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How does degree heterogeneity affect nucleation on complex networks?

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Abstract. Nucleation is an initiating process of a stable phase from a metastable phase in a first-order phase transition. Taking the Ising model as a paradigm, we investigate the dynamics of nucleation on complex networks and focus on the role played by the heterogeneity of degree distribution on nucleation rate. Using Monte Carlo simulation combined with forward flux sampling, we find that for a weak external field the nucleation rate decreases monotonically as degree heterogeneity increases. Interestingly, for a relatively strong external field the nucleation rate exhibits a nonmonotonic dependence on degree heterogeneity, in which there exists a maximal nucleation rate at an intermediate level of degree heterogeneity. Furthermore, we develop a heterogeneous mean-field theory for evaluating the free-energy barrier of nucleation. The theoretical estimations are qualitatively consistent with the simulation results. Our study suggests that degree heterogeneity plays a nontrivial role in the dynamics of phase transitions in networked Ising systems.

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Contents

1. Introduction

Since many social, biological, and physical systems can be properly described by complex networks, dynamics on complex networks have received considerable attention in the last decade [1]–[4]. In particular, phase transitions on complex networks have been a subject of intense research in the field of statistical physics and many other disciplines [5]. Owing to the heterogeneity in degree distribution, phase transitions on complex networks are drastically different from those on regular lattices in Euclidean space. For instance, degree heterogeneity can lead to a vanishing percolation threshold [6], the whole infection of disease with any small spreading rate [7], the Ising model to be ordered at all temperatures [8]–[10], the transition from order to disorder in voter models [11], synchronization to be suppressed [12, 13] and different paths towards synchronization in oscillator network [14], to list just a few. However, there is much less attention paid to the dynamics of phase transition itself on complex networks, such as the nucleation process in a first-order phase transition.

Nucleation is a fluctuation-driven process that initiates the decay of a metastable state into a more stable one [15]. Many important phenomena in nature, like crystallization [16], glass formation [17], and protein folding [18], are closely related to the nucleation process. In the context of complex networks, the study of the nucleation process is not only of theoretical importance for understanding how a first-order phase transition happens in networked systems, but also may have potential implications in real situations, such as the transitions between different dynamical attractors in neural networks [19], the genetic switch between high- and low-expression states in gene regulatory networks [20, 21], and opinion revolution [22] as well as language replacement [23, 24] in social networks.

Recently, we have made a tentative step in the study of the nucleation process of the Ising model on complex networks, where we have identified nucleation pathways using a rare-event sampling technique, such as nucleating from nodes with smaller degree on heterogeneous networks [25] and a multi-step nucleation process on modular

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networks [26]. In addition, we identified a size-effect of the nucleation rate on mean-field-type networks [25] and a nonmonotonic dependence of the nucleation rate on the modularity of networks [26]. As mentioned above, degree heterogeneity has a significant effect on the dynamics on complex networks. Therefore, a natural question arises: how does degree heterogeneity affect nucleation of the Ising model on complex networks? To answer this question, in this paper, we study the dynamics of nucleation on various network models whose heterogeneity of degree distribution can be continuously changed by adjusting a single parameter. We use Monte Carlo (MC) simulation combined with forward flux sampling (FFS) to compute the nucleation rate and consider the effect of degree heterogeneity on the rate. Since the critical temperature of the Ising model on uncorrelated random networks increases with the heterogeneity of degree distribution [5], [8]–[10], one may come to the intuitive conclusion that if both the temperature and external field are fixed, the nucleation rate will decrease monotonically as degree heterogeneity increases. Here, we show that such an intuition is not the case: the nucleation rate can change monotonically or nonmonotonically with degree heterogeneity depending on the level of driving force, i.e., the value of external field. For a weak external field, the nucleation rate decreases monotonically with degree heterogeneity, whereas for a relatively strong external field there exists a maximal nucleation rate corresponding to a moderate level of degree heterogeneity. Furthermore, we present a heterogeneous mean-field theory for calculating the free-energy barrier of nucleation. The theoretical results qualitatively agree with the simulation ones.

