Cluster geometry and survival probability in systems driven by reaction–diffusion dynamics

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Abstract. We consider a reaction–diffusion model incorporating the reactions $A \rightarrow \phi$, $A \rightarrow 2A$ and $2A \rightarrow 3A$. Depending on the relative rates for sexual and asexual reproduction of the quantity $A$, the model exhibits either a continuous or first-order absorbing phase transition to an extinct state. A tricritical point separates the two phase lines. While we comment on this critical behaviour, the main focus of the paper is on the geometry of the population clusters that form. We observe the different cluster structures that arise at criticality for the three different types of critical behaviour and show that there exists a linear relationship for the survival probability against initial cluster size at the tricritical point only.

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1. Introduction

Being able to identify the important geometrical structures of a system is known to greatly facilitate the understanding of the underlying physical mechanism [1]. In this paper, we describe how the tricritical point in a certain class of nonequilibrium population models is characterized by the unique structure of the spatial cluster.

Nonequilibrium phase transitions are of great relevance to disciplines as wide-ranging as traffic flow [2], chemical reactions [3] and atmospheric studies [4]. Of particular interest is the idea of universality, where different models display identical scaling functions and critical exponents close to the critical point. By far the largest and most well-known universality class out of equilibrium is directed percolation (DP). In fact, the robustness of DP led Janssen [5] and Grassberger [6] to the conjecture that all models involving short-range processes, with a single, scalar order parameter that exhibit a continuous phase transition from an active to a single absorbing state belong to the class. A universality class closely associated with DP is tricritical directed percolation (TDP), which has recently been studied by both steady-state [7] and dynamical [8] simulations.

The process of TDP incorporates higher order terms than DP, with the multicritical behaviour occurring if the lower order reactions vanish on a coarse-grained scale [9]. Lübeck [7] examined tricritical behaviour by adding the pair reaction $2A \rightarrow 3A$ to the contact process [10], whereas Grassberger [8] used a generalization of the Domany–Kinzel model [11] in $2+1$ dimensions.

Recently, we examined a simple reaction–diffusion model with the reactions $A \rightarrow \phi$ and $2A \rightarrow 3A$ [12] (see also [6, 13]), which exhibited a phase transition that is continuous, and DP, in $1+1$ dimensions, and first-order in higher dimensions. Although, from the mean field, the first-order phase transition was expected in all dimensions, the larger fluctuations in the $(1+1)$-dimensional case are likely to destabilize the ordered phase [14], resulting in the observed DP transition. Following on from Lübeck [7], we introduce a lower order proliferation reaction to our original model. By allowing both asexual and sexual reproduction, we have a phase space exhibiting both first-order and continuous phase transitions. While the critical behaviour of such a system has been previously studied [7, 8], the geometrical structure of the population at the different types of critical behaviour has so far been ignored. Sample snapshots of the population for sexual reproduction only and both asexual and sexual reproduction are shown in figure 1, highlighting the range of structures that are observed.

We show in this paper that the study of the geometrical structure can give additional insight into the behaviour of the model. In particular, we find that the tricritical point represents the unique point at which the spatial structure and event probabilities combine to give a birth rate that is independent of population size. This appears to give rise to the remarkable result that the relationship between initial cluster size and the survival probability up to some finite time $t$ is linear at the tricritical point only.

2. The model

We have a $d$-dimensional square lattice of linear length $L$ where each site is either occupied by a single particle or is empty. A site is chosen at random. The particle on an occupied site dies with probability $p_d$, 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.
and produces a new individual at the site that it has just left with probability $k$. If the chosen site is, however, occupied, the particle reproduces with probability $p_b$ producing a new particle on another randomly selected neighbouring site, conditional on that site being empty. A time step is defined as the number of lattice sites $N = L^d$, which corresponds to approximately one update per site. Periodic boundary conditions are used.

