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Phase transitions and correlations in the bosonic pair contact process with diffusion: exact results

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Abstract

The variance of the local density of the pair contact process with diffusion is investigated in a bosonic description. At the critical point of the absorbing phase transition (where the average particle number remains constant) it is shown that for a lattice dimension $d > 2$ the variance exhibits a phase transition: for high enough diffusion constants, it asymptotically approaches a finite value, while for low diffusion constants the variance diverges exponentially in time. This behaviour also appears in the density correlation function, implying that the correlation time is negative. Yet one has dynamical scaling with a dynamical exponent calculated to be $z = 2$.

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1. Introduction

A prototypical example for critical phenomena in nonequilibrium statistical physics is the absorbing phase transition. This is a transition from an active fluctuating phase with a finite particle density to an absorbing state where any dynamics is suppressed. One has found rather robust universality classes, e.g. the class of directed percolation (DP) and the parity conserving (PC) universality class. A member of the DP-class is the pair contact process where two neighbouring particles may create an offspring on a third lattice site or may annihilate each other.

This model extended by particle diffusion—the pair contact process with diffusion (PCPD)—has attracted much interest because it is not known to which universality class it belongs. Several possibilities have been discussed: it was found that some exponents are very close to those of the PC class [1], more recent investigations however give hints of a DP behaviour [2]. It was also suggested that the critical behaviour of the PCPD defines a new universality class [3, 4], or may depend on the diffusion constant [7]. Analytical results are rare in this field and one has to revert to numerical methods such as the density matrix renormalization group (DMRG) or Monte Carlo simulations. An exception is [5] where the PCPD is investigated by a renormalization group approach by applying an ϵ-expansion around the upper critical dimension $d_c = 2$. The computation of the scaling exponents leads to the conclusion that the PCPD belongs to a universality class not known before, but it is not yet settled that these results are applicable to the one-dimensional case [5]. For a comprehensive review of the current state of the art we refer to [6].

Analytical treatment becomes easier for the bosonic description of the model where the exclusion interaction—which constraints the number of particles at one site to at most one—is dropped. In this case a field theoretic approach due to Howard and Täuber [8] is available. A drawback of this approach is that it is not suitable for deciding the universality class of the model with particle number restriction. In this paper, we show by an exact treatment of the model that the diffusion constant and the lattice dimension have considerable impact on the phase transition and correlations of the bosonic PCPD. Although the particle exclusion interaction is crucial for the behaviour of the system this investigation gives some insight into the role of diffusion in the PCPD.

2. Model

We define the following process: on an infinite d-dimensional cubic lattice particles ('A') are diffusing with rate D in each spatial direction. Additionally they branch and annihilate: $k \geqslant 1$ particles A are created with rate μ out of any set of $m \geqslant 1$ particles (m fixed), and $l \geqslant 1$ particles are annihilated with rate λ out of any set of $p \geqslant l$ particles (l fixed):

$$mA \stackrel{\mu}{\rightarrow} (m+k)A \qquad pA \stackrel{\lambda}{\rightarrow} (p-l)A \qquad A\cdot \stackrel{D}{\leftrightarrow} \cdot A. \tag{1}$$

The number of particles on each lattice site is not restricted—the creation and annihilation processes take place on one lattice site. Thus the bosonic representation of the process is used. We try to keep the description as general as possible, but as we will see, analytical results are available only for few cases. In this paper, we investigate the two cases where $p = m = 1$ or $p = m = 2$ and arbitrary k and $l \leqslant p$. One special case is the PCPD, where $m = p = l = 2$ and $k = 1$.

Following the notation and formalism introduced in [9, 10] we define the site occupation numbers as $\vec{n} = \{n(\mathbf{x})\}$. Then the time-dependent probability vector describing the system can be expressed as

$$|F(t)\rangle = \sum_{n(\mathbf{x})} P(\vec{n}, t)|\vec{n}\rangle \tag{2}$$

where the $|\vec{n}\rangle$ are the basis vectors spanning the state space and $P(\vec{n}, t)$ is the probability distribution of the site occupation numbers. The master equation describing the time evolution of the probability distribution can then be written as

$$\frac{\partial}{\partial t}|F(t)\rangle = -\mathcal{H}|F(t)\rangle \tag{3}$$

where $\mathcal{H}$ is the stochastic generator of the system, often called 'Hamiltonian' by analogy of the master equation with the Schrödinger equation (in imaginary time) [11]. Let $a(\mathbf{x})$ and $a(\mathbf{x})^\dagger$ be the space-dependent annihilation and creation operators and $n(\mathbf{x}) = a^\dagger(\mathbf{x})a(\mathbf{x})$ the particle number operator, then the Hamiltonian is given by

$$\begin{aligned}\mathcal{H} = &-D\sum_{k=1}^{d}\sum_{\mathbf{x}}[a(\mathbf{x})a^{\dagger}(\mathbf{x}+\mathbf{k}) + a^{\dagger}(\mathbf{x})a(\mathbf{x}+\mathbf{k}) - 2n(\mathbf{x})]\\ &- \lambda\sum_{\mathbf{x}}\left[(a^{\dagger}(\mathbf{x}))^{(p-l)}(a(\mathbf{x}))^{p} - \prod_{i=1}^{p}(n(\mathbf{x}) - i + 1)\right]\\ &- \mu\sum_{\mathbf{x}}\left[(a^{\dagger}(\mathbf{x}))^{(m+k)}(a(\mathbf{x}))^{m} - \prod_{i=1}^{m}(n(\mathbf{x}) - i + 1)\right]\end{aligned} \tag{4}$$

where $\mathbf{k} \equiv \mathbf{k}(k) = (\ldots, 0, 1, 0, \ldots)^T$ is the kth unit space vector. The time evolution of an operator $b(\mathbf{y})$ is calculated by

$$\frac{\partial}{\partial t}b(\mathbf{y}) = [\mathcal{H}, b(\mathbf{y})]. \tag{5}$$