2. Model and simulation descriptions

The Ising model in a network comprised of N nodes is described by the Hamiltonian

$$\mathcal{H} = -J \sum_{i<j} a_{ij} s_i s_j - h \sum_i s_i, \tag{1}$$

where spin variable s_i at node i takes either $+1$ (up) or -1 (down). $J(>0)$ is the coupling constant and h is the external field imposed on each node. The elements of the adjacency matrix of the network take $a_{ij} = 1$ if nodes i and j are connected and $a_{ij} = 0$ otherwise.

The simulation is performed by standard Metropolis spin-flip dynamics, in which we attempt to flip each spin once, on average, during each MC cycle. In each attempt, a randomly chosen spin is flipped with the probability $\min(1, \mathrm{e}^{-\beta\Delta E})$, where $\beta = 1/(k_{\mathrm{B}}T)$ with the Boltzmann constant k_{B}, temperature T, and ΔE the energy change due to the flipping process. We set $J = k_{\mathrm{B}} = 1$, $h > 0$ and $T < T_{\mathrm{c}}$, where T_{c} is the critical temperature. The initial configuration is prepared with a metastable state in which $s_i = -1$ for most of the spins. The system will stay in that state for a significantly long time before undergoing a nucleating transition to the thermodynamic stable state with most spins pointing up.

Since nucleation is an activated process that occurs extremely slowly, brute-force simulation is prohibitively expensive. To overcome this difficulty, we will use a recently developed simulation method, FFS [27]. This method allows us to calculate nucleation rate and determine the properties of ensemble towards nucleation pathways. This method uses a series of interfaces in phase space between the initial and final states to force the system from the initial state A to the final state B in a ratchet-like manner. Before the simulation begins, an order parameter λ is first defined, such that the system is in state A if $\lambda < \lambda_0$ and

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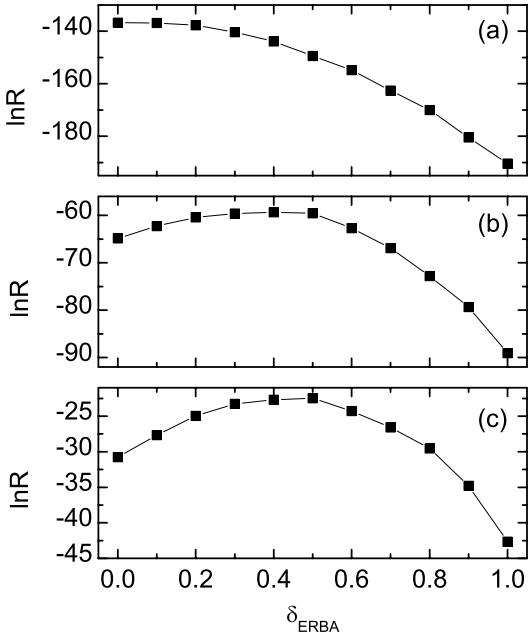

Figure 1. The logarithm of the nucleation rate $\ln R$ as a function of the strength of degree heterogeneity δ_{ERBA} for $h = 0.5$ (a), $h = 0.8$ (b), and $h = 1.0$ (c). Other parameters are $N = 1000$, the mean degree $\langle k \rangle = 6$, and $T = 2.5$.

