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Phase transitions in a lattice population model

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Abstract

We introduce a model for a population on a lattice with diffusion and birth/death according to $2A \longrightarrow 3A$ and $A \longrightarrow \phi$ for a particle A. We find that the model displays a phase transition from an active to an absorbing state which is continuous in 1 + 1 dimensions and of first-order in higher dimensions in agreement with the mean field equation. For the (1 + 1)-dimensional case, we examine the critical exponents and a scaling function for the survival probability and show that it belongs to the universality class of directed percolation. In higher dimensions, we look at the first-order phase transition by plotting a histogram of the population density and use the presence of phase coexistence to find an accurate value for the critical point in 2 + 1 dimensions.

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1. Introduction

Non-equilibrium phase transitions have long been a major area of investigation (see [1] for a review). Studies are wide-ranging, involving atmospheric precipitation [2], sandpile models [3], epidemics [4] and many more. One of the great achievements in the field has been the discovery that a broad range of models belong to one of a few universality classes, whose members share the same critical exponents and scaling functions (see for example [5]). In particular, it has been conjectured that all models with a scalar order parameter that exhibit a continuous phase transition from an active state to a single absorbing state belong to the same universality class of *directed percolation* (DP) [6, 7]. Although not proven, the conjecture is strongly supported by numerical evidence and seems to be even more general since, for example, a system with multiple absorbing states is known to belong to the class [8].

Here, we introduce a lattice model representing a population in a habitat and include the processes of birth, death and diffusion. Due to the conflict between growth and decay, with steady state population density $\bar{\rho}$ as our order parameter, we expect a phase transition to an absorbing state to occur under certain conditions. The expected phase transition may be either

continuous or of first-order. The latter, however, is rarely seen in low spatial dimensions due to the destabilization of the ordered phase caused by the larger fluctuations that are present in such systems. Hinrichsen has hypothesized that first-order phase transitions are impossible in $(1+1)$-dimensional systems provided that there are no additional conservation laws, long-range interactions, macroscopic currents or special boundary conditions [9]. Since our model does not fulfil any of these criteria, we expect at least the $(1+1)$-dimensional version of our model to exhibit a continuous phase transition and thus to belong to DP.

Thanks to series expansions, the critical exponents of DP are now known to a high degree of accuracy [10]. We therefore proceed in section 2 by describing our model and then, in sections 3 and 4, examine the critical exponents and a scaling function respectively to compare them with those of DP. In section 5, we examine the first-order phase transitions and conclude with some remarks in section 6.

2. The model

We have a d-dimensional square lattice of linear length L where each square is either occupied by a single particle (1) or is empty (0). A site is chosen at random. With probability p_d the particle on an occupied site dies, leaving the site empty. If the particle does not die, a nearest-neighbour site is randomly chosen. If the neighbouring site is empty the particle moves there; otherwise, the particle reproduces with probability p_b producing a new particle on another randomly selected neighbouring site, conditional on that square being empty. A time step is defined as the number of lattice sites $N = L^\mathrm{d}$ and periodic boundary conditions are used. We have the following reactions for a particle A for proliferation and annihilation respectively,

$$A + A \longrightarrow 3A \qquad \text{and} \qquad A \longrightarrow \phi. \tag{1}$$

Our model is similar to that of Schlögl's second model [11] with similar cases being previously studied [6, 12, 13].

Assuming the particles are spaced homogeneously, the mean field equation for the density of active sites $\rho(t)$ is given by

$$\frac{\partial \rho(t)}{\partial t} = p_\mathrm{b}(1-p_\mathrm{d})\rho(t)^2(1-\rho(t)) - p_\mathrm{d}\rho(t). \tag{2}$$

This has three stationary states

$$\bar{\rho}_0 = 0, \qquad \bar{\rho}_\pm = \frac{1}{2}\left(1 \pm \sqrt{1 - \frac{4p_\mathrm{d}}{p_\mathrm{b}(1-p_\mathrm{d})}}\right). \tag{3}$$