Using the commutator rule $[a(\mathbf{x}), a^{\dagger}(\mathbf{y})] = \delta_{\mathbf{x},\mathbf{y}}$ we get after straightforward calculations

$$\frac{\partial}{\partial t}\langle a(\mathbf{x})\rangle = D\sum_{k=1}^{d}\{\langle a(\mathbf{x}-\mathbf{k})\rangle + \langle a(\mathbf{x}+\mathbf{k})\rangle - 2\langle a(\mathbf{x})\rangle\} - \lambda l\langle a(\mathbf{x})^{p}\rangle + \mu k\langle a(\mathbf{x})^{m}\rangle \tag{6}$$

$$\begin{aligned}\frac{\partial}{\partial t}\langle a(\mathbf{x})a(\mathbf{y})\rangle \underset{\mathbf{x}\neq\mathbf{y}}{=} &D\sum_{k=1}^{d}\{\langle a(\mathbf{x})a(\mathbf{y}-\mathbf{k})\rangle + \langle a(\mathbf{x})a(\mathbf{y}+\mathbf{k})\rangle + \langle a(\mathbf{x}-\mathbf{k})a(\mathbf{y})\rangle\\ &+ \langle a(\mathbf{x}+\mathbf{k})a(\mathbf{y})\rangle - 4\langle a(\mathbf{x})a(\mathbf{y})\rangle\} - \lambda l\{\langle a(\mathbf{x})a(\mathbf{y})^{p}\rangle + \langle a(\mathbf{x})^{p}a(\mathbf{y})\rangle\}\\ &+ \mu k\{\langle a(\mathbf{x})a(\mathbf{y})^{m}\rangle + \langle a(\mathbf{x})^{m}a(\mathbf{y})\rangle\}\end{aligned} \tag{7}$$

$$\begin{aligned}\frac{\partial}{\partial t}\langle(a(\mathbf{x}))^{2}\rangle = &2D\sum_{k=1}^{d}\{\langle a(\mathbf{x})a(\mathbf{x}-\mathbf{k})\rangle + \langle a(\mathbf{x})a(\mathbf{x}+\mathbf{k})\rangle - 2\langle a(\mathbf{x})^{2}\rangle\}\\ &+ \lambda l\{(1+l-2p)\langle a(\mathbf{x})^{p}\rangle - 2\langle a(\mathbf{x})^{p+1}\rangle\}\\ &- \mu k\{(1-k-2m)\langle a(\mathbf{x})^{m}\rangle - 2\langle a(\mathbf{x})^{m+1}\rangle\}.\end{aligned} \tag{8}$$

Using $\langle n(\mathbf{x})\rangle = \langle a(\mathbf{x})\rangle$ and $\langle n(\mathbf{x})^2\rangle = \langle a(\mathbf{x})^2\rangle + \langle a(\mathbf{x})\rangle$ this set of coupled difference-differential equations allows for the analytical calculation of the time-dependent expectation value of the particle density and its autocorrelation in some special cases.

We restrict ourselves to the case $p = m$ where the creation and annihilation processes are balanced and an absorbing phase transition can be found. For $\lambda l > \mu k$ the particles die out exponentially ($p = m = 1$) or according to a power law ($p = m > 1$), while for $\lambda l < \mu k$ the particle density diverges. Here a crucial difference between the description with and without particle number restriction can be seen: while in the models with exclusion interaction the absorbing phase transition is of a second order, the bosonic model exhibits a first-order transition.

In analogy with the exclusion model we call the rate which divides the two different behaviours the 'critical' rate, which from equation (6) can be read off as

$$\lambda_{\mathrm{c}} = \mu k/l \tag{9}$$

for a given μ. For this rate the particle density is constant for all times $\langle a(\mathbf{x}, t)\rangle = \rho_0$ (for homogeneous initial conditions), as can be seen from equation (6) which reduces to a diffusion equation. Thus the interesting quantity is the variance $\sigma^2 = \langle n(\mathbf{x})^2\rangle - \langle n(\mathbf{x})\rangle^2$ which we shall investigate in what follows.

Eliminating p and λ in equations (6)–(8) one gets

$$\begin{aligned}
\frac{\partial}{\partial t}\langle a(\mathbf{x})\rangle &= D\sum_{k=1}^{d}\{\langle a(\mathbf{x}-\mathbf{k})\rangle + \langle a(\mathbf{x}+\mathbf{k})\rangle - 2\langle a(\mathbf{x})\rangle\} \\
\frac{\partial}{\partial t}\langle a(\mathbf{x})a(\mathbf{y})\rangle &\underset{\mathbf{x}\neq\mathbf{y}}{=} D\sum_{k=1}^{d}\{\langle a(\mathbf{x})a(\mathbf{y}-\mathbf{k})\rangle + \langle a(\mathbf{x})a(\mathbf{y}+\mathbf{k})\rangle + \langle a(\mathbf{x}-\mathbf{k})a(\mathbf{y})\rangle \\
&\qquad + \langle a(\mathbf{x}+\mathbf{k})a(\mathbf{y})\rangle - 4\langle a(\mathbf{x})a(\mathbf{y})\rangle\} \\
\frac{\partial}{\partial t}\langle (a(\mathbf{x}))^2\rangle &= 2D\sum_{k=1}^{d}\{\langle a(\mathbf{x})a(\mathbf{x}-\mathbf{k})\rangle + \langle a(\mathbf{x})a(\mathbf{x}+\mathbf{k})\rangle - 2\langle a(\mathbf{x})^2\rangle\} + \mu k(k+l)\langle a(\mathbf{x})^m\rangle.
\end{aligned} \tag{10}$$

We see that this set of equations is only closed for the cases $m = 1$ or $m = 2$.

In the case of a vanishing diffusion constant, $D = 0$, the lattice sites are independent of each other. Thus the description of the process reduces to the zero-dimensional case $d = 0$,

$$\frac{\partial}{\partial t}\langle a(\mathbf{x})\rangle = 0 \qquad \frac{\partial}{\partial t}\langle (a(\mathbf{x}))^2\rangle = \mu k(k+l)\langle a(\mathbf{x})^m\rangle \tag{11}$$

and has to be treated separately.

2.1. Contact process with diffusion, $m = 1$

Here, only $l = 1$ is possible. Additionally by rescaling μ we may fix $k = 1$. This case has already been considered in [13] as a model for the clustering of biological organisms [14]. For convenience we summarize the main results here.