it is in state B if $\lambda > \lambda_M$. A series of nonintersecting interfaces λ_i $(0 < i < M)$ lie between states A and B, such that any path from A to B must cross each interface without reaching λ_{i+1} before λ_i. The algorithm first runs a long-time simulation which gives an estimate of the flux $\bar{\Phi}_{\mathrm{A},0}$ escaping from the basin of A and generates a collection of configurations corresponding to crossings of interface λ_0. The next step is to choose a configuration from this collection at random and use it to initiate a trial run which is continued until it either reaches λ_1 or returns to λ_0. If λ_1 is reached, store the configuration of the end point of the trial run. Repeat this step, each time choosing a random starting configuration from the collection at λ_0. The fraction of successful trial runs gives an estimate of the probability of reaching λ_1 without going back into A, $P(\lambda_1|\lambda_0)$. This process is repeated, step by step, until λ_M is reached, giving the probabilities $P(\lambda_{i+1}|\lambda_i)$ $(i = 1, \ldots, M-1)$. Finally, we get the nucleation rate R from A to B, which is the product of the flux $\bar{\Phi}_{\mathrm{A},0}$ and the probability $P(\lambda_M|\lambda_0) = \prod_{i=0}^{M-1} P(\lambda_{i+1}|\lambda_i)$ of reaching λ_M from λ_0 without going into A.

In the present work, we define the order parameter λ as the total number of up-spins in the network. The spacing between adjacent interfaces is fixed at three up-spins, but the computed results do not depend on this spacing. The simulation results below are obtained by averaging over at least five independent FFS samplings and ten different network realizations.

3. Results

To study the effect of degree heterogeneity on nucleation, we first adopt a network model proposed in [28]. The network model allows us to construct networks with the same mean degree, interpolating from Erdo–Reènyi (ER) graphs to Barabaèsi–Albert (BA) scale-free

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networks by tuning a single parameter δ_{ERBA}. For $\delta_{\mathrm{ERBA}} = 0$ one gets ER graphs with a Poissonian degree distribution whereas for $\delta_{\mathrm{ERBA}} = 1$ the resulting networks are SF with $P(k) \sim k^{-3}$. Increasing δ_{ERBA} from 0 to 1, the degree heterogeneity of the network increases. Figure 1 shows the logarithm of the nucleation rate, $\ln R$, as a function of δ_{ERBA} for three different external fields: $h = 0.5$, 0.8, and 1.0. For $h = 0.5$, $\ln R$ decreases monotonically with δ_{ERBA}, implying that degree heterogeneity is unfavorable for the occurrence of nucleation events. Interestingly, for $h = 0.8$, $\ln R$ is no longer monotonically dependent on δ_{ERBA}: as degree heterogeneity increases, $\ln R$ first increases slowly until $\delta_{\mathrm{ERBA}} = 0.5$ and then decreases rapidly. Further increasing h to $h = 1.0$, $\ln R$ clearly exhibits a nonmonotonic change with δ_{ERBA}. That is, there exists a maximal nucleation rate that occurs at a moderate strength of degree heterogeneity.

To understand the above simulation results, we shall give a heterogeneous mean-field theory on complex networks for evaluating the nucleation barrier. First, we define m_k as the average magnetization of a node with degree k, i.e., $m_k = N_k^{-1}\sum_{i|k_i=k} s_i$, where N_k is the number of nodes with degree k. Furthermore, for a network without degree correlation, the probability that a randomly chosen nearest-neighbor node has degree k is $kP(k)/\langle k\rangle$, where $P(k) = N_k/N$ is degree distribution and $\langle k\rangle = \sum_k kP(k)$ is the mean degree. Thus, the interaction energy between a node with degree k and its neighboring nodes can be expressed as $-Jkm_k\sum_{k'} k'P(k')m_{k'}/\langle k\rangle$. The total energy of the network can be written as

$$\begin{aligned} E &= -\frac{1}{2}J\sum_k N_k k m_k \sum_{k'} \frac{k'P(k')m_{k'}}{\langle k\rangle} - h\sum_k N_k m_k \\ &= -\tfrac{1}{2}NJ\langle k\rangle m'^2 - Nhm, \end{aligned} \tag{2}$$

where

$$m' = \sum_k \frac{kP(k)m_k}{\langle k\rangle} \tag{3}$$

is the average magnetization of a randomly chosen nearest-neighbor node, and $m = \sum_k P(k)m_k$ is the average magnetization of a randomly chosen node. Note that m' differs from m in general. Special cases for which $m' = m$ are provided by k-independent quantities $m_k = m$. In particular, for the all-spin-down configuration with $m_k = -1$ for all k and for the all-spin-up configuration with $m_k = 1$ for all k, one has $m' = m = -1$ and $m' = m = 1$, respectively.

