Nanotechnology Perceptions
ISSN 1660-6795
www.nano-*ntp.com*

Absorbing Phase Transition In A Class Of Models Of Polydisperse K-Mers In One Dimension

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We study diffusion, split and reconstitution of hard k-mers on a one-dimensional periodic lattice, subjected to a constraint that the lengths of the k-mers do not increase beyond a fixed value n, however initially, at t=0 the k-mers can have lengths larger than n. For higher values of packing fractions (i.e. higher ρ, where $\rho = \frac{N}{L}$, N is number of sites covered by the k-mers, L is system size) the system gets stuck into absorbing state. On the other hand, for lower ρ, the system remains in the active state. In this article it is shown that in this class of models, the system continuously undergoes an active to absorbing state phase transition when the density crosses a critical threshold $\rho_c = \frac{n}{n+1}$. The active steady state of these models can be exactly solved using matrix product ansatz, and it is shown that the density of active rods $\rho_a = \frac{N_a}{L}$, (where, N_a is number of active rods) vanishes at the transition point as $\rho_a \sim 2(n+1)\,(\rho_c - \rho)$.

Keywords: *Polydisperse k-mers, Absorbing Phase Transition, Non-equilibrium Systems, Stochastic Process, Driven Diffusive Systems, Statistical Mechanics*

1. Introduction

Absorbing state phase transition (APT) [1] is the most studied non-equilibrium phase transition in the recent times. In APT, by tuning a control parameter, the system can be driven from an active phase to an absorbing one where the dynamics ceases. Unlike equilibrium systems, generally these systems do not obey the detailed balance condition all over the accessible phase space, which makes analytical treatment of these systems highly nontrivial, giving rise to varied class of distributions as well as novel correlations and unconventional critical behavior. The most robust universality class of APT of such systems is directed percolation (DP) [2]. DP plays a paradigmatic role in non-equilibrium statistical mechanics like that of Ising class in the equilibrium counterpart. Other examples include the class of compact directed percolation, the parity-conserving universality class, the pair-contact process with diffusion, the Manna class etc. [1]. These types of critical behavior are observed in context of synchronization [3], damage spreading [4], depinning transition [5], catalytic reactions [6], forest fire [7], extinction of species [8] etc. The study of statistical mechanics of extended objects has started long ago by Tonks, Onsager etc. [9, 10, 11]. In context of non-equilibrium systems, there has been lot of

interest in the study of driven diffusion of extended objects. In this article we will focus on driven diffusive systems with polydisperse k-mers in 1D lattice, i.e. extended objects with various integer length k, occupying consecutive k lattice sites without violating hard-core exclusion. A driven diffusive system of k-mers was first studied in context of protein synthesis in prokaryotic cells [12]. Reconstitution dynamics has been studied for one-dimensional systems consisting of only monomers and dimers [13, 14]; these systems generally exhibit ergodicity breaking. Later studies [15, 16] generalized these models to consider asymmetric diffusion of k-mers up to a maximum length k_{max} . In another work [17], an asymmetric fragmentation process was studied where k-mers could break or combine when separated by one vacancy; for specific rates the model can be mapped to the TASEP [18]. Existence of phase separation is also seen in these type of models [19, 20].

In this paper we study a class of models where k-mers diffuse on a 1D periodic lattice, and these k-mers can reconstitute into k-mers of different sizes, provide that the only k-mers with length $k \leq n$ can undergo such activities, where n is a integer parameter which defines this class of models. It is shown that the number of active k-mers in these models will diminish as the density of covered sites ρ is increased beyond a critical density ρ_c. The active steady state of this APT is solved using matrix product ansatz (MPA).

2. Model:

The model is defined on a one-dimensional periodic lattice of length L, where sites (site number i=1,2,3 .... L) can be occupied by polydisperse k-mers of length 0<k<L. These k-mers are hard in the sense that no site can be occupied by more than one k-mer. Although the length of the k-mers can change through the processes of split and reconstitution, the total length of all of the k-mers (i.e. total no. of sites occupied by all of the k-mers) remains constant. Let us understand how