Clearly, for $4p_\mathrm{d} > p_\mathrm{b}(1-p_\mathrm{d})$, $\bar{\rho}_0$ is the only real stationary state, resulting in a phase transition occurring at the critical death rate $p_{\mathrm{d}_\mathrm{c}} = p_\mathrm{b}/(4+p_\mathrm{b})$. Simple analysis shows that $\bar{\rho}_+$ and $\bar{\rho}_0$ are stable stationary states, whereas $\bar{\rho}_-$ is unstable and therefore represents a critical density ρ_c below which extinction will occur in all cases. So, for $p_\mathrm{d} < p_{\mathrm{d}_\mathrm{c}}$,

$$\rho(t) \longrightarrow \begin{cases} 0 & \text{for} \quad \rho(t) < \rho_\mathrm{c} \\ \bar{\rho}_+ & \text{for} \quad \rho(t) > \rho_\mathrm{c} \end{cases} \qquad \text{as} \quad t \longrightarrow \infty. \tag{4}$$

At $p_\mathrm{d} = p_{\mathrm{d}_\mathrm{c}}$, the stationary density jumps from $1/2$ to 0, resulting in a first-order phase transition. We investigate whether the Monte Carlo (MC) simulations agree with the mean field by plotting, in figure 1, the steady state population density against p_d in $1+1$, $2+1$ and $3+1$ dimensions with $\rho(0) = 1$. From now on, we use a constant value of $p_\mathrm{b} = 0.5$. We note that, although we keep p_b constant, the actual *birth rate* is dependent on p_d since the probability of birth is proportional to $p_\mathrm{b}(1-p_\mathrm{d})$. To find the steady state, we examine

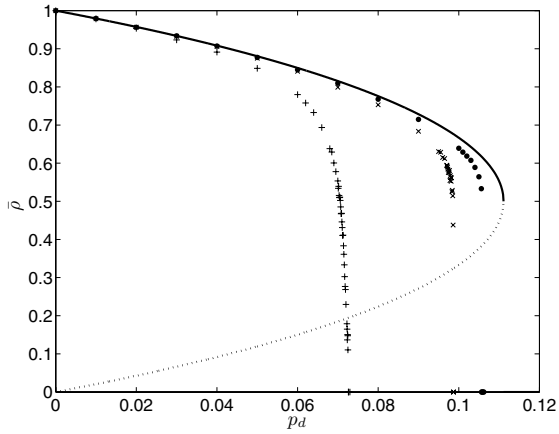

Figure 1. Steady state population densities for the mean field (line) and the (1 + 1) (+), (2 + 1) (×) and (3 + 1) (•) dimensional Monte Carlo simulations. The solid line represents the stable stationary state and the dashed line the unstable one.

surviving runs only, looking at an increasing number of time steps up to 2×10^5 and increments in p_d of 5×10^{-5} as the critical point is approached.

We see from the results that we have a strong indication of a first-order phase transition in 2 + 1 and 3 + 1 dimensions whilst a continuous phase transition in 1 + 1 dimensions. While these results are compelling, we note that since the simulations were performed on finite lattices and for finite times, we cannot take them to be conclusive since in such simulations there is always a non-zero probability of survival for finite t even for $p_d > p_{d_c}$. Instead we look for power-law behaviour in $\rho(t)$ close to the critical point. For a continuous phase transition we expect asymptotic power-law behaviour of the order parameter at the critical point (see [14] for a review) of the form

$$\rho(t) \sim t^{-\delta}. \tag{5}$$

In log–log plots, positive curvature for large t indicates the system is in the active phase whereas negative curvature implies that the system is in the absorbing phase. A first-order phase transition will therefore be marked by non power-law behaviour, rather exponential decay of the order parameter for $p_d > p_{d_c}$. Figure 2 shows the (1 + 1)-dimensional case with $\rho(t)$ for different values of p_d close to the critical point clearly showing power-law behaviour at the critical point. No power-law behaviour is however observed in 2 + 1 or 3 + 1 dimensions; instead, with the inclusion of spontaneous particle creation at rate $\kappa = 0.005$, hysteresis occurs in both cases as plotted in figure 3, which is indicative of first-order phase transitions. However, no hysteresis is observed in the (1 + 1)-dimensional case. We examine the first-order phase transitions in more detail in section 5.