Defining S_k as the entropy of a node with degree k, the total entropy of the network is

$$S = \sum_k N_k S_k = N\sum_k P(k)S_k, \tag{4}$$

with

$$S_k = -k_{\mathrm{B}}\left[\frac{1+m_k}{2}\ln\left(\frac{1+m_k}{2}\right) + \frac{1-m_k}{2}\ln\left(\frac{1-m_k}{2}\right)\right]. \tag{5}$$

Combining equations (2) and (4), we can get the expression of free energy, i.e., $F = E - TS$.

At the minimum and maximum points of free energy, we have $\partial F/\partial m_k = 0$, which yields the mean-field equation of m_k [5, 9],

$$m_k = \tanh\left[\beta h + \beta Jkm'\right]. \tag{6}$$

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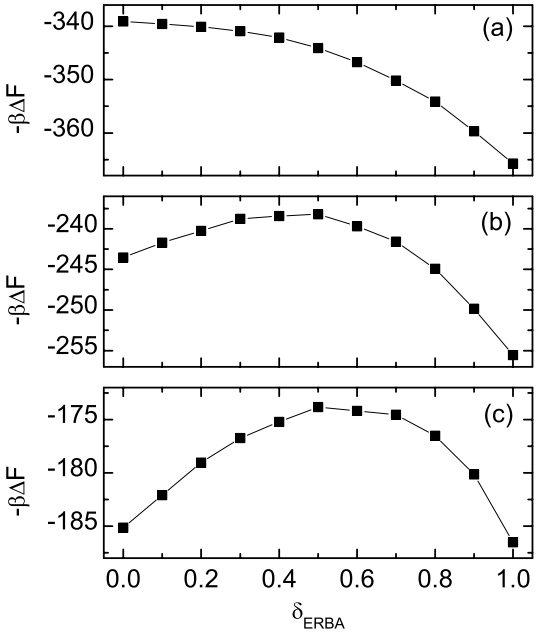

Figure 2. Theoretical results of $-\beta\Delta F$ as a function of δ_{ERBA} for $h = 0.5$ (a), $h = 0.8$ (b), and $h = 1.0$ (c). Other parameters are the same as those in figure 1.

Substituting equation (6) into (3), we get

$$m' = \sum_k \frac{kP(k)}{\langle k\rangle} \tanh\left[\beta h + \beta J k m'\right]. \tag{7}$$

Equation (7) is a self-consistent equation of m' that can be numerically solved. In the present settings, equation (7) has three solutions: m'_-, m'_0, and m'_+, where $m'_\pm$ are stable solutions and m'_0 is unstable one. Inserting the three solutions of m' into the right-hand side of equation (6), we can obtain m_k, and then get E_α, S_α and F_α ($\alpha = -, 0, +$) according to equations (2) and (4). Since $h > 0$, we have $F_0 > F_- > F_+$, which gives the free-energy barrier from metastable to stable states $\Delta F = F_0 - F_-$, and thus we estimate the nucleation rate $R \sim \exp(-\beta\Delta F)$.

Theoretical results of $-\beta\Delta F$ as a function of δ_{ERBA} are shown in figure 2, where the parameters are the same as those in figure 1. It is clear that the theoretical results are qualitatively consistent with the simulation ones.