For $D = 0$ or $d = 0$ equation (11) directly yields $\langle a(\mathbf{x})^2\rangle = c_0 + c_1 t$ and thus the variance diverges. For $D \neq 0$ the fluctuations of the particle density diverge for dimensions $d \leqslant 2$ while they remain finite for $d > 2$,

$$\langle a(\mathbf{x})^2\rangle = \begin{cases} c_1 t^{-d/2+1} & d < 2 \\ c_2 \ln t & d = 2 \\ c_3 + c_4 t^{-d/2+1} & d > 2 \end{cases} \tag{12}$$

where $t \gg 1$ and $c_0, \ldots, c_4$ are positive constants.

2.2. Pair contact process with diffusion, $m = 2$

We now derive analytically the late-time behaviour of the solution for $m = 2$.

For $D = 0$ or $d = 0$ equation (11) yields

$$\langle a(\mathbf{x}^2)\rangle = \rho_0^2 \exp(t/\tau) \qquad \tau = \frac{1}{\mu k(k+l)}. \tag{13}$$

The variance diverges exponentially in time as opposed to $m = 1$ where the divergence is linear. Only for times small compared to τ the variance (13) grows linearly.

For $D \neq 0$ we get the solution by applying Fourier and Laplace transformations. We also present the crossover from short- to late-time behaviour, which has to be calculated numerically.

First we rescale time by

$$t \to \frac{t}{2D} \tag{14}$$

and define

$$F_{\mathbf{x}}(\mathbf{r},t) = \langle a(\mathbf{x})a(\mathbf{x}+\mathbf{r})\rangle = \langle n(\mathbf{x})n(\mathbf{x}+\mathbf{r})\rangle - \delta_{\mathbf{r},\mathbf{0}}\langle n(\mathbf{x})\rangle$$
$$\alpha = \frac{\mu k(k+l)}{2D}. \tag{15}$$

The parameter α is a measure for the weighting of reaction rates to diffusion, small α corresponds to dominant diffusion, while large α corresponds to dominating reaction rates. In what follows, we consider only translational-invariant initial conditions, in which case $F_{\mathbf{x}}(\mathbf{r},t)$ is independent of $\mathbf{x}$. Using equation (10) we get the following difference-differential equation for F:

$$\begin{aligned}\frac{\partial}{\partial t}F(\mathbf{r},t) &= \sum_{k=1}^{d}\{F(\mathbf{r}-\mathbf{k},t)+F(\mathbf{r}+\mathbf{k},t)-2F(\mathbf{r},t)\}+\delta_{\mathbf{r},\mathbf{0}}\alpha F(\mathbf{0},t)\\ &= \sum_{k=1}^{d}\Delta_k F(\mathbf{r},t)+\delta_{\mathbf{r},\mathbf{0}}\alpha F(\mathbf{0},t)\end{aligned} \tag{16}$$

where Δ_k is the discrete Laplacian concerning the kth component. The variance σ^2 is related to F as follows:

$$\sigma(t)^2 = F(\mathbf{0},t)+\rho_0-\rho_0^2. \tag{17}$$

Here, we see that there is no qualitative difference between parity conserving models (k and l even) and non-parity conserving models—models with different k and l differ only by different creation and annihilation rates.

This kind of equation can be solved using the Fourier transformation:

$$f(\mathbf{q},t) = \sum_{\mathbf{r}} \mathrm{e}^{-\mathrm{i}\mathbf{q}\mathbf{r}}F(\mathbf{r},t) \qquad F(\mathbf{r},t) = \int \frac{\mathrm{d}^d\mathbf{q}}{(2\pi)^d}\,\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}}f(\mathbf{q},t). \tag{18}$$

We get

$$\frac{\partial}{\partial t}f(\mathbf{q},t) = -w(\mathbf{q})f(\mathbf{q},t)+\alpha F(\mathbf{0},t) \tag{19}$$

with the dispersion relation $w(\mathbf{q}) = -2\sum_{k=1}^{d}(\cos(q_k)-1)$. Integration yields

$$f(\mathbf{q},t) = \mathrm{e}^{-w(\mathbf{q})t}\left\{f(\mathbf{q},0)+\alpha\int_0^t \mathrm{d}\tau\, F(\mathbf{0},\tau)\,\mathrm{e}^{w(\mathbf{q})\tau}\right\}. \tag{20}$$

As the initial condition we choose a Poisson-distribution $F(\mathbf{r},0) = \rho_0^2$ so that $f(\mathbf{q},0) = \delta_{\mathbf{q},\mathbf{0}}\rho_0^2$. Thus we get

$$F(\mathbf{r},t) = \rho_0^2+\alpha\int_0^t \mathrm{d}\tau\, F(\mathbf{0},\tau)b(\mathbf{r},t-\tau) \tag{21}$$

with

$$\begin{aligned}b(\mathbf{r},t) &= \int\frac{\mathrm{d}^d\mathbf{q}}{(2\pi)^d}\,\mathrm{e}^{-w(\mathbf{q})t+\mathrm{i}\mathbf{q}\mathbf{r}}\\ &= \mathrm{e}^{-2\,\mathrm{d}t}I_{r_1}(2t)\cdots I_{r_d}(2t)\end{aligned} \tag{22}$$

where $I_r(t)$ is the modified Bessel function of order r. The dimension d is now just a parameter which can formally take real values. Although this is not physical it allows for the investigation of the dependence on the dimension.