Since the model shows a continuous phase transition in 1 + 1 dimensions, we must ask ourselves to which universality class it belongs. By Grassberger and Janssen's conjecture [6, 7], we would expect it to belong to the universality class of DP. We investigate this now by looking at the critical exponents and a scaling function in turn for 1 + 1 dimensions only.

3. Critical exponents

Finding the critical exponents through steady state simulations is notoriously difficult due to critical slowing down, finite-size effects, large fluctuations and the difficulties that arise in

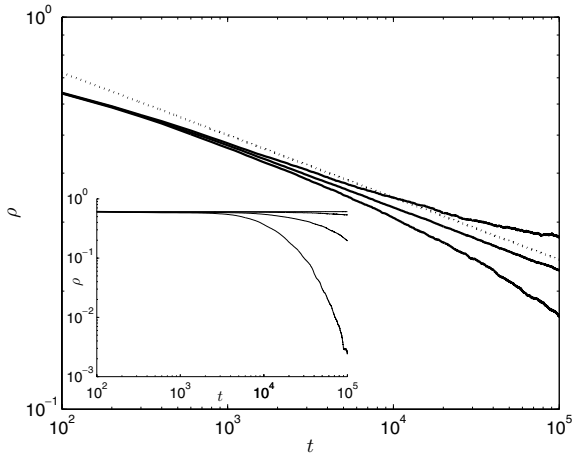

Figure 2. Power-law behaviour for the (1 + 1)-dimensional model. Solid lines represent (from top to bottom) $p_d = 0.071\,654$, 0.071 754 and 0.071 854. The hashed line represents the gradient -0.159 as a guide for the eye. The inset shows non-power law behaviour for various values of p_d close to the critical point for the (2 + 1)-dimensional model. The (3 + 1)-dimensional case is very similar. Information on how the critical points were found are detailed later in the paper.

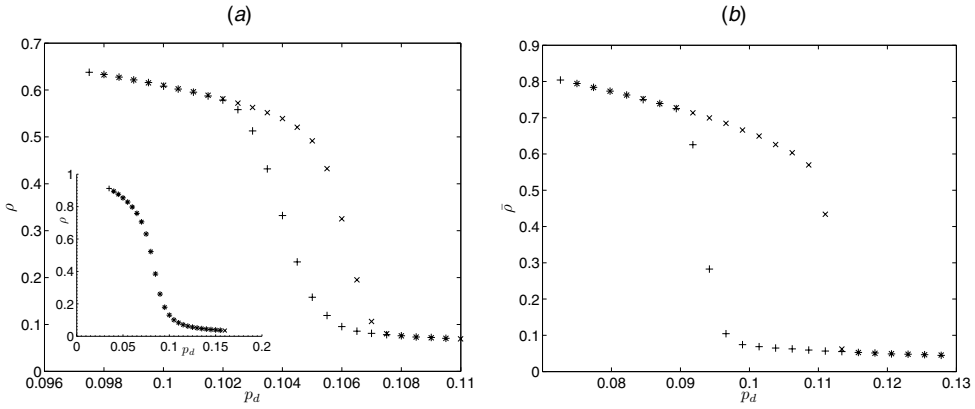

Figure 3. Hysteresis loop for the (*a*) 2 + 1 and (*b*) (3 + 1)-dimensional models with p_d increasing (×) and decreasing (+). The inset in (*a*) shows no hysteresis occurring in the (1 + 1)-dimensional model.

finding the critical point. A much more effective method is that of time-dependent simulations, which has proved to be a very efficient way of determining the critical exponents and the critical point for models exhibiting absorbing phase transitions [15]. Using this method, the time evolution of the model is observed up to some time t_M, after beginning with a configuration that is very close to the absorbing state—two adjacent particles in this model. The size of the lattice is made large enough so that the particles never reach the boundary before t_M.