In order to check the generality of the above results, we shall calculate nucleation rate on some other network models by both numerical simulations and theory. Firstly, we construct a network with uniform degree distribution in which node degree is randomly selected in the range $[\langle k\rangle - \delta_{\mathrm{uni}}, \langle k\rangle + \delta_{\mathrm{uni}}]$, where δ_{uni} is an integer between 0 and $\langle k\rangle - 1$ that controls the strength of degree heterogeneity. The network is generated according to the Molloy–Reed algorithm [29]. This construction eliminates the degree correlations between neighboring nodes. Figure 3 shows the simulation and theoretical results, in which the same phenomenon is also present: for weak external field the nucleation rate decreases monotonically with degree heterogeneity, while for strong external field the nucleation rate varies nonmonotonically with degree heterogeneity. Moreover, we construct a network with

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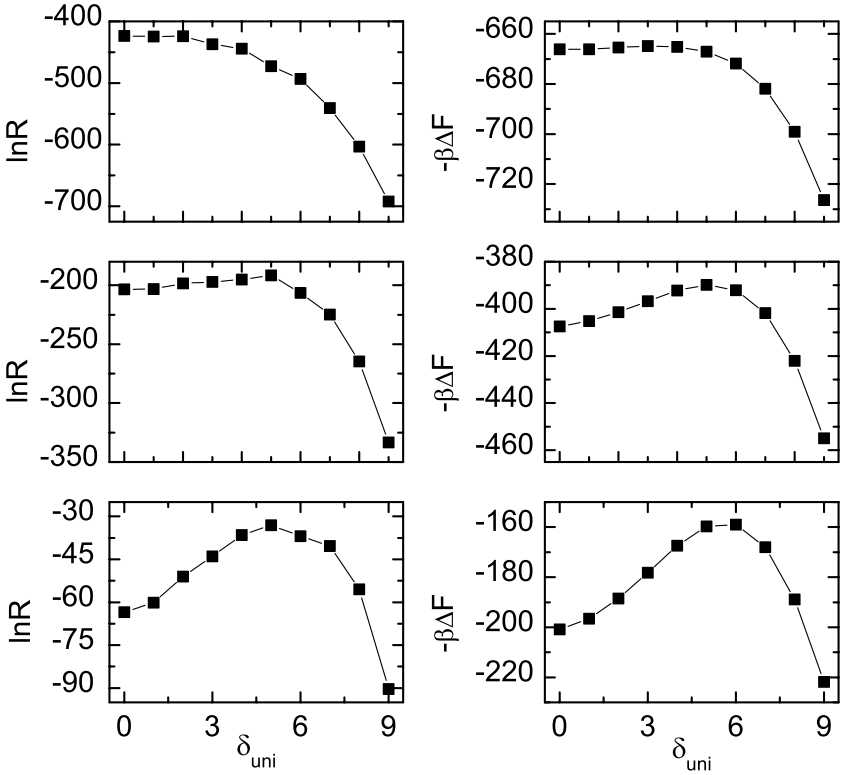

Figure 3. Simulation (left panels) and theoretical (right panels) results on networks with uniform degree distribution. The external fields from top to bottom are $h = 1.0$, 2.0, and 3.0, respectively. Other parameters are $N = 1000$, the mean degree $\langle k \rangle = 10$, and $T = 3$.

Gaussian degree distribution with fixed mean degree $\langle k \rangle$ and variance δ_{gau}. As shown in figure 4, both the simulation and theoretical results again display the same phenomenon.

4. Summary and discussions

In summary, using the Ising model on complex networks we have shown how degree heterogeneity affects the rate of nucleation. The main results of the present paper are that for a weak external field the nucleation rate decreases monotonically as degree heterogeneity increases, whereas for a relatively strong external field the nucleation rate first increases and then decreases with the increment of degree heterogeneity. Therefore, the nucleation rate can change monotonically or nonmonotonically with degree heterogeneity depending on the value of the external field. The results are robust to different network models, thereby verifying the generality of the results. Moreover, we have developed the so-called heterogeneous mean-field theory for calculating the free-energy barrier to nucleate and thus estimate the nucleation rate. The theory is effective in qualitatively predicting the simulation results. Our findings indicate that degree heterogeneity plays a nontrivial role in the nucleation events of the Ising model on complex networks.