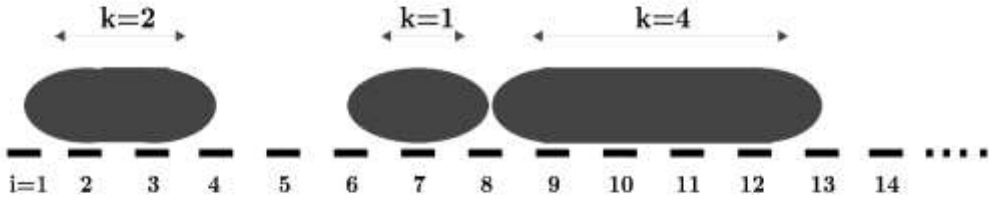

Figure 1: Three k-mers of length 2, 1, and 4 occupies site no. 2-3, 7 and 9-12 respectively.

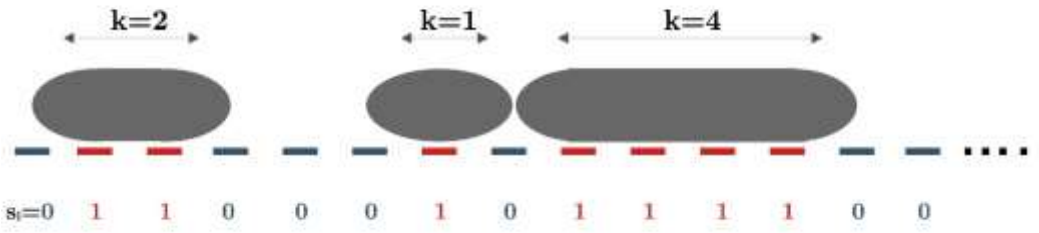

Figure 2: The sites occupied by the k-mers are represented by site variable s_i=1

the k-mers occupy the lattice sites through Figure 1 and Figure 2. In the Figure 1 three k-mers of length 2, 1, and 4 are seen to occupy sites with number 2-3, 7 and 9-12. States of the sites occupied by the k-mers are represented by the site variables s_i=1 and that of the unoccupied sites are represented by s_i=0. In the Figure 2 the states of the sites are depicted in red (s_i=1, i.e. occupied) and blue (s_i=0, i.e. unoccupied). Here we must note that the nearest unoccupied sites adjacent to any k-mer, can not be occupied by any other k-mer. Thereby we can represent the configuration of the sites 1-14 shown in Figure 1 and Figure 2, as {01100010111100}.

Now, let us define the dynamics of the model. The k-mers which have at least one vacant next-nearest neighbor, can diffuse symmetrically with rate 1/k, for $k \leq n$. Here n is an integer parameter which defines this class of models. With the same rate it can also split into two k-mers of length k_1 and k_2 (such that $k_1+k_2 = k$). Here we should remember that the nearest neighbor of the k-mer is not occupiable unless the next-nearest neighbor is vacant. Furthermore, two adjacent k-mers of length k_1 and k_2, reconstitute or merge with rate $1/(k_1+k_2)$ to form k-mers of length $k_1 \pm \Delta$ and $k_2 \mp \Delta$; here the value of Δ is such that, the length of the resulting k-mer(s) do not increase beyond n, although there is no such restriction on decrement of the length. The cases $\Delta = k_2$ and $\Delta = k_1$ correspond to the merger of k-mers. Below we summarize these rules of the dynamics with the help of site variables:

Diffusion:

$$\begin{gathered} 001^{k}0 \xrightarrow{1/k} 01^{k}00 \\ 01^{k}00 \xrightarrow{1/k} 001^{k}0 \quad \text{where,} \quad k \leq n \end{gathered} \tag{1}$$

Split:

$$\begin{gathered} 001^{k}0 \xrightarrow{1/k} 01^{k_1}01^{k_2}0 \\ 01^{k}00 \xrightarrow{1/k} 01^{k_1}01^{k_2}0 \text{ where}, k = k_1 + k_2 \end{gathered} \tag{2}$$

Reconstitution (including merger):

$$01^{k_1}01^{k_2}0 \xrightarrow{1/k} 01^{k_1+\Delta}01^{k_2-\Delta}0 \text{ where, } k_1 + \Delta \leq n$$

$$01^{k_1}01^{k_2}0 \xrightarrow{1/k} 01^{k_1-\Delta}01^{k_2+\Delta}0 \text{ where, } k_2 + \Delta \leq n \quad (3)$$