We measure the survival probability $P(t)$, defined as the probability that the system has not reached the absorbing state at time t and the average number of occupied sites $n(t)$. At $p_d = p_{d_c}$, we expect the following asymptotic power-law behaviour [16]:

$$P(t) \sim t^{-\delta}, \tag{6}$$

$$n(t) \sim t^{\eta}. \tag{7}$$

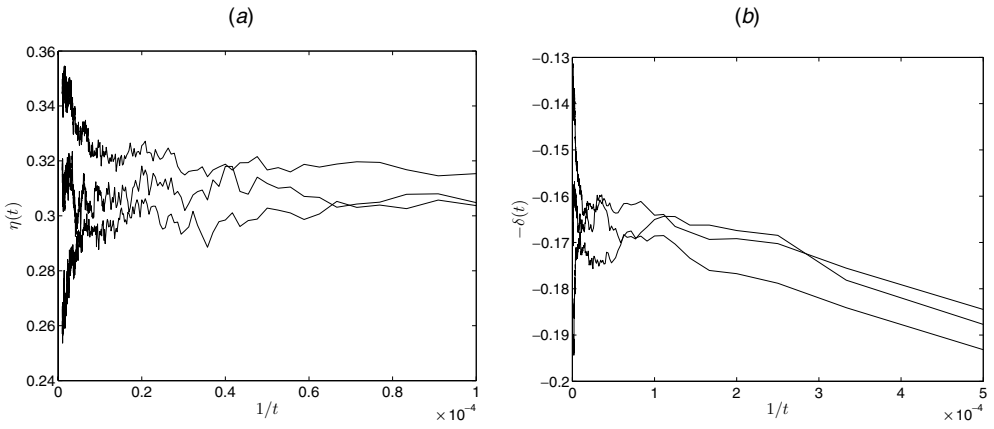

Figure 4. Plots of (*a*) $\eta(t)$ and (*b*) $-\delta(t)$ up to $t = 10^6$. From top to bottom, $p_d = 0.071\,746$, 0.071 754 and 0.071 762.

Away from the critical point, the evolution departs from pure power-law and so by examining log–log plots of $P(t)$ and $n(t)$ versus t we can find the critical point by finding the value of p_d that gives a straight line. Generally, however, we expect corrections to the pure power-law behaviour so that $P(t)$ is more accurately given as [16]

$$P(t) \sim t^{-\delta}(1 + at^{-1} + bt^{-\delta'} + \cdots) \tag{8}$$

and similarly for $n(t)$. Here, δ' represents the correction-to-scaling exponent for δ. More precise estimates for the critical exponents are obtained by examining the local slope

$$-\delta(t) = \frac{\ln[P(t)/P(t/m)]}{\ln(m)} \tag{9}$$

and similarly for $n(t)$, where the critical exponent δ is given by $\lim_{t\to\infty}\delta(t)$. Here, m is given as the local range over which the slope is measured and is typically 5 [17, 18] or 8 [16]. Grassberger [16] has shown that for the local slope defined in (9), we have the following behaviour

$$\delta(t) = \delta + at^{-1} + b\delta' t^{-\delta'} + \cdots \tag{10}$$

and again, similarly for $n(t)$. Thus if we plot $\delta(t)$ versus t^{-1}, we have that the critical exponent δ is given by the intercept with the y-axis and any curvature would indicate a correction-to-scaling exponent less than 1.