For $\mathbf{r} = \mathbf{0}$ the long-time behaviour of the solution of the Volterra integral equation (21) with the function $b(t)$ given by equation (22) is known from the mean spherical model[1]. In this context α plays the role of temperature. This analogy enables us to use known results from the spherical model. Equation (21) can be solved using a temporal Laplace transformation [15],

$$\tilde{F}(p) = \int_0^\infty \mathrm{d}t\, \mathrm{e}^{-pt} F(\mathbf{0}, t). \tag{23}$$

We get

$$\tilde{F}(p) = \frac{\rho_0^2}{p} + \alpha \tilde{F}(p)\tilde{b}(p) \quad \Leftrightarrow \quad \tilde{F}(p) = \frac{\rho_0^2}{p(1 - \alpha\tilde{b}(p))}. \tag{24}$$

For late times $F(\mathbf{0}, t)$ is given by the behaviour of $\tilde{b}(p)$ for small p, which crucially depends on the dimension d (see for example [15]):

$$\tilde{b}(p) = \begin{cases} (4\pi)^{-d/2}\Gamma(1 - d/2)p^{-(1-d/2)} & d < 2 \\ 2A_1 - (4\pi)^{-d/2}|\Gamma(1 - d/2)|p^{d/2-1} & 2 < d < 4 \\ 2A_1 - 4A_2 p & d > 4 \end{cases}$$
$$A_k = \int \frac{\mathrm{d}^d\mathbf{q}}{(2\pi)^d} \frac{1}{(2w(\mathbf{q}))^k}. \tag{25}$$

This results in different behaviour of $F(\mathbf{0}, t)$ as we shall see in the next sections.

For all even integral dimensions $d = 2, 4, \ldots$ logarithmic corrections arise whose investigation goes beyond the scope of this paper.

Case 1: $d < 2$. As for $d < 2$ the quantity $\tilde{b}(p)$ diverges for $p \to 0$, the denominator of equation (24) has always a zero for $p \neq 0$, so that $\tilde{F}(p)$ has a pole at a positive value $p = 1/\tau$. A pole of the Laplace transform corresponds to the exponential behaviour of the original function and we get

$$F(\mathbf{0}, t) \underset{t\to\infty}{\propto} \mathrm{e}^{t/\tau}. \tag{26}$$

For $d = 1$ the exact expression of $\tilde{b}$ is known [15]:

$$\tilde{b}(p) = \frac{1}{\sqrt{p(p+4)}} \tag{27}$$

which yields

$$\tau_{d=1} = \frac{1}{\sqrt{4 + \alpha^2} - 2}. \tag{28}$$

For any finite value of α the time scale τ is finite but diverges if $\alpha \searrow 0$. This is in analogy with the spherical model, where in one dimension the critical temperature is zero.

In order to investigate how the predicted asymptotic behaviour for large times is approached we have performed a numerical integration of $F(\mathbf{0}, t)$, which is shown in figure 1. For details of the numerical calculation see [12], where a similar integral equation is calculated. We see that the asymptotic behaviour is approached quickly and the solution (26) is a good approximation for times $t > 1$.

[1] In the mean spherical model the spherical constraint is parametrized mathematically by a Lagrangian multiplier. This multiplier is determined by the Volterra integral equation (21) where ρ_0^2 is replaced by $b(\mathbf{0}, t)$ which does not change the long time–time behaviour.

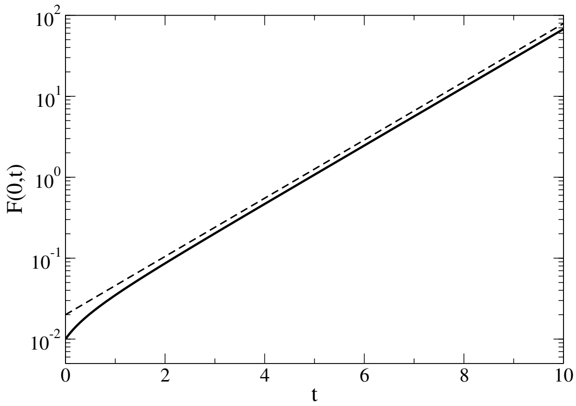

Figure 1. Numerical calculation of $F(\mathbf{0}, t)$ for $d = 1, \alpha = 2, \rho_0 = 0.1$. The dashed line shows the theoretical predicted slope $\tau \approx 1.2071$.

Case 2: $2 < d < 4$. For $d > 2$ the quantity $\tilde{b}(p)$ shows a qualitatively different behaviour: it approaches the finite value $2A_1$ for $p \to 0$. Therefore the $\tilde{F}(p)$ has a pole for positive p only for α larger than a critical value given by

$$\alpha_c = \frac{1}{2A_1} \tag{29}$$

which is identical to the critical temperature in the spherical model. Thus we find a phase transition in the behaviour of the autocorrelation $F(\mathbf{0}, t)$: for $\alpha > \alpha_c$ (low diffusion constant) we recover the exponential divergence

$$F(\mathbf{0}, t) \underset{t\to\infty}{\propto} e^{t/\tau}. \tag{30}$$

with a time scale

$$\tau = \left(\frac{\alpha'}{c_2\alpha}\right)^{-\frac{1}{d/2-1}} \tag{31}$$

with the reduced control parameter

$$\alpha' = \frac{\alpha - \alpha_c}{\alpha_c} \tag{32}$$

and $c_2 = (4\pi)^{-d/2}|\Gamma(1 - d/2)|$. This time scale diverges if we approach $\alpha \searrow \alpha_c$.

For $\alpha < \alpha_c$ (high diffusion constant) the pole of $\tilde{F}(p)$ vanishes and $F(\mathbf{0}, t)$ asymptotically approaches a finite value

$$F_\infty = \lim_{t\to\infty} F(\mathbf{0}, t) = \frac{\rho_0^2}{1 - \alpha/\alpha_c} > \rho_0^2 \tag{33}$$

which diverges if we approach $\alpha \nearrow \alpha_c$.

Therefore, a suitable order parameter for this phase transition is F_∞^{-1} which decreases linearly to zero for $\alpha \nearrow \alpha_c$ and is equal to zero for $\alpha > \alpha_c$.

For $\alpha = \alpha_c$ we get

$$\tilde{F}(p) = \frac{(4\pi)^{d/2}\rho_0^2}{|\Gamma(1 - d/2)|\,\alpha_c}\frac{1}{p^{d/2}} \tag{34}$$

which results in a power law

$$F(\mathbf{0}, t) \propto t^{d/2-1} \tag{35}$$

and hence in a power law divergence of the variance.