With these rules, at an instant, the system will have two types of k-mers, a) k-mers which can move/split/reconstitute, b) k-mers which do not have such activity. The density of the sites covered by the k-mers, i.e. ρ=N/L, plays a crucial role in determining the state of the system. Here, $N = \sum_{i=1}^{r} k_i$, r is total number of k-mers, k_i is the length of the i-th k-mer. For sufficiently higher values of ρ, the k_i's are larger than n, thus all of the k-mers are inactive. As a result the system gets stuck into an absorbing state. On the other hand for sufficiently lower values of ρ, the k_i 's are smaller than n, therefore the system remains in active state forever. In between these higher and lower density regimes, there exist a critical density ρ_c, below which the system remains in active phase and above which the system gets stuck into an absorbing state. Thus, there occurs an APT at critical density ρ_c. Here in this article, we focus on the active steady state of this class of models, which will help us understand the characteristics of these phase transitions. Below critical density ρ_c the system starts from an initial state, where k-mers of various possible sizes (k<L) are randomly placed over the lattice. As the time elapses, k-mers of sizes k> n are destroyed gradually. On the contrary no k-mer with length k>n are produced by the rules of dynamics. Consequently, after a long relaxation period ($t \sim L^{\frac{1}{2}}$) the system reaches steady state where, there are no k-mers of length greater than n. This property of the active steady is crucial to get the exact solution of these models through MPA.

3. Study of active steady state:

As discussed in the previous section, we can guess that there exists an APT at a critical density $\rho = \rho_c$. Below $\rho = \rho_c$, the system remains in active steady state. In this active steady state, all the k-mers in the system have length $k \leq n$. All possible configurations in the accessible phase space in the active steady state are equally probable, as the dynamics given in Eq. 1, 2, and 3 follow detailed balance condition. Thus, without loss of generality, weight of an arbitrary configuration in the steady state $C = \{0^{m_1}1^{k_1}0^{m_2}1^{k_2}\ldots.0^{m_r}1^{k_r}\}$ can be taken:

$$w\left(\{\, 0^{m_1}1^{k_1}0^{m_2}1^{k_2}\ldots.0^{m_r}1^{k_r}\}\right) = \begin{matrix} 1 & \forall\, k_i \leq n \\ 0 & \text{otherwise} \end{matrix} \quad (4)$$

Where m_i and k_i follow the constraints given below:

$$\sum_{i=1}^{r}(m_i + k_i) = L, \qquad \sum_{i=1}^{r} k_i = N \quad (5)$$

We try to write down the weight function as product of matrices. For that purpose, we consider V and K matrices for vacant and filled sites and write down the weight function as:

$$w(\{\, 0^{m_1}1^{k_1}0^{m_2}1^{k_2}\ldots.0^{m_r}1^{k_r}\}) = Tr[V^{m_1}K^{k_1}V^{m_2}K^{k_2}\ldots.V^{m_r}K^{k_r}] \quad (6)$$

Here V and K matrices follow: $K^i = 0$, for $i > n$; $VK^i = V$, for $i \leq n$. V, K are (n+1)×(n+1) matrices, which have following form:

$$V = \begin{pmatrix} 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & ... & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 1 & 0 & 0 & \cdots & 0 & 0 \\ 1 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}_{(n+1)\times(n+1)} \qquad K = \begin{pmatrix} 0 & 1 & 0 & 0 & \cdots & 0 & 0 \\ 0 & 0 & 1 & 0 & ... & 0 & 0 \\ 0 & 0 & 0 & 1 & ... & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 0 & 0 \end{pmatrix}_{(n+1)\times(n+1)}$$

Now we can write down the partition function of the system in active steady state as: $\mathcal{Z}_L = T(z)^L$, where $T(z) = (zK + V)$. Here z is a fugacity which tunes ρ. Partition function in variable length ensemble can be written as:

$$\mathcal{Q}(z,\gamma) = \sum_{L=1}^{\infty} \gamma^L \, Tr(T^L) = Tr[\gamma T.(1-\gamma T)^{-1}] \tag{7}$$

Here γ is a fugacity which tunes system size L. After simplification, we get

$$\mathcal{Q}(z,\gamma) = \frac{\gamma \frac{\partial}{\partial \gamma}\left(\gamma \, g(\gamma z)\right)}{1-\gamma g(\gamma z)} \tag{8}$$

where,

$$g(\gamma z) = 1 + (\gamma z) + (\gamma z)^2 + (\gamma z)^3 \ldots . + (\gamma z)^n \tag{9}$$