We plot in figure 4, $\eta(t)$ and $\delta(t)$ for up to $t = 10^6$ and over 10^5 runs with $m = 5$. We find that the data are in fact very noisy, leading to inaccurate results for the critical exponents. However, it is clear that the gradient increases for $p_d = 0.071\,746$ and decreases for $p_d = 0.071\,762$ for large t whereas we have an approximately straight line for $p_d = 0.071\,754$, especially for $\eta(t)$. This therefore gives a value of $p_{d_c} = 0.071\,754 \pm 0.000\,004$. We plot in figure 5, $\eta(t)$ and $\delta(t)$ for $p_d = 0.071\,754$ but this time up to $t = 10^4$ and over 2.5×10^6 runs to improve the accuracy of the results. From this plot we can read off the values $\eta = 0.314 \pm 0.002$ and $\delta = 0.160 \pm 0.002$, which are in agreement with the best currently known DP values of $\eta = 0.313\,686$ and $\delta = 0.159\,464$ [10].

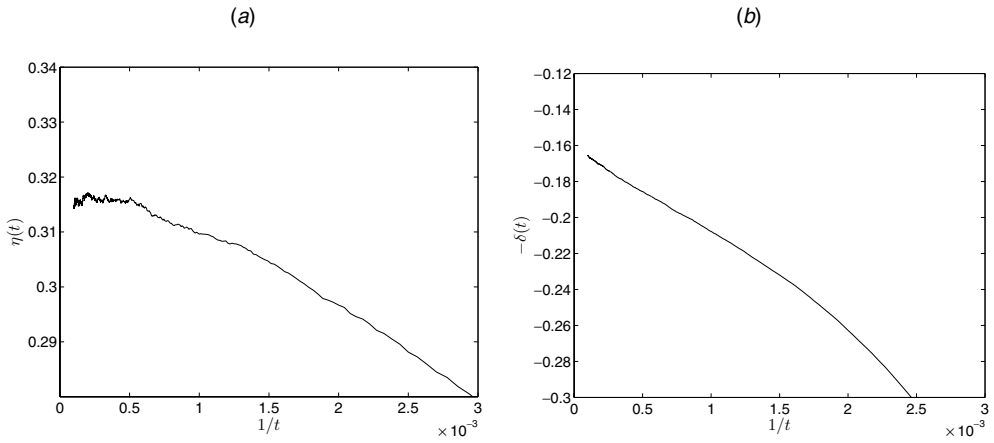

Figure 5. Plots of (*a*) $\eta(t)$ and (*b*) $-\delta(t)$ up to $t = 10^4$ at $p_d = p_{d_c} = 0.071754$.

4. Scaling functions

For models to belong to the same universality class, both the critical exponents and the scaling functions must be the same. Having shown that the critical exponents δ and η for our model are in agreement with the DP values, we turn our attention now to the scaling function for the probability of survival, $P(\Delta, L, t)$, where $\Delta = p_{d_c} - p_d$. We have the scaling ansatz [5]

$$P(\Delta, L, t) \sim \lambda^{-\beta} R_1(\Delta\lambda, L\lambda^{-\nu_\perp}, t\lambda^{-\nu_\parallel}) \tag{11}$$

for any $\lambda > 0$. β ($=\beta'$ in DP) is the critical exponent associated with the survival probability according to

$$P \sim \Delta^\beta \tag{12}$$

as $t \longrightarrow \infty$ and $\nu_\parallel$ and $\nu_\perp$ are the critical exponents associated with the temporal and spatial correlation lengths respectively. As in the previous section, we begin our simulations from a single seed with L large enough so that we can ignore the L-dependence in (11) and examine

$$P(\Delta, t) \sim \lambda^{-\beta} R_2(\Delta\lambda, t\lambda^{-\nu_\parallel}), \tag{13}$$

only. The functions R_i are non-universal, i.e. they are unique to each model. However, we may introduce metric factors a_Δ and a_t,

$$P(\Delta, t) \sim \lambda^{-\beta} \bar{R}(a_\Delta \Delta\lambda, a_t t\lambda^{-\nu_\parallel}) \tag{14}$$

so that $\bar{R}$ is a universal scaling function. Now all of non-universal, system-dependent features, such as the update scheme, boundary conditions, lattice structure, etc. are contained in these non-universal metric factors.

