Physica A 424 (2015) 97–104

Contents lists available at ScienceDirect

Physica A

journal homepage: www.elsevier.com/locate/physa

# Nucleation of a three-state spin model on complex networks

Hanshuang Chen [a,*], Chuansheng Shen [b]

[a] School of Physics and Materials Science, Anhui University, Hefei, 230039, People's Republic of China
[b] Department of Physics, Anqing Normal University, Anqing, 246011, People's Republic of China

## HIGHLIGHTS

- Nucleation of a three-state spin model on complex networks is studied.
- Heterogeneous mean-field theory is developed for evaluating free-energy barrier.
- Four regions are distinguished as distinct nucleation scenarios.
- A maximal nucleation rate is found at the two-step nucleation region.

## ARTICLE INFO

*Article history:*
Received 24 September 2014
Received in revised form 9 November 2014
Available online 10 January 2015

*Keywords:*
Nucleation
Complex networks
Metastable
Blume–Capel model
Heterogeneous mean-field theory

## ABSTRACT

We study the metastability and nucleation of the Blume–Capel model on complex networks, in which each node can take one of three possible spin variables $\{-1, 0, 1\}$. We consider the external magnetic field $h$ to be positive, and let the chemical potential $\lambda$ vary between $-h$ and $h$ in a low temperature, such that the 1 configuration is stable, and $-1$ configuration and/or 0 configuration are metastable. Combining the heterogeneous mean-field theory with simulations, we show that there exist four regions with distinct nucleation scenarios depending on the values of $h$ and $\lambda$: the system undergoes a two-step nucleation process from $-1$ configuration to 0 configuration and then to 1 configuration (region I); nucleation becomes a one-step process without an intermediate metastable configuration directly from $-1$ configuration to 1 configuration (region II(1)) or directly from 0 configuration to 1 configuration (region II(2)) depending on the sign of $\lambda$; the metastability of the system vanishes and nucleation is thus irrelevant (region III). Furthermore, we show that in the region I nucleation rates for each step intersect that results in the occurrence of a maximum in the total nucleation rate.



## 1. Introduction

Complex networks describe not only the pattern discovered ubiquitously in the real world, but also provide a unified theoretical framework to understand the inherent complexity in nature [1,2]. A central topic in this field is to unveil the relationship between the topology of a network and dynamics taking place on it [3–6]. In particular, phase transitions on complex networks have been a subject of intense research in the field of statistical physics and many other disciplines [7]. Extensive research interests have focused on the onset of phase transitions in diverse network topologies. 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 [8], the whole infection of disease with any small spreading rate [9], the Ising model to be ordered at all temperatures [10–12], the

* Corresponding author.
*E-mail address:* chenhshf@ahu.edu.cn (H. Chen).

http://dx.doi.org/10.1016/j.physa.2015.01.015
0378-4371/

disorder–order transition in voter models [13], synchronization to be suppressed [14,15] and different paths toward synchronization in oscillator network [16], spontaneous differentiation of nonequilibrium pattern [17], to list just a few. However, there is much less attention paid to the dynamics of a phase transition itself on complex networks, such as nucleation 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 [18]. Many important phenomena in nature, like crystallization [19], glass formation [20], and protein folding [21], 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 for controlling fluctuation-driven system-wide transitions in real situations, such as the transitions between different dynamical attractors in neural networks [22], the genetic switch between high- and low-expression states in gene regulatory networks [23,24], a new opinion [25] or scientific paradigm formation [26] as well as language replacement [27,28] in social networks, and spontaneous traffic jamming [29], synchronization [30,31], cascading failure [32] and recovery [33] close to an explosive phase transition.

Recently, we have made a tentative step in the study of the nucleation process of the two-state Ising model on complex networks, where we have identified nucleation pathways, such as nucleating from nodes with smaller degree on heterogeneous networks [34] and a multi-step nucleation process on modular networks [35]. In addition, a size-effect of the nucleation rate on mean-field-type networks [34] and a nonmonotonic dependences of the nucleation rate on the modularity of networks [35] and on the degree heterogeneity [36] were reported. However, many real systems possess complicated free-energy landscape with several local minima where phase transition happens usually via these intermediate metastable states [37]. The presence of intermediate metastable states has been shown to play a key role in determining the pathway and rate of nucleation. For example, it was recently reported that an intermediate metastable phase can provide an easier pathway for the growth of crystal nuclei from fluids, with implications for the crystallization of protein and colloid [38–42]. Thus, it is natural to generalize the nucleation of the two-state Ising model to a three-state spin model on complex networks in which an intermediate metastable state may exist.

In this paper, we shall use the three-state Blume–Capel (BC) model to investigate the nucleation on complex networks. The BC model is a spin-1 Ising model that has been introduced, by Blume [43] and Capel [44] independently, as a model for magnetic systems and then applied to multicomponent fluids [45]. The BC model defined on a two-dimensional lattice has been previously used to study the metastability and nucleation in the limit of zero temperature [46] and in the absence of external magnetic field [47]. Recently, a reentrance phase transition has been observed in the BC model defined on heterogeneous networks [48]. Here, we show, by using mean-field analysis and simulation, that there are four distinct regions corresponding to different nucleation scenarios for the networked BC model. Depending on the model's parameters, the system undergoes either a two-step nucleation process with an intermediate metastable state or a one-step nucleation process. We also calculate the rates of nucleation by a rare-event sampling method that agree with the theoretical predictions by evaluating the free-energy barrier to nucleate.

## 2. Model

We consider the BC model defined on a network, where spin variable of each node can take three possible values $\sigma_i \in \{-1, 0, 1\}$, and interacting according to the Hamiltonian

$$\mathcal{H} = J \sum_{i<j} a_{ij} \left(\sigma_i - \sigma_j\right)^2 - \lambda \sum_i \sigma_i^2 - h \sum_i \sigma_i, \tag{1}$$

where $J$ is the ferromagnetic interaction constant among nodes, $\lambda$ and $h$ have the meaning of the chemical potential and the external magnetic field imposed on each node, respectively. 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 present paper is devoted to the study of metastability and nucleation of the networked three-state BC model at the low temperature. For the purpose, we first consider the stability of the system in the zero temperature limit. In this case, the (local) stable equilibrium refer to the configurations with all the spins equal to $-1$, 0, 1, respectively. For the sake of convenience, we use $\underline{-1}$, $\underline{0}$, $\underline{1}$ to denote these stable ordered configurations, respectively. Their energy are as follows: $h - \lambda$, 0, and $-h - \lambda$. Since we want to study the nucleation from $\underline{-1}$ to $\underline{0}$, and then to $\underline{1}$, we set $\underline{-1} < \underline{0} < \underline{1}$ as the relative stabilities of these configurations. To the end, it is required that $h - \lambda > 0 > -h - \lambda$, or equivalently, $-h < \lambda < h$ and $h > 0$. Due to the small thermal fluctuation at the low temperature, it is expected that the behavior at the low temperature is similar to that at the zero temperature. However, in the presence of small thermal fluctuation the notations $\underline{-1}$, $\underline{0}$, $\underline{1}$ refer to the configurations with most instead of all the spins equal to $-1$, 0, 1, respectively. Here, the temperature is fixed at $T = 5$ (in unit of $J/k_B$) throughout the paper where $k_B$ is the Boltzmann constant.

## 3. Theory and simulation

To proceed the heterogeneous mean-field theory, we first define $X_k^{(\alpha)}$ as the probability that a node of degree $k$ is in the state $\alpha \in \{-1, 0, 1\}$. The interaction energy of an edge connecting a $k$-degree node and a $k'$-degree node is thus