We therefore have the following reactions for a particle $A$ for proliferation and annihilation, respectively,

$$ A + A + \phi \rightarrow 3A, \quad A + \phi \rightarrow 2A \quad \text{and} \quad A \rightarrow \phi. $$ (1)

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

$$ \frac{d\rho(t)}{dt} = p_b (1 - p_d) \rho(t)^2 (1 - \rho(t)) + k (1 - p_d) \rho(t) (1 - \rho(t)) - p_d \rho(t), $$ (2)

where, here, we synonymously define the probabilities as rates. The first two terms consider the sexual and asexual reproduction reactions, respectively, and the final term death of an individual. Equation (2) has three stationary states:

$$ \bar{\rho}_0 = 0, \quad \bar{\rho}_\pm = \frac{1}{2} \left[ 1 - \frac{k}{p_b} \pm \sqrt{\left( \frac{k}{p_b} - 1 \right)^2 + \frac{4}{p_b} \left( k - \frac{p_d}{1 - p_d} \right)} \right]. $$ (3)

For $k \geq p_b$, $\bar{\rho}_+ \rightarrow 0$ continuously as $p_d \rightarrow k/(1 + k)$, indicative of a continuous phase transition with critical point

$$ p_{d_c}(k \geq p_b) = \frac{k}{1 + k}. $$ (4)

For $k < p_b$, we have a jump in steady state density from $(p_b - k)/2p_b$ to zero, this time with

$$ p_{d.c}(k < p_b) = \frac{(k + p_b)^2}{4p_b + (k + p_b)^2}. $$ (5)

Further, for $k < p_b$, we have a region

$$ \frac{k}{1 + k} < p_d \leq \frac{(k + p_b)^2}{4p_b + (k + p_b)^2}. $$ (6)
where the survival of the population is dependent on the population density. In fact, we have extinction for
\[
\rho(t) < \bar{\rho}_-(k < p_b, p_d).
\]
For \(k < p_b\), we therefore have a first-order phase transition. The two phase transition lines meet at the point \(k = p_b\), defining the position of the tricritical point \(k^*\). From our mean field analysis, we therefore have a phase diagram as shown in figure 2. We note that in our earlier paper [12], we examined the case \(k = 0\) and so were restricted, at the mean field level, to the first-order regime only.

Due to the false assumptions of spatial homogeneity and the neglect of fluctuations, we turn now to examining the model by Monte Carlo simulations with fixed \(p_b = 0.5\). From these simulations we find that for 1 + 1 dimensions, continuous phase transitions are observed for all \(k\). In order to examine tricritical behaviour we therefore proceed in 2 + 1 dimensions. Since the focus in this paper is on the geometrical structure of the population at criticality, we give here only a brief summary of how we obtained the critical points and refer the reader to [7, 8] for a more detailed overview of the techniques involved.

To find the values of \(p_d\) in the first-order regime we adopt an approach inspired by Lee and Kosterlitz [15] (see also [12]), due to the lack of power-law behaviour. For \(k < k^*\) we examine
Figure 3. Plots showing the critical behaviour of the model through power-law behaviour for the continuous phase transitions ($k \geq k^*$) and a histogram of population density for the first-order transitions ($k < k^*$). The main plot shows $n(t)$ (top) and $P(t)$ outlined in equations (8) and (9) at the tricritical point with $k = k^* = 0.12$ and $p_d = p_{d_c} = 0.1502195$. The dashed lines show our critical exponent values $\eta = -0.4875$ and $\delta' = 1.365$. The top right inset shows DP power-law behaviour for (from top to bottom) $k = 0.5$, $0.75$ and $1$. The values of $p_d$ are found to be $0.30302(0)$, $0.36765(0)$ and $0.41626(0)$ respectively, and the dashed lines show the power-law with DP values. The other inset shows the double-peaked structure of the frequency of population density for $k = 0.1 < k^*$. The equal heights of the peaks implies criticality with $p_{d_c} = 0.1418(1)$.

histograms of population density against frequency for different values of $p_d$. Due to the phase-coexistence at the critical point, we observe a double-peaked structure in the histogram for $p_d$ close to $p_{d_c}$, where the peaks are at equal heights for $p_d = p_{d_c}$ (see bottom inset of figure 3). For $p_d < p_{d_c}$, the peak at $\rho_\scriptscriptstyle C$ is greater than that at $\rho_\scriptscriptstyle B$ and vice versa for $p_d > p_{d_c}$.