If we choose $\lambda = (a_t t)^{1/\nu_\parallel}$, then, since $\delta = \beta/\nu_\parallel$,

$$P(\Delta, t) \sim (a_t t)^{-\delta} \bar{R}(a_\Delta \Delta (a_t t)^{1/\nu_\parallel}, 1) \tag{15}$$

so we would expect to observe a data collapse by plotting $(a_t t)^\delta P$ versus $a_\Delta \Delta (a_t t)^{1/\nu_\parallel}$ for all models belonging to the same universality class. To find the metric factors a_t and a_Δ, we use the normalizations

$$\bar{R}(1, \infty) = \bar{R}(0, 1) = 1. \tag{16}$$

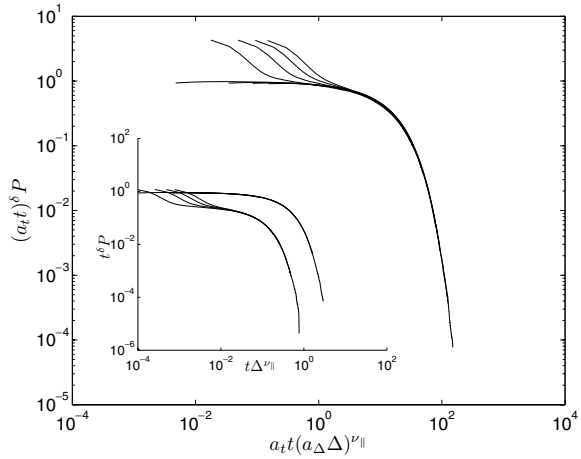

Figure 6. Data collapse for both the directed bond percolation model and our own using metric factors. Inset: data collapse for both the directed bond percolation model (top right) and our own (bottom left).

Then, choosing $\Delta = 0$ and $\lambda = (a_t t)^{1/\nu_\parallel}$ we have that a_t is given by the amplitude of

$$P \sim (a_t t)^{-\delta}. \tag{17}$$

Similarly, setting $\lambda = (a_\Delta \Delta)^{-1}$ and letting $t \longrightarrow \infty$, a_Δ is given by the amplitude of

$$P \sim (a_\Delta \Delta)^{\beta}, \tag{18}$$

where, since $\lambda > 0$, we must have $\Delta > 0$.

We now compare the scaling function for our model with that for *directed bond percolation* which belongs to DP. The model begins with an initial number of active sites and proceeds in time with site i becoming active at time $t + 1$ if site $i + 1$ and/or site $i - 1$ is active at time t and there exists a bond (with probability p) between this active site and the site i. The best estimate of the critical value of p is $p_c = 0.644\,700\,185(5)$ [19] where, for $p \geqslant p_c$, the active sites percolate the infinite system.

As was the case in our model, we begin with a single seed—just one active site at the origin here—and record the probability of survival $P_{DP}(t)$, i.e. the probability that there is at least one active site at time t. We denote the metric factors with a subscript DP for the *directed bond percolation* model and subscript P for our model. Excluding the metric factors, we plot in the inset in figure 6 the two separate data collapses for P for both the directed bond percolation model and for our own by plotting Pt^δ versus $t\Delta^{\nu_\parallel}$. We use the best known DP values of $\delta = 0.159464$ and $\nu_\parallel = 1.733\,847$ [10] and see clear data collapses in both models, especially for large t. Using now the obtained values for the metric factors, $a_{t,DP} = 1.57$, $a_{\Delta,DP} = 7.51$, $a_{t,P} = 3137.30$ and $a_{\Delta,P} = 0.2$, we have a complete data collapse of all the data from both models as shown in the main plot in figure 6, indicating that the scaling function for both models is identical.

Having examined both the critical exponents and the scaling functions, we conclude that our model belongs to DP in 1 + 1 dimensions.