Now, with the help of this variable length partition function (i.e. Eq. 8), we can write down the expression of average number of occupied sites $\langle N \rangle$ and average system size $\langle L \rangle$:

$$\langle N \rangle = \frac{z}{\mathcal{Q}} \frac{\partial \mathcal{Q}}{\partial z}, \qquad \langle L \rangle = \frac{\gamma}{\mathcal{Q}} \frac{\partial \mathcal{Q}}{\partial \gamma} \tag{10}$$

Using Eq. 8 & 9 we get:

$$\langle N \rangle = z\gamma \frac{\partial_z g}{1-\gamma g} + z \frac{\partial_z g + \partial_{\gamma z}^2 \, g}{g + \gamma \partial_\gamma g} \tag{11}$$

$$\langle L \rangle = \frac{g + 3\gamma \partial_\gamma g + \gamma^2 \partial_\gamma^2 g}{g + \gamma \partial_\gamma g} + \frac{\gamma g + \gamma^2 \partial_\gamma g}{1-\gamma g} \tag{12}$$

$\gamma \to 1/g(\gamma z)$ corresponds to the thermodynamic limit $\langle L \rangle \to \infty$. In this limit the expression of density $\rho = \langle N \rangle / \langle L \rangle$ comes out:

$$\rho = \frac{\beta g'(\beta)}{g(\beta) + \beta g'(\beta)} = \frac{\beta + 2\beta^2 + 3\beta^3 + \cdots \ldots + n\beta^n}{1 + 2\beta + 3\beta^2 + \cdots \ldots + (n+1)\beta^n} \tag{13}$$

Here we have used the fact that g is function of $\beta = \gamma z$ (see Eq. 9). With the given description of the active steady state, $\rho(\beta)$ is an analytic function of β. As β is increased, the density of the system increases and at $\beta \to \infty$ the density saturates to $\frac{n}{n+1}$. Beyond this density the system can not remain in active steady state. Hence $\rho_c = \frac{n}{n+1}$ is the critical density of the APT. As ρ is expanded as a function of β^{-1}, around 0, near criticality we get

$$\rho(\beta^{-1}) = \rho_c - \frac{1}{(n+1)^2}\frac{1}{\beta} + \mathcal{O}\left(\frac{1}{\beta^2}\right)$$

$$\Rightarrow (\rho_c - \rho) \sim \frac{1}{(n+1)^2}\frac{1}{\beta} \tag{14}$$

In Fig. 3, ρ is plotted against 1/β for n=2 and n=3. As $\beta^{-1} \to 0$ the density $\rho \to \rho_c$. For n=2 and 3, the critical density is seen to be $\rho_c = 2/3 \; and \; 3/4$ respectively.

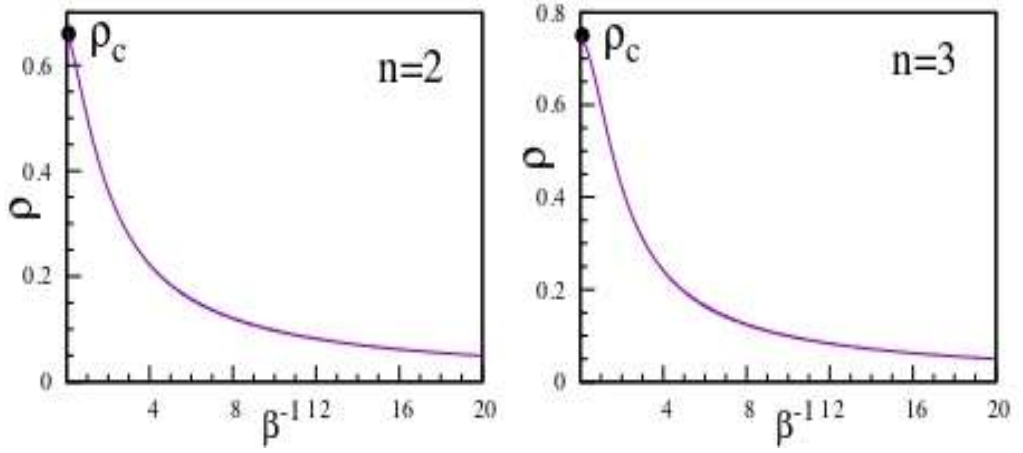

Figure 3: ρ is plotted against β^{-1} for n=2 and n=3. In the limit $\beta^{-1} \to 0, \; \rho \to \rho_c$ For n=2 and 3, the critical density is seen to be $\rho_c = 2/3 \; and \; 3/4$ respectively.

