the marginal case $d = 2$, the annihilation decay is $\ln t/t$, and the incriminated terms in Eqs. 3 have to be completed by logarithmic factors ($\pm \rho_A^2 / \ln(1/\rho_A)$). From these “bare” equations, one readily realizes that some extra terms — in particular a cross term $\omega \rho_A \rho_B$ in the $\rho_B$ equation or a noise term $\sigma' \sqrt{\rho_B} \eta_A$ in the $\rho_A$ equation — are generated perturbatively once the effect of fluctuations is taken into account. Thus these terms should be incorporated from the beginning, and disregarding now all noises and derivatives, one arrives at the mean-field decay equations

$$\begin{align*}
\partial_t \rho_B &= D_B \nabla^2 \rho_B + a_B \rho_B - b_B \rho_A^2 + c_B \rho_A^2 + \sigma_B \rho_B \eta_B \\
\partial_t \rho_A &= D_A \nabla^2 \rho_A - e \rho_A^2 + f \rho_B,
\end{align*}$$

(3)

which themselves change with dimension: for $d = 1$, one has $\alpha = 3$ since the singlet-field must decay like $1/\sqrt{t}$ for pure annihilation, while for $d > 2$ the mean-field pure-annihilation decay $1/t$ imposes $\alpha = 2$. In the marginal case $d = 2$, the annihilation decay is $\ln t/t$, and the incriminated terms in Eqs. 3 have to be completed by logarithmic factors ($\pm \rho_A^2 / \ln(1/\rho_A)$). From these “bare” equations, one readily realizes that some extra terms — in particular a cross term $\omega \rho_A \rho_B$ in the $\rho_B$ equation or a noise term $\sigma' \sqrt{\rho_B} \eta_A$ in the $\rho_A$ equation — are generated perturbatively once the effect of fluctuations is taken into account. Thus these terms should be incorporated from the beginning, and disregarding now all noises and derivatives, one arrives at the mean-field decay equations

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(3)

where the nonlinear terms for the singlet-field so that it decays, for the space dimension of interest and when the pair-field is set to zero, with the appropriate decay at least on average 21. The abstract fields $\psi_A, \psi_B$ in Eqs. 2 then become the real particle density fields $\rho_A$ and $\rho_B$, governed by the following effective Langevin equations:

as calculated between neighboring blocks of size 64. Two-species PCPD model described in text implemented as in 3 (d = 1, 23 sites, 16 runs).

\begin{graph}
\begin{center}
\includegraphics[width=\textwidth]{Fig1.png}
\end{center}
\end{graph}

FIG. 1: (Color online) Evolution, during a slightly subcritical quench, of the densities of isolated particles $A$ and pair particles $B$, together with the absolute value of the singlet-field noise variance $(b \rho_A)^2$ measured as the connected correlation function of the local density of $A$s calculated between neighboring blocks of size 64. Two-species PCPD model described in text implemented as in 3 (d = 1, 23 sites, 16 runs).
DP one (1) and, therefore, the accurate and efficient integration scheme recently presented in 4 can be employed. Varying the “temperature-like” parameter $a$, an absorbing phase transition is observed, with (apparently) clean scaling behavior at and around the critical point in all tested physical dimensions. As expected from our model building, subcritical quenches show a quasi-exponential departure from the scaling regime, followed by a late annihilation-like decay (without local anti-correlations). In $d = 1$ critical quenches allow to estimate the decay exponent $\theta = \beta/\nu_\parallel = 0.19(1)$ (Fig. 2). Measuring steady-state activity above threshold determines $\beta = 0.33(2)$, while finite-size lifetime statistics at criticality or seed simulations yield differently $z = \nu_\perp/\nu_\parallel = 1.64(3)$ (not shown). Even though the quality of these results, at par with those of the “best” microscopic models, leads to suggest asymptotic values different from that of the DP class in $d = 1$, we prefer in view of recent large-scale simulations in PCPD problems [11], to avoid drawing a conclusion on whether the “true” asymptotic behavior is DP-like or not, based solely on such a small quantitative difference (for the DP class $\theta \simeq 0.16$, $\beta \simeq 0.28$, and $z \simeq 1.58.$) We have extensively checked that these results are robust against both changes in parameter values and inclusion of the extra perturbatively generated terms.

In higher dimensions, the difference with DP transitions becomes qualitative: our simulations in $d = 2$ show that at threshold both fields decay with the same exponent $\theta^{d=2} \simeq 0.50(2)$, the remaining curvature in log-log plots (not shown) indicating the presence of logarithmic behavior for the ratio $\langle \rho_B \rangle/\langle \rho_A \rangle$ characteristic of the marginal dimension (in agreement with microscopic models). For $d = 3$, simulations of Eqs. (3) with $\alpha = 2$ show different scaling at threshold for the two fields: $\theta^{d=3}_A \simeq 0.50(5)$ and $\theta^{d=3}_B \simeq 1.0(1)$, values according with those found in microscopic models (Fig. 3) and with the previously found mean-field predictions. This, and the behavior in $d = 2$ suggests that $d_c = 2$.

We now turn our attention to power-counting arguments aimed at identifying the critical dimension analytically and determining the relevance or irrelevance of the different terms of our Langevin equations. As usual in problems with multiple fields, one has some freedom to perform naive scaling analyses. If we enforce, as usual, the coefficient of $\partial_t \rho_B$ to scale as a constant (fixing in this way the dominant time-scale) and the associated action to be dimensionless, one is ineluctably led to the conclusion that the noise term in the $\rho_B$-equation is the dominant nonlinearity together with the saturation term $-b\rho_B^2$, and that both become relevant below $d_c = 4$ as in DP. This being in contradiction with our findings, it is mandatory to scale in a different way. If we now impose the coefficient of the other time-derivative, $\partial_t \rho_A$, to scale as a constant, we conclude that the main nonlinearity is the (generated) noise term of the $\rho_A$ equation, proportional to $\sqrt{\rho_B}$, which becomes relevant below $d_c = 4/\alpha$.