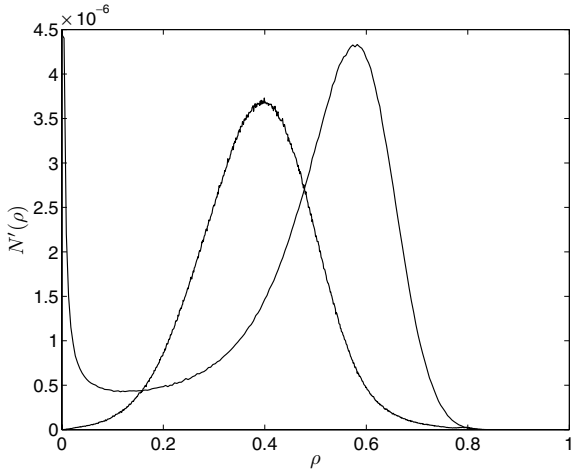

Figure 7. Normalized histogram, $N'(\rho)$ for different population densities in the (1+1)-dimensional (left) and 2 + 1 dimensional (right) cases showing the results for a continuous and first-order phase transition respectively.

5. First-order phase transitions

Due to DP having a critical dimension, $d_c = 4$ [20], it is surprising that this model belongs to DP in 1 + 1 dimensions only due to the first-order transition in higher dimensions. This is not a unique property to this model. A stochastic cellular automaton model developed by Bidaux, Boccara and Chaté (BBC) [21] is known to belong to DP in 1 + 1 dimensions [22] yet also displays a first-order transition in higher dimensions.

In order to examine the first-order phase transitions, we borrow a technique developed by Lee and Kosterlitz [23], which allows one to determine the order of a phase transition in an equilibrium system. The method detects a temperature-driven first-order phase transition by MC simulations in a finite system of volume L^d with periodic boundary conditions by examining the histogram of the energy distribution

$$N(E;\beta,L) = \mathcal{N} Z^{-1}(\beta,L)\Omega(E,L)\exp(-\beta E). \tag{19}$$

$\mathcal{N}$ is the number of MC sweeps, Z is the partition function and Ω is the number of states with energy E. For the q-state Potts models with q ordered and one disordered state, N has a characteristic double-peak close to $T = T_c$ for energy values $E_1(L)$ and $E_2(L)$ corresponding to the ordered and disordered states. The peaks are separated by a minimum at $E_m(L)$. If we define

$$A(E;\beta,L,\mathcal{N}) = -\ln N(E;\beta,L,\mathcal{N}), \tag{20}$$

then at $\beta = \beta_c(L)$ defined by $A(E_1;\beta,L) = A(E_2;\beta,L)$,

$$A(E_m;\beta,L,\mathcal{N}) - A(E_1;\beta,L,\mathcal{N}) = \Delta F \tag{21}$$

where ΔF is the bulk free-energy barrier between the states. At a first-order phase transition, $\Delta F \sim L^{d-1}$ for $L \gg \xi$, where ξ is the correlation length, whereas ΔF is independent of L at a continuous phase transition.

Due to our model being out of equilibrium, we continue only in the spirit of the above method and examine the histogram for the population density $N(\rho)$. For a first-order phase

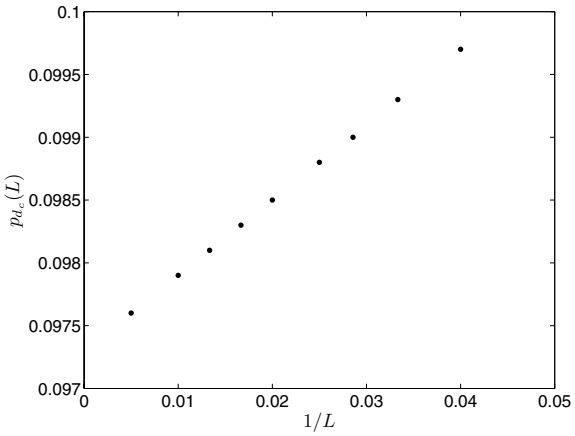

Figure 8. Plot to obtain an approximation for the critical point in the $(2+1)$-dimensional model by extrapolation of the points to the intersection with the y-axis.