4. The order-parameter:

Till this point we have studied the properties of the active steady state of this class of models, and using MPA we have obtained the critical density of the APT. Qualitatively we have discussed how the activity of the system depends upon the density ρ. Now let us define the activity of the system, which is the order-parameter of the APT, and can be studied as a function of ρ. If total number of active k-mers is N_a, then activity in the system is given by $\rho_a = N_a/L$. In the active steady state,

$$\rho_a = \sum_{l=1}^{n}\left[\langle 001^l 0\rangle + \langle 01^l 00\rangle\right] + \sum_{\substack{l_1,l_2=1 \\ l_1+l_2<2n}}^{n} \langle 01^{l_1}01^{l_2}0\rangle \tag{15}$$

In Eq. 15, the first two terms correspond to the number of active k-mers which can diffuse and split; the last term counts number of active k-mers which can reconstitute among them. As the lattice follow periodic boundary condition, $\langle 001^l 0\rangle = \langle 01^l 00\rangle$. Treating vacancies and occupancies with matrices V and K, as given in Eq. 6, we calculate following quantities:

$$\sum_{l=1}^{n}\langle 001^l 0\rangle = \frac{\gamma^3}{Q} Tr[V(I-\gamma T)^{-1}]\sum_{l=1}^{n}\beta^l \tag{16}$$

$$\sum_{\substack{l_1,l_2=1 \\ l_1+l_2<2n}}^{n} \langle 01^{l_1}01^{l_2}0\rangle = \frac{\gamma^3}{Q}\, Tr[V(I-\gamma T)^{-1}](\beta^2 + 2\beta^3 \ldots + n\beta^{n+1} + (n-1)\beta^{n+2} \ldots + 2\beta^{2n-1}) \tag{17}$$

In thermodynamic limit, using Eq. 8, and $Tr[V(I-\gamma T)^{-1}] = g/(1-\gamma g)$, we get

$$\rho_a(\beta) = \frac{2\beta + 3\beta^2 + 4\beta^3 \ldots + n\beta^{n+1} + (n-1)\beta^{n+2} \ldots + 2\beta^{2n-1}}{g(\beta)(1 + 2\beta + 3\beta^2 \ldots + (n+1)\beta^n)} \tag{18}$$

Near criticality i.e. $\beta \to \infty$

$$\rho_a(\beta) \sim \frac{2}{n+1}\frac{1}{\beta}$$

Using Eq. 14, we obtain $\rho_a \sim 2(n+1)(\rho_c - \rho)$, hence the order-parameter exponent in this class of models is 1, which is similar to the class of models discussed in [21].

Eq. 13 and Eq. 18 are used to eliminate β, and ρ_a is plotted as a function of ρ for n=2 and 3. In Figure 4 these plots are compared with the data points obtained from Monte Carlo simulations with system with lattice size $L=10^5$. Here we have not shown any result for the simplest case n=1, because that corresponds to the CLG model [22].