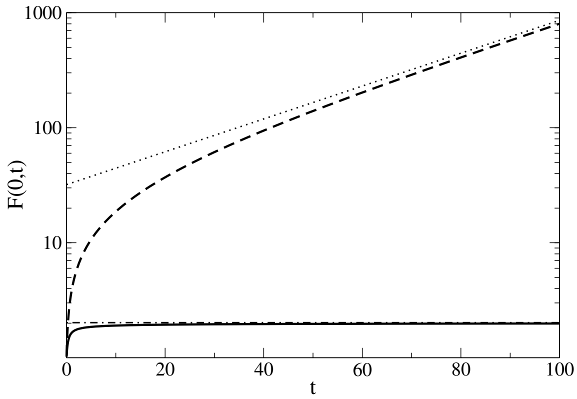

Figure 2. Numerical calculation of $F(\mathbf{0}, t)$ for $d = 3, \rho_0 = 1, \alpha = 2 < \alpha_c$ (solid line) and $\alpha = 4.2 > \alpha_c$ (dashed line). The dotted line shows the theoretical predicted slope $\tau \approx 30.4$, the dashed-dotted line the theoretical predicted asymptotic value $F(\mathbf{0}, t = \infty) \approx 2.02$.

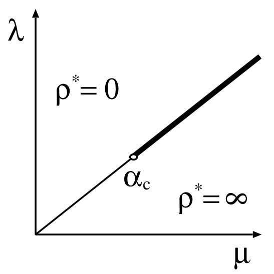

Figure 3. The phase diagram of the system for a fixed diffusion constant D: in the limit of $t \to \infty$ for $\lambda > \mu k/l$ the stationary density ρ^* is zero while it diverges for $\lambda < \mu k/l$. For $\lambda = \mu k/l$ the density is constant, $\rho^* = \rho_0$ and the variance function is bounded for $\alpha < \alpha_c$, while it diverges exponentially for $\alpha > \alpha_c$ and algebraically for $\alpha = \alpha_c$, where $\alpha = \mu k(k + l)/(2D)$.

In figure 2 the numerical calculation of the crossover to the behaviour for large times is shown for $\alpha < \alpha_c$ and $\alpha > \alpha_c$.

Case 3: $d > 4$. For $d > 4$ we find qualitatively the same behaviour as for $2 < d < 4$. Like in the previous case, $\tilde{F}(p)$ has a pole at a positive p only for values $\alpha > \alpha_c = 1/(2A_1)$. For $\alpha > \alpha_c$ the time scale of the exponential increase is given by

$$\tau = \left(\frac{\alpha'}{4A_2\alpha}\right)^{-1}. \tag{36}$$

The difference from the case $2 < d < 4$ is that this time scale is now independent of the dimension d, indicating that we are in the mean-field region.

For $\alpha < \alpha_c$, $F(\mathbf{0}, t)$ approaches the asymptotic value given by equation (33). For $\alpha = \alpha_c$ we get

$$\tilde{F}(p) = \frac{\rho_0^2}{4A_2\alpha_c p^2} \tag{37}$$

which results in a power law

$$F(\mathbf{0}, t) \propto t. \tag{38}$$

These results are summed up in the phase diagram in figure 3.

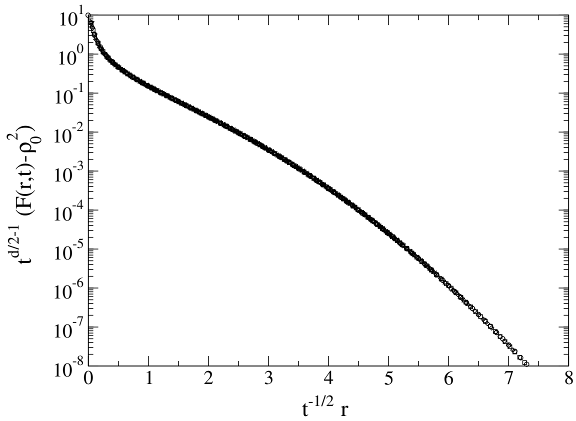

Figure 4. Numerical calculation of $F(\mathbf{r} = (r, 0, \ldots), t)$ for $d = 3$, $\alpha = 2 < \alpha_c$, $\rho_0 = 1$ and times $t = 50, 100, 150, \ldots, 400$.

3. Spatial correlations

In the mean-field regime ($d > 4$) the behaviour of the correlation function $F(\mathbf{r}, t)$ can be calculated analytically in the limit of large $\mathbf{r}$ and t. As derived in the appendix we get

$$F(\mathbf{r}, t) - \rho_0^2 = \begin{cases} \dfrac{\rho_0^2 \alpha}{4\pi^{d/2}|\alpha'|} r^{2-d} \Gamma\left(\dfrac{d}{2} - 1, \dfrac{r^2}{4t}\right) & \alpha' < 0 \\ \dfrac{\rho_0^2}{64 A_2 \pi^{d/2}} r^{4-d} \Psi\left(d, \dfrac{r^2}{4t}\right) & \alpha' = 0 \\ \dfrac{\rho_0^2}{(8\pi)^{(d-1)/2} A_2^{(d-2)/2}} \left(\dfrac{\alpha'}{\alpha}\right)^{(d-4)/2} \left(\dfrac{r}{\xi}\right)^{(1-d)/2} \exp(t/\tau - r/\xi) & 1 \gg \alpha' > 0 \end{cases} \tag{39}$$

where $\alpha' = (\alpha - \alpha_c)/\alpha_c$ is the reduced control parameter, Γ is the incomplete Gamma function and Ψ is a scaling function defined by

$$\Psi(d, u) = \int_u^\infty \mathrm{d}y \frac{\Gamma\left(\frac{d}{2} - 1, y\right)}{y^2}. \tag{40}$$

Above the critical point the correlations diverge; the time scale τ is given by equation (36) and the correlation length by

$$\xi = \sqrt{\tau} = \sqrt{\frac{4A_2\alpha}{\alpha'}}. \tag{41}$$

Interestingly, as for $\alpha_c > 0$ the correlations increase with time, what in usual dynamical critical phenomena would be called the correlation time is *negative* while the correlation length is positive. For $\alpha' \leqslant 0$ the dependence on r^2/t directly shows that the dynamical exponent is $z = 2$. For $\alpha' > 0$ the time scale τ is the square of the length scale ξ, therefore also in this case the dynamical exponent is $z = 2$. The same dynamical exponent appears in a field theoretical treatment of the fermionic PCPD [5].