transition, we expect a double-peaked structure at ρ_0 and at $\rho_+ = \rho_- = 0.5$ due to the corresponding phase coexistence. For $p_d > p_{d_c}$ we expect $N(\rho_0) > N(\rho_+)$ due to the greater chance of extinction, and likewise for $p_d < p_{d_c}$ we expect $N(\rho_0) < N(\rho_+)$ due to the greater chance of survival. This in fact gives us an excellent method for determining the critical point since it will be marked by $N(\rho_0)$ and $N(\rho_+)$ being equal. At a continuous phase transition, however, due to the power-law behaviour $\rho \sim t^{-\delta}$, we expect $N(\rho_0) = 0$ at the critical point. Both expectations are confirmed in figure 7, where we plot the histogram at the critical points for both the $(1+1)$- and $(2+1)$-dimensional cases.

As has been mentioned, the phase-coexistence enables the critical value p_{d_c} to be estimated. Iteratively finding the critical value for large enough t and different values of L and then plotting $p_{d_c}(L)$ versus $1/L$ in figure 8, we are able to obtain, by an extrapolation to the intercept with the y-axis, the value of the critical point in $2+1$ dimensions to be 0.0973 ± 0.0001. Unfortunately, no conclusive numerical evidence has yet been obtained in $3+1$ dimensions to give an accurate value for p_{d_c}.

6. Concluding remarks

By examining the critical exponents δ and η and the scaling function for the survival probability, we have shown that the $(1+1)$-dimensional version of our model belongs to the class of DP. Higher dimensions however do not, surprisingly, belong to this class due to the observed first-order phase transitions. In order to examine these transitions we used a technique inspired by equilibrium systems to find the value of the critical point in $2+1$ dimensions.

In order to answer the question about why our model does not belong to DP in all dimensions, we must look at how our model differs from others in the class. One difference to other models such as the *contact process* [24] or the *Domany–Kinzel* [25, 26] model is that, here, population growth requires two particles meeting, whereas death involves one particle only. This requirement results in the mean field exhibiting a first-order phase transition and also the existence of the critical population density, meaning that extinction can occur either because the death rate is too large and/or because the population density is too small. The previously mentioned BBC model shares this feature since they too observed a critical value of the initial concentration of 'alive' sites below which the system decayed to a zero concentration

state. With this inclusion, it is remarkable that the (1 + 1)-dimensional version of our model belongs to DP at all and only goes to highlight the robust nature of the universality class.

It seems likely that the unusual behaviour of both our model and that of BBC displaying DP behaviour in 1 + 1 dimensions, whilst first-order transitions in higher dimensions, is due to the critical population density/concentration present in both models. In our model, with the given rules for growth and decay, it is clear that the population will become more dependent on the density as the dimensionality of the system increases since particles will find it progressively harder to meet one another before they die. Time-dependent simulations carried out in higher dimensions, for example, needed increasingly large populations at $t = 0$ for *initial* population growth as p_d was increased, whereas two particles were sufficient in 1 + 1 dimensions even for $0 < p_d - p_{d_c} \ll 1$.

To examine whether the first-order transitions are a result of the critical population density, we changed our model to include single-particle reproduction, $A \longrightarrow 2A$, at rate c. From mean field analysis, this inclusion eradicates the critical population density for $c > p_b$ and initial numerical analysis appears to show that this changes the transition to continuous in at least the (2 + 1)-dimensional case. Similar observations were made if the particle diffusion mechanism was removed, i.e. if we turned the model into a simple growth process.

In the (1 + 1)-dimensional case, not only is it easier for particles to meet, but the larger fluctuations in the population are likely to be enough to induce the observed continuous phase transition as has been known to happen [27]. This was tested by introducing two separate types of particles into the system, L and R particles, where the L particles could only move left and R particles to the right. All other rules remained the same except that both an L and a R particle were required for reproduction. This modification to our model reduced the size of the fluctuations in the overall population and, again, early numerical simulations appear to show that this results in the transition changing to first-order.

Clearly, more work will however have to be carried out to confirm the above observations and to find out exactly what is happening at the phase transition.

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