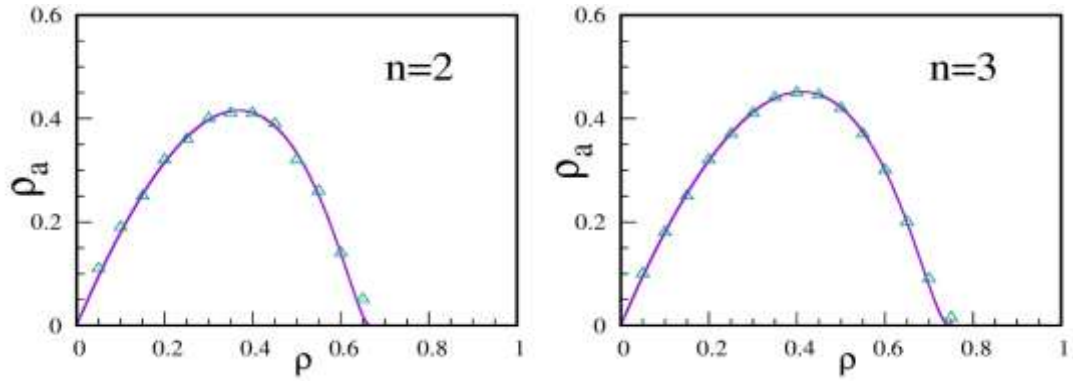

Figure 4: The order-parameter ρ_a is plotted against tuning parameter ρ, for n=2 & 3. The solid lines are from theoretical calculations and the dots are obtained from Monte Carlo simulation of system with $L=10^5$. Below ρ_c the system remains in active steady state, above ρ_c the system gets stuck into absorbing state.

5. Conclusion:

Phase transition in a system with extended objects can be very interesting in regards to both theoretical and experimental research. First such studies in equilibrium systems were done by Tonks, Onsager etc. [9, 10, 11]. Those simple systems are enriched with complex phases and transition between those phases are also of great interest. Here, in this article we have noticed that a diffusive system of reconstituting k-mers in a 1D chain undergoes a phase transition from active to absorbing phase, as the density of the system is increased beyond a critical density. In the time evolution of the system, a constraint is imposed that the length of the k-mers do not increase beyond a certain integer parameter n. Although the length of the k-mers can decrease. In this APT density of k-mers is considered as the tuning parameter, and the density of active k-mers is the order parameter. With the help of MPA we solve the active steady state of the model exactly. The critical density of the transition is found to be $\rho_c = \frac{n}{n+1}$. The order parameter exponent of the APT is 1. Theoretically obtained expression of order-parameter as a function of tuning parameter is compared with the Monte Carlo simulation data for the cases n=2 and 3. Presently, study of complex behaviour of active extended objects has received considerable attention [22]. Exactly solved models with extended objects will be of great help for future studies in this field.

6. References:

1. M. Henkel, H. Hinrichsen, and S. Lubeck, Non-Equilibrium phase transitions, vol.-**1**, Springer, Berlin (2008).
2. H. Hinrichsen, Advances in physics 49 (7), 815-958 (2000)
3. P. Grassberger, Phys. Rev. E 59, R2520 (1999)
4. P. Grassberger, J. Stat Phys. 79, 13 (1995)
5. F. D. A. A. Reis, Braz. J. Phy. 33, 501 (2003).
6. R. M. Ziff, E. Gulari, and Y. Barshad, Phys. Rev. Lett. 56, 2553 (1986).
7. E. V. Albano, J. Phys. A 27, L881 (1994).
8. A. Lipowski and M. Lopata, Phys. Rev. E 60, 1516 (1999).

9. L. Tonks, Phys. Rev. 50, 955 (1936).
10. L. Onsager, Ann NY Acad. Sci. 51, 627 (1949).
11. B. J. Alder and T. E. Wainwright, J. Chem. Phys. 27, 1208 (1957).
12. C. T. MacDonald, J. H. Gibbs, and A. C. Pipkin, Biopolymers 6, 11 (1968).
13. G. I. Menon, M. Barma, and D. Dhar, J. Stat. Phys. 86, 1237 (1997).
14. D. Dhar, Physica A 315, 5 (2002).
15. M. Barma, M. D. Grynberg, and R. B. Stinchcombe, J. Phys. Condens. Matter 19, 065112 (2007).
16. M. D. Grynberg, Phys. Rev. E 84, 061145 (2011).
17. A. Rakos and G.M. Schutz, J. Stat. Phys. 118, 511 (2005).
18. F. Spitzer, Adv. in Math. 5, 246 (1970).
19. B. Daga and P. K. Mohanty, JSTAT P04004 (2015).
20. AK Chatterjee, B Daga, PK Mohanty, Physical Review E 94 (1), 012121 (2016).
21. A. Chatterjee and P. K. Mohanty, Phys. Rev. E 94, 062141 (2016).
22. M.Rossi, R.Pastor-Satorras, and A.Vespignani, Phys.Rev.Lett. 85, 1803 (2000).
23. A. Baskaran, M. C. Marchetti, Phys. Rev. E **77**, 011920 (2008)