No analytical solution is available in the case $2 < d < 4$, thus we evaluate the integral (21) numerically. Figure 4 shows the spatial dependence of the correlation function along the

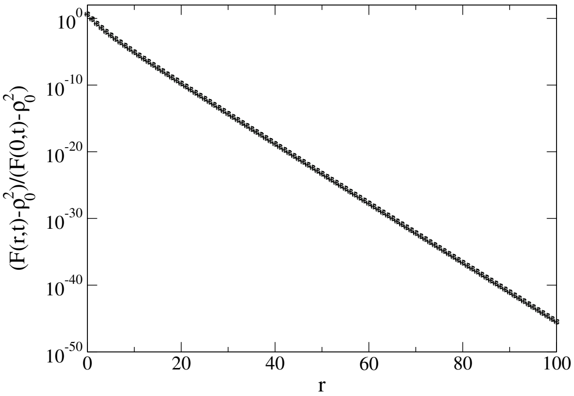

Figure 5. Numerical calculation of $F(\mathbf{r} = (r, 0, \ldots), t)$ for $d = 3$, $\alpha = 6 > \alpha_c$, $\rho_0 = 1$ and times $t = 50, 100, 150, \ldots, 400$.

axis $\mathbf{r} = (r, 0, \ldots)$, for $\alpha < \alpha_c$; figure 5 shows the case $\alpha > \alpha_c$. A collapse of the calculated data points is achieved if we assume the following functional dependence:

$$F(r,t) - \rho_0^2 \propto \begin{cases} r^{2-d} f_1(r^2/t) & \alpha' < 0 \\ F(0,t) f_2(d,r) & \alpha' > 0, \end{cases} \tag{42}$$

where f_1 is a scaling function and $f_2(d, r)$ is a function that only depends on d and r. This result is in qualitative agreement with the previously derived formula for $d > 4$.

4. Discussion

Apart from the spherical model this phase transition is related to a much simpler model: on a d-dimensional cubic lattice non-interacting particles are diffusing with rate D and additionally at site $\mathbf{x} = \mathbf{0}$ particles may branch as $A \to 2A$ with rate $\alpha' = \alpha D$. The equation for the time evolution of the particle density $\langle n(\mathbf{x}, t)\rangle$ is just given by equation (16). We can adopt the solutions for $F(\mathbf{r}, t)$ by substituting the initial condition by $\rho_0^2 \to \rho_0$. In particular, we recover a phase transition for the particle density at the origin. While in the original process it is rather complicated to understand the physical meaning of the behaviour of the second moment, in this model we understand the behaviour of the first moment: for $d = 1$ diffusion does not suffice to spread the particles on the lattice fast enough and the particle density at $\mathbf{x} = \mathbf{0}$ diverges for any given parameters. For higher dimensions additional spatial directions are accessible to spread particles and as a consequence the particle density at $\mathbf{x} = \mathbf{0}$ remains finite for high enough diffusion constant D.

The fact that the autocorrelation function is diverging while the particle density remains constant allows some conclusions concerning the distribution function for the particles $p(n)$ for late times. On the one hand, if $\langle n\rangle = \sum_n np(n)$ is finite then for large n the distribution function $p(n) < c_1 n^{-\beta}$ with $\beta > 2$. On the other hand, if $\langle n^2\rangle = \sum_n n^2 p(n)$ is infinite then for large n the distribution function $p(n) > c_2 n^{-\beta}$ with $\beta < 3$ with some positive constants c_1, c_2. Thus the distribution function follows for large n a power law $p(n) \propto n^{-\beta}$ with $2 < \beta < 3$.

In summary, we have shown that for $d > 2$ the bosonic PCPD exhibits a phase transition for $\langle a(\mathbf{x})^2\rangle$ and thus for the autocorrelation function $\sigma(t)^2 = \langle n(\mathbf{x})^2\rangle - \langle n(\mathbf{x})\rangle^2 = \langle a(\mathbf{x})^2\rangle + \langle n(\mathbf{x})\rangle - \langle n(\mathbf{x})\rangle^2$. The order parameter F_∞^{-1} decreases linearly to zero for $\alpha \nearrow \alpha_c$

and is equal to zero for $\alpha > \alpha_c$, where α is proportional to the ratio of the reaction rates and the diffusion constant. Thus diffusion has a large influence in this process, and it must be high enough in order to avoid a divergence of the autocorrelation.

We have also shown that the critical properties of this process are related to the mean spherical model. As the spherical model is a model for magnetism this analogy is rather intriguing and the question arises whether it is just accidental.

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Appendix

For the mean-field case $d > 4$ the solution of $F(\mathbf{r}, t)$ in the limit of large $\mathbf{r}$ and t can be derived analytically, as presented in what follows:

With the definition

$$G(\mathbf{r}, t) = F(\mathbf{r}, t) - \rho_0^2 \tag{A.1}$$

the integral equation can be transformed to

$$G(\mathbf{r}, t) = \alpha \int_0^t \mathrm{d}\tau\, G(\mathbf{0}, \tau) b(\mathbf{r}, t - \tau) + \alpha\rho_0^2 \int_0^t \mathrm{d}\tau\, b(\mathbf{r}, t). \tag{A.2}$$

Using a Laplace transformation we get

$$\tilde{G}(\mathbf{r}, p) = \alpha \tilde{G}(\mathbf{0}, p)\tilde{b}(\mathbf{r}, p) + \alpha\rho_0^2 \frac{\tilde{b}(\mathbf{r}, p)}{p} \tag{A.3}$$

setting $\mathbf{r} = \mathbf{0}$ determines $\tilde{G}(\mathbf{0}, p)$ which yields

$$\tilde{G}(\mathbf{r}, p) = \alpha\rho_0^2 \frac{\tilde{b}(\mathbf{r}, p)}{p(1 - \alpha\tilde{b}(\mathbf{0}, p))}. \tag{A.4}$$

The Fourier transform of this equation is

$$\tilde{g}(\mathbf{q}, p) = \rho_0^2 \alpha \frac{1}{p(1 - \alpha\tilde{b}(\mathbf{0}, p))} \frac{1}{p + w(\mathbf{q})}. \tag{A.5}$$