Therefore $d_c^{PCPD} = 2$ (as $\alpha = 2$ in PCPD above its critical dimension), in agreement with our numerics. One can thus consider that the (activity) pair-field $\rho_B$ is “slaved” to the singlet field $\rho_A$ (which is the leading one, controlling the scaling). This viewpoint is further supported by the numerical observation that the decay-exponent $\theta_B$ experiences a discontinuity at $d_c$ where it jumps from its mean-field value $\theta_B = 1$ above $d_c$ to $\theta_B = \theta_A$ at or below.

Following the above discussion, our final minimal set of effective equations yielding the correct scaling laws (as we have verified numerically) both when fluctuations are relevant and when they can be neglected reads:

$$\begin{align*}
\partial_t \rho_B &= D_B \nabla^2 \rho_B + \alpha \rho_B - \beta \rho_B^2 + c \rho_A^2 + \omega \rho_A \rho_B \\
\partial_t \rho_A &= D_A \nabla^2 \rho_A - \epsilon \rho_A^2 + f \rho_B + \sigma A \rho_B^2 \eta.
\end{align*}$$

(4)

Note the change of perspective from Eqs. (3), which leads to consider the PCPD (and related models) as a system of annihilating random walks wandering between high-activity (pair) clusters, themselves of course self-consistently determined by the complex interplay of the two modes of the dynamics. These clusters act not only as non-trivial boundaries for the isolated particles, but also as fluctuating sources. Since fluctuation effects for $2A \rightarrow \emptyset$ (or $2A \rightarrow A$) in the presence of even a constant source term are known to be relevant up to and including $d = 2$, 22, this provides, in our opinion, an intuitive mechanism which can explain, among other things, why $d_c = 2$ for the PCPD and also why the dynamical exponent is not that of simple random walks 23.

The two-species/two-fields description put forward above is easily extended to the TCPD and QCPD cases 3, 14, 17, by replacing the pair field by a triplet or
FIG. 3: (Color online) Decay of singlet and pair densities during near-critical quenches for \( d = 3 \) PCPD models. (a) Reaction-diffusion model \( 2A \rightarrow 3A, 2A \rightarrow \emptyset \) implemented as in [3]; (b) Integration of the Langevin Eqs. [3] with \( \alpha = 2 \).

quadruplet field: the interpretation of the fields changes but the governing equations [14] remain identical, with an exponent \( \alpha \) chosen according to the corresponding behavior of the pure annihilation processes (\( 3A \rightarrow \emptyset \) or \( 4A \rightarrow \emptyset \)). For \( 3A \rightarrow \emptyset \), the particle density decays as \( \sqrt{\ln t/t} \) in \( d = 1 \), which can be accounted for by \( \alpha = 3 \) with a logarithmic correction, while for \( d > 1 \) mean-field decay \( 1/\sqrt{t} \) (corresponding to \( \alpha = 3 \)) emerges. A striking consequence is that the TCPD class should not exist per se in \( d = 1 \), since its effective Langevin equations are identical to those of the PCPD class (the logarithmic term plays no rôle on asymptotic scaling). Moreover, following the power-counting analysis sketched above, \( d_{c}^{TCPD} = \frac{3}{4} \) (in agreement with [16]), with the mean-field exponents \( \theta_{A} = \frac{1}{3} \) and \( \theta_{B} = 1 \). Now for quadruplet models, the pure-annihilation mean-field decay \( t^{-\frac{1}{2}} \) holds in all physical dimensions and thus \( \alpha = 4 \) always, leading to \( d_{c}^{TCPD} = 1 \). Indeed, in \( d = 1 \) both fields decay with exponent \( \theta = \frac{2}{3} \) with strong log corrections (most likely \( \langle \rho_{A} \rangle / \rho_{B} \) \( \sim \) \( (\ln t)^{1/3} \)), while for \( d > 1 \), \( \theta_{A} = \frac{1}{d} \) and \( \theta_{B} = 1 \) (mean-field results). All these results (in disagreement with some previously published ones) have been verified by simulations of the Langevin equations and of microscopic two-species reaction-diffusion models, and will be reported elsewhere.

Finally, let us discuss the rôle of biased diffusion (anisotropy) for the isolated particles within our picture [14]. Starting either directly from microscopic models, or from symmetry considerations, one realizes that an additional \( \nabla \rho_{A} \) term needs to be introduced in the \( \rho_{A} \) equation. A power counting analysis, analogous to the one discussed above, then reveals that \( d_{c} \) is reduced by one unit, so \( d_{c} = 1 \) for \( \alpha = 2 \) (biased-PCPD) and it is below \( d = 1 \) for larger values of \( \alpha \): the biased TCPD and QCPD are expected to exhibit mean-field behavior in any physical dimension. All these results are in agreement with known ones [14] and have been verified numerically.

Summing up, we have proposed effective coupled Langevin equations governing the densities of a \( n \)-uplet field and a singlet field in reaction-diffusion problems where at least \( n \) particles are required for creation or annihilation to occur. A combination of numerical and analytical arguments have shown that they do reproduce the behavior of microscopic models, and thus provide a sound framework to further study these problems. Such future work should concentrate on a renormalization group treatment of these equations, possibly in a non-perturbative approach. Due to the closeness of estimated exponent values for the PCPD case in \( d = 1 \) with those of the DP class, this appears as the only solution to put an end to the crucial question of whether such problems, below their upper critical dimension, exhibit genuinely novel critical behavior or not.

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