To examine the continuous critical behaviour of our model, we study instead the dynamical behaviour of the system after starting from a single-seed at the centre of a large lattice. The lattice is sufficiently large so that no individuals reach the boundary during the running of the simulation. For fixed $p_b = 0.5$ we find the critical value $p_{d_c}$ for a given $k$. For the continuous phase transitions, at $p_d = p_{d_c}$, we expect asymptotic power-law behaviour

\begin{equation}
\bar{n}(t) \propto t^\eta,
\end{equation}

\begin{equation}
\bar{P}(t) \propto t^{-\delta'}
\end{equation}

for the population size and survival probability, respectively. For $k$ sufficiently greater than $k^*$, we find DP values for the critical exponents $\eta = 0.231$ and $\delta' = 0.451$ ([16] and references therein) as shown in the top right inset of figure 3.

Due to the continuous phase transition at $k = k^*$, we again expect power-law behaviour at the critical point, but this time with different values for the exponents [9, 17]. The tricritical point

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Figure 4. (a) Typical plots of the population structure at the critical point for (from left to right) $k = 0, 0.05, 0.5$ and 1. (b) Four different population structures for identical parameter values $k = k^* = 0.12$ and $p_d = p_{d_c} = 0.1502195$ showing no typical population structure. The simulations began from an initially fully occupied $128 \times 128$ lattice and ran until the population size reached 400 for the first time.

itself then can be obtained by seeking this power-law behaviour. The problem with this method is that a lack of power-law behaviour could be the result of an incorrect value of $k$, or $p_d$, or in fact both. Other methods, such as examining the scaling at the critical point, are also known to exhibit certain inaccuracies. These difficulties have led to discrepancies between values for the critical exponents at the tricritical point [7, 8]. Since our focus in this paper is on the geometrical structure of the population, we do not wish to review the approaches made, nor do we claim to have the definitive values. Instead, we give only our best estimate for the tricritical values which are $k = k^* = 0.12 \pm 0.005$ with $p_d = p_{d_c} = 0.150219(5)$, where the number in the parenthesis show the uncertainty in the last figure. Using these parameter values, we obtain the critical exponents $\eta = -0.487(5)$ and $\delta' = 1.36(5)$ as shown in figure 3. These values differ from those found by Grassberger [8] which is perhaps not surprising given the difficulties faced in finding the location of the tricritical point. The population structure is, however, not very sensitive to the parameter values, so we continue in the following section to examine the cluster geometry at different parameter values.

3. Cluster geometry

In this paper, we are particularly interested in the heterogeneous population distribution and in particular the geometrical structure of the clusters at criticality and how this changes
with $k$. From figure 4(a), we see that for $k \ll k^*$, after starting from a fully occupied lattice, the population becomes densely clustered. This is certainly not unexpected since, for $k = 0$, reproduction is only possible if an individual finds another. In contrast, in the DP region, the population is much more dispersed. For $k \gg k^*$, an individual has a greater chance of reproduction if it is surrounded by empty sites and so being heavily clustered is a disadvantage. For $k \neq k^*$, the plots shown in figure 4(a) are very typical plots, whereas at the tricritical point, the plots are very varied. For $k = k^*$, figure 4(b) shows that the population has little preference as to its structure. There are often areas where the population is heavily clustered as well as those where the structure is DP-like.

We find that there is no difference in the structure of the individual clusters themselves for different values of $k$. For example, plots of the radius of gyration against cluster size show identical plots for different values of $k$. In contrast, the probability of there being a cluster of size $n$ and the probability of such a cluster size surviving depends greatly on $k$. To examine this survival probability, we run simulations from an initially fully occupied lattice up to the point when a certain population is reached. We ensure that this population is sufficiently small so that the resulting density does not ‘force’ the population to take on certain cluster sizes. Clearly, if the density was too high, the population would naturally display large clusters since the population would be so tightly packed. Once this population has been reached, we make a copy of each cluster and place each one in turn at the centre of a sufficiently large lattice. The survival probability $P_s$ up to some time $t_{\text{max}}$ of the population is then measured for each individual initial cluster. The average results for each initial cluster size are shown in figure 5.

We see that the gradient of $P_s$ with respect to cluster size increases for $k = 0$ whereas it decreases for $k = 1$. Consistent with the snapshots from figure 4, we have that additional
individuals give an increasing advantage to the survival probability for \( k = 0 \) but have a negative effect for \( k = 1 \). Due to the curvature of the plots for \( k = 1 \) and \( k = 0 \), we would expect a linear relationship for some \( 0 < k < 1 \). Surprisingly, this occurs at the tricritical point \( k = k^* = 0.12 \).