For the mean-field case, $d > 4$, $\tilde{b}(\mathbf{0}, p)$ takes the simple form

$$\tilde{b}(\mathbf{0}, p) = 1/\alpha_c - p\gamma/\alpha \tag{A.6}$$

and we get

$$\tilde{g}(\mathbf{q}, p) = \frac{\rho_0^2 \alpha}{\gamma} \frac{1}{p\,(p - \alpha'/\gamma)} \frac{1}{p + w(\mathbf{q})}. \tag{A.7}$$

Here we defined the reduced control parameter $\alpha' = (\alpha - \alpha_c)/\alpha_c$ and $\gamma = 4A_2\alpha$. Although the function $\tilde{b}$ does not depend on dimension for $d > 4$, generally a dependence of the solution $G(\mathbf{r}, t)$ on dimension is still possible as the inverse Fourier transform depends on d, which does not affect the critical exponents. Using an expansion into partial fractions we get

$$\tilde{g}(\mathbf{q}, p) = \rho_0^2 \alpha \left(-\frac{1}{\alpha' w(\mathbf{q})} \frac{1}{p} + \frac{1}{\alpha'(w(\mathbf{q}) + \alpha'/\gamma)} \frac{1}{p - \alpha'/\gamma} + \frac{1}{\gamma w(\mathbf{q})(w(\mathbf{q}) + \alpha'/\gamma)} \frac{1}{p + w(\mathbf{q})} \right). \tag{A.8}$$

The inverse Laplace transform of this expression reads

$$g(\mathbf{q},t) = \rho_0^2\alpha\left(-\frac{1}{\alpha' w(\mathbf{q})} + \frac{1}{\alpha'\left(w(\mathbf{q})+\alpha'/\gamma\right)}\exp\left(\frac{\alpha'}{\gamma}t\right)\right.$$
$$\left. + \frac{1}{\gamma w(\mathbf{q})\left(w(\mathbf{q})+\alpha'/\gamma\right)}\exp\left(-w(\mathbf{q})t\right)\right). \tag{A.9}$$

Although the second term is not Laplace transformable for $\alpha' > 0$ this result is correct and can be derived by transforming the function $H(\mathbf{r},t) = \exp\left(-\left(\frac{\alpha'}{\gamma}+\epsilon\right)t\right)G(\mathbf{r},t)$ with $\epsilon > 0$.

The inverse Fourier transform of the first term of (A.9) is

$$\begin{aligned}\int \frac{\mathrm{d}^d\mathbf{q}}{(2\pi)^d}\,\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}}\frac{1}{w(\mathbf{q})} &= \int_0^\infty \mathrm{d}x \int \frac{\mathrm{d}^d\mathbf{q}}{(2\pi)^d}\exp(-w(\mathbf{q})x)\,\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}} \\ &= \int_0^\infty \mathrm{d}x\,\mathrm{e}^{-2\,\mathrm{d}x} I_{r_1}(2x)\cdot\ldots\cdot I_{r_d}(2x) \\ &\underset{|\mathbf{r}|\gg 1}{\approx} \int_0^\infty \mathrm{d}x\,(4\pi x)^{-d/2}\exp\left(-\frac{r^2}{4x}\right) \\ &= \frac{\Gamma\left(\frac{d}{2}-1\right)}{4\pi^{d/2}}r^{2-d}.\end{aligned} \tag{A.10}$$

For the long-time limit the second term contributes significantly only for $\alpha' > 0$. Defining $b^2 = \alpha'/\gamma$ we get for this case:

$$\begin{aligned}\int \frac{\mathrm{d}^d\mathbf{q}}{(2\pi)^d}\frac{\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}}}{w(\mathbf{q})+b^2} &= \int_0^\infty \mathrm{d}x \int \frac{\mathrm{d}^d\mathbf{q}}{(2\pi)^d}\exp(-(w(\mathbf{q})+b^2)x)\,\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}} \\ &= \int_0^\infty \mathrm{d}x\,\exp(-b^2x)\,\mathrm{e}^{-2\,\mathrm{d}x} I_{r_1}(2x)\cdot\ldots\cdot I_{r_d}(2x) \\ &\underset{b^2\ll 1,|\mathbf{r}|\gg 1}{\approx} (4\pi)^{-d/2}\int_0^\infty \mathrm{d}x\,x^{-d/2}\exp\left(-\frac{r^2}{4x}-b^2x\right) \\ &= (4\pi)^{-d/2}\left(\frac{r^2}{4}\right)^{1-d/2}\int_0^\infty \mathrm{d}z\,z^{d/2-2}\exp\left(-z-\frac{b^2r^2}{4z}\right) \\ &= (4\pi)^{-d/2}\left(\frac{r^2}{4}\right)^{1-d/2} 2^{2-d/2}\,(br)^{d/2-1}\,K_{d/2-1}\,(br) \\ &\underset{r\gg 1}{\approx} (4\pi)^{-d/2}\left(\frac{r^2}{4}\right)^{1-d/2} 2^{2-d/2}\,(br)^{d/2-1}\sqrt{\frac{\pi}{2}}\frac{\exp(-br)}{\sqrt{br}} \\ &= \frac{1}{2^{(d+1)/2}\pi^{(d-1)/2}}b^{(d-3)/2}r^{(1-d)/2}\exp(-br) \\ &= \frac{1}{2^{(d+1)/2}\pi^{(d-1)/2}}\left(\frac{\alpha'}{\gamma}\right)^{(d-3)/4} r^{(1-d)/2}\exp\left(-\sqrt{\frac{\alpha'}{\gamma}}r\right),\end{aligned} \tag{A.11}$$

where $K_{d/2-1}$ is the modified Bessel function of second kind.