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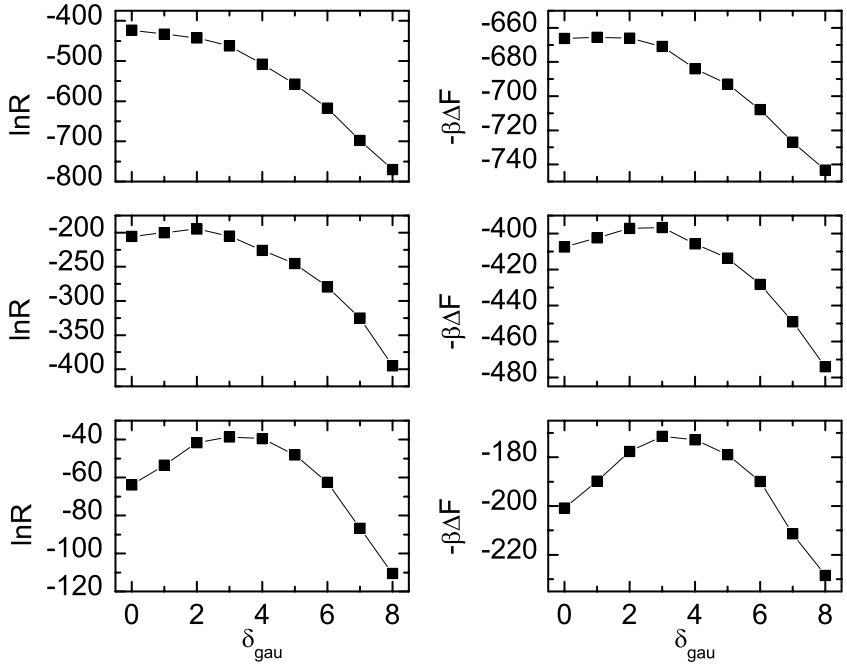

Figure 4. Simulation (left panels) and theoretical (right panels) results on networks with Gaussian degree distribution. The external fields from top to bottom are $h = 1.0$, 2.0, and 3.0, respectively. Other parameters are $N = 1000$, the mean degree $\langle k \rangle = 10$, and $T = 3$.

It is possible to find some practical implications of the present results in more realistic networked systems in which nucleation or nucleation-like phenomena are also important. This is because, on the one hand, the Ising model and its variants have been successfully used to understand social and biological problems [30]–[32]. In the social context, binary spins can represent two opposite opinions, or competitive language features, the concept of physical temperature corresponds to a measure of noise due to imperfect information or uncertainty on the part of the agent, and the external field imitates the effect of mass media, yielding a bias of the agents in favor of either state. In the biological context, the binary states may correspond to a neuron being fired or not, or a gene being on or off. Furthermore, physical temperature can be interpreted as stochastic fluctuations at the cellular level, and the external field naturally represents external stimuli. On the other hand, some practical problems in social networks can be interpreted by nucleation processes such as revolutions of opinion [22, 33], changes in a language feature [23, 24] and swings in business confidence [34]. There are also some examples in biological networks related to nucleation processes such as the functional transition between different dynamical attractors in neural networks [19] and the genetic switch between high- and low-expression states in gene regulatory networks [20, 21]. Our findings imply that when considering the role played by degree heterogeneity on such nucleation or nucleation-like processes on real networks the strength of external field should be delicately involved.

In particular, we have noticed two recent works that addressed the question of how one language is replaced by another language [23] and the question of how a new scientific idea replaces the old one [35], respectively. Therein, by simulating theoretical models on diverse

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networks the authors have shown that both the rate of language change and the mean spreading time of a new scientific idea strongly depend on the topology of the underlying networks. These social phenomena are reminiscent of our study on the nucleation process of the networked Ising model. We hope that our theoretical findings will provide useful hints for future studies by empirical data and experiments.

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