In order to understand why this linear behaviour might occur at the tricritical point, we plot in figure 6 the average number of births and deaths that occur per individual per time step, \( B_i(n) \) and \( D_i(n) \) respectively, as a function of population size \( n \). The simulations were carried out at the critical point for different \( k \), using the same initial clusters as for figure 5. Rather than examining \( P_s \), here we found \( D_i(n) \) and \( B_i(n) \) averaged over \( t_{\text{max}} \) time steps, after starting from a variety of cluster sizes. We note that most of the cluster sizes used were small, with approximately 90\% of them being of size \(< 10\).

As expected, for all values of \( k \), \( D_i(n) \) remains constant for all population sizes since it is independent of the local density. In contrast, an increasing population seems to have a positive influence on \( B_i(n) \) for \( k = 0 \) whereas a negative influence for \( k = 1 \). At \( k = k^* \), for sufficiently large population sizes, \( B_i(n) \) is independent of the population size. In fact, for \( n > 40 \), \( B_i(n) \approx D_i(n) \). It appears then that at the tricritical point only, the unique combination of both the spatial structure and the event probabilities, result in a constant value for \( B_i(n) \).

The plots in figure 6 appear to show the systems out of criticality since we would expect \( D_i(n) = B_i(n) \) as \( n \to \infty \) at criticality. In particular, the results for \( k = 1 \) appear to show a typical population size due to the crossover of \( D_i(n) \) and \( B_i(n) \) at some \( n = n_c \), seemingly contradicting the scale-free nature one would expect to observe at criticality. We find however these effects are a result of the finite \( t_{\text{max}} \) used. In all cases, \( B_i(n) \to D_i(n) \) as \( t_{\text{max}} \to \infty \) and \( n \to \infty \) as shown in the inset in figure 6 for \( k = 1 \).\(^4\) For finite \( t_{\text{max}} \) and a sufficiently large population size,

\[^4\text{We note at this asymptotic limit that although } B_i(n) > D_i(n) \text{ leads to a growing population, the density is still zero in the thermodynamic limit.}\]
however, it is only at the tricritical point that we see equality in the number of births and deaths per individual per time step. We examine now whether it is this equality in the number of births and deaths that results in the observed linear relationship between initial cluster size and $P_s$. We simplify our model by considering the macroscopic population size $n(t)$ only and ignoring the microscopic individuals. Analogous to a random walk, the population increases by one with probability $p$, decreases by one with probability $q$ and stays the same with probability $1 - p - q$. We again examine the probability that the population survives up to some time $t_{\text{max}}$ where a time step at time $t$ is defined as $n(t)$ updates. We note that this is the same definition of a time step that we use when running simulations that begin with a single-seed. In the simulations, it corresponds to approximately one update per individual.

With $p = q$ only we find that the probability of survival increases linearly with initial population size (see inset of figure 5). This finding seems to indicate the equality in the number of births/deaths per individual per time step results in the observed linear behaviour at the tricritical point.

4. Conclusions

We have examined the critical behaviour in our model which exhibited DP, first-order and tricritical phase transitions. We noted the key geometrical differences in the cluster structure for each type of transition caused by the different values of the rate of asexual reproduction $k$. Of particular importance was the surprising result of the linear increase in probability of survival with cluster size. We hypothesized that this was due to the number of births and deaths per time step being equal at the tricritical point. Unfortunately, the lack of sensitivity of this linear behaviour to the parameters do not make this an effective method to obtain the position of the tricritical point. To do this, we believe seeking the power-law behaviour for $n(t)$ (often found to be the most sensitive parameter) to be the best approach. One area of future study is the discrepancy between our values for $\eta$ and $\delta'$ at the tricritical point with Grassberger’s who found $\eta = -0.353(9)$ and $\delta' = 1.218(7)$ [8]. Indeed, he had disagreement between his values for $\beta$, $\nu_\perp$ and $\phi$ and Lübeck’s [7]. The difficulties in finding the parameters at the tricritical point have been mentioned and need to be addressed before accurate values for the tricritical exponents can be conclusively obtained.

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