For $\alpha' > 0$ the third term is transformed to

$$\begin{aligned}&\int \frac{\mathrm{d}^d\mathbf{q}}{(2\pi)^d}\frac{\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}}\exp\left(-w(\mathbf{q})t\right)}{w(\mathbf{q})(w(\mathbf{q})+b^2)} \\ &\quad= \int_0^\infty \mathrm{d}x \int \frac{\mathrm{d}^d\mathbf{q}}{(2\pi)^d}\exp(-(w(\mathbf{q})+b^2)x)\frac{\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}}\exp(-w(\mathbf{q})t)}{w(\mathbf{q})} \\ &\quad= \int_0^\infty \mathrm{d}x\,\exp(-b^2x)\int_{t+x}^\infty \mathrm{d}y \int \frac{\mathrm{d}^d\mathbf{q}}{(2\pi)^d}\exp(-w(\mathbf{q})y)\,\mathrm{e}^{\mathrm{i}\mathbf{q}\mathbf{r}}\end{aligned}$$

$$
\begin{aligned}
&= \int_0^\infty \mathrm{d}x \exp(-b^2 x) \int_{t+x}^\infty \mathrm{d}y\, \mathrm{e}^{-2\,\mathrm{d}y} I_{r_1}(2y)\cdot \ldots \cdot I_{r_d}(2y) \\
&\underset{|\mathbf{r}|\gg 1}{\approx} (4\pi)^{-d/2} \int_0^\infty \mathrm{d}x \exp(-b^2 x) \int_{t+x}^\infty \mathrm{d}y\, y^{-d/2} \exp\left(-\frac{r^2}{4y}\right) \\
&= (4\pi)^{-d/2} t^{1-d/2} \left(\frac{r^2}{4t}\right)^{1-d/2} \int_0^\infty \mathrm{d}x \exp(-b^2 x) \int_0^{\frac{r^2}{4t(1+x/t)}} \mathrm{d}z\, z^{d/2-1} \exp(-z) \\
&\underset{t\gg 1}{\approx} \frac{r^{2-d}}{4\pi^{d/2}} \int_0^\infty \mathrm{d}x \exp(-b^2 x) \left(\int_0^{\frac{r^2}{4t}} \mathrm{d}z\, z^{d/2-1} \exp(-z) \right. \\
&\quad \left. - \left(\frac{r^2}{4t}\right)^{d/2-1} \exp\left(-\frac{r^2}{4t}\right) \frac{x}{t} \right) \\
&= \frac{r^{2-d}}{4\pi^{d/2}} \int_0^\infty \mathrm{d}x \exp(-b^2 x) \left(\Gamma\left(\frac{d}{2}-1\right) - \Gamma\left(\frac{d}{2}-1, \frac{r^2}{4t}\right) \right. \\
&\quad \left. - \left(\frac{r^2}{4t}\right)^{d/2-1} \exp\left(-\frac{r^2}{4t}\right) \frac{x}{t} \right) \\
&= \frac{r^{2-d}}{4\pi^{d/2}} b^{-2} \left(\Gamma\left(\frac{d}{2}-1\right) - \Gamma\left(\frac{d}{2}-1, \frac{r^2}{4t}\right) \right. \\
&\quad \left. - \frac{b^{-2}}{t} \left(\frac{r^2}{4t}\right)^{d/2-1} \exp\left(-\frac{r^2}{4t}\right) \right)
\end{aligned}
\tag{A.12}
$$

with the incomplete Gamma-function $\Gamma(a, x) = \int_x^\infty \mathrm{d}t\, t^{a-1}\, \mathrm{e}^{-t}$.

For $\alpha' < 0$ the same result can be derived by substituting $x \to -x$.

At the critical rate $\alpha' = 0$ equation (A.7) reduces to

$$
\tilde{g}(\mathbf{q}, p) = \frac{\rho_0^2 \alpha}{\gamma} \frac{1}{p^2} \frac{1}{p + w(\mathbf{q})}. \tag{A.13}
$$

The inverse Laplace transform of this expression is given by

$$
\begin{aligned}
\mathcal{L}^{-1}\left(\frac{1}{p^2\,(p + w(\mathbf{q}))}, t \right) &= \int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\tau' \mathcal{L}^{-1}\left(\frac{1}{p + w(\mathbf{q})}, \tau' \right) \\
&= \int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\tau' \exp(-w(\mathbf{q})\tau').
\end{aligned}
\tag{A.14}
$$

The necessary conditions for this equality are fulfilled [16]:

$$
\begin{aligned}
&\lim_{t\to\infty} \left(\mathrm{e}^{-pt} \int_0^t \mathrm{d}\tau \exp(-w(\mathbf{q})\tau) \right) = 0 \\
&\lim_{t\to\infty} \left(\mathrm{e}^{-pt} \int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\tau' \exp(-w(\mathbf{q})\tau') \right) = 0.
\end{aligned}
\tag{A.15}
$$

This yields

$$
\begin{aligned}
G(\mathbf{r}, t) &= \frac{\rho_0^2 \alpha}{\gamma} \int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\tau' \int \frac{\mathrm{d}^d \mathbf{q}}{(2\pi)^d} \exp(-w(\mathbf{q})\tau') \\
&= \frac{\rho_0^2 \alpha}{\gamma} \int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\tau'\, \mathrm{e}^{-2\,\mathrm{d}x} I_{r_1}(2x)\cdot \ldots \cdot I_{r_d}(2x)
\end{aligned}
$$

$$\begin{aligned}
&\underset{|\mathbf{r}|\gg 1}{\approx} \frac{\rho_0^2\alpha}{\gamma}\int_0^t \mathrm{d}\tau \int_0^\tau \mathrm{d}\tau'(4\pi\tau')^{-d/2}\exp\left(-\frac{r^2}{4\tau'}\right)\\
&= \frac{\rho_0^2\alpha}{\gamma(4\pi)^{d/2}}\left(\frac{r^2}{4}\right)^{-d/2+1}\int_0^t \mathrm{d}\tau\int_{\frac{r^2}{4\tau}}^\infty \mathrm{d}z\, z^{d/2-2}\exp(-z)\\
&= \frac{\rho_0^2\alpha}{4\gamma\pi^{d/2}}r^{2-d}\int_0^t \mathrm{d}\tau\,\Gamma\left(\frac{d}{2}-1,\frac{r^2}{4\tau}\right)\\
&= \frac{\rho_0^2\alpha}{16\gamma\pi^{d/2}}r^{4-d}\int_{\frac{r^2}{4t}}^\infty \mathrm{d}z\frac{\Gamma\left(\frac{d}{2}-1,z\right)}{z^2}.
\end{aligned}\tag{A.16}$$

Thus we get the expressions (39) in the limit of large $\mathbf{r}$ and t.

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