Study of Nucleation Processes in Two-dimensional Ising Model via Network Analysis

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Background

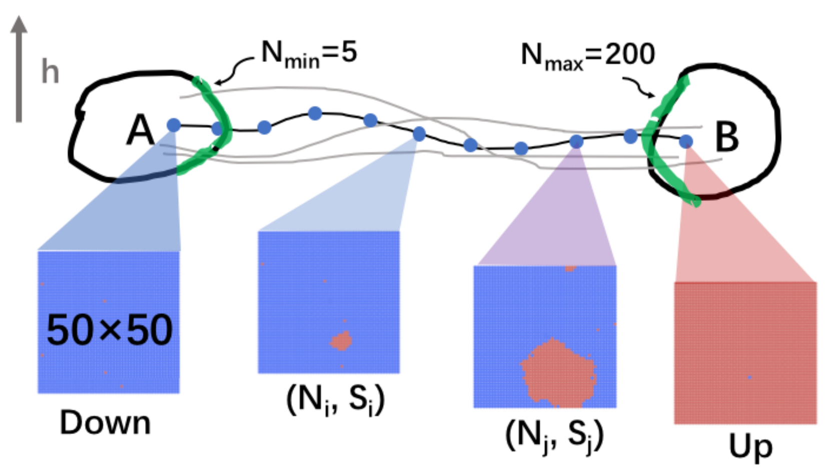


Fig. 1 The schematic diagram of the nucleation of 2D Ising model. N=50×50. Initially, all the spins are down With the presence of weak magnetic field, nucleation may take place with rare chance. Maximum cluster size N in the lattice is used as the criteria. N<5 (region A) is when nucleation not taking place and N>200 (region B) is when nucleation having taken place. Along the transition routes, there are different configurations. Another reaction coordinate (order parameter) perimeter S is introduced in order to characterize the shape of the cluster.

Hamiltonian of Ising model

$$H = -J\sum_{\langle i,j\rangle} s_i s_j - h\sum_i s_i$$

Magnetic fields

Mechanism of Nucleation[1]:

The competition between

1. An unfavorable contribution from the formation of a surface – Prefer smaller perimeter S.
2. A favorable contribution from nucleating the stable phase – Achieve all the spins up with the existence of magnetic fields.

Research Objectives

Study the effects of varying magnetic field on the topology of the nucleation pathways.

1. If the process is equilibrium or non-equilibrium.
2. If any favored paths exist
3. Interpret nucleation rates with pathway topology.

Methods

1. Transition path sampling[2] (TPS) - a method used to study and sample rare events (trajectories) in computer simulations. TPS codes were written by Aaron Keys[3] and data were collected with some modifications on codes in order to sample (N,S).

2. First-order network

- Construction: 1000 trajectories with length ~20 configurations extracted are used. Every (N,S) is binned properly to get networks with fewest self-loop. All the constructions and calculations were done with python codes and Networkx package[4].
- The probability distribution of edge weights
- The probability distribution of in and out degree of nodes
- Pagerank[5]: Measure a node's influence extending beyond their direct connections to the wider network. Basically, it represents the static probability distribution of the nodes by viewing the system as a Markov state model, i.e. $\pi=\pi P$.
- Load centrality[6]: Similar to betweenness centrality, measure the number of times a node lies on the shortest path between other nodes, to find the nodes (typical configurations) which influence the flow or serve as the bridges.

3. High-order network[7] – a method to display the memory issues hidden in the trajectories.

- Construction: Generated with Higher-order Network[7] (HON) automatically.
- Pagerank analysis: Rebuild the pagerank for each nodes in first order network, also done by Higher-order Network (HON).

1. Bolhuis, P. G.; Dellago, C.; Chandler, D. Proc. Natl. Acad. Sci. U.S.A. 2000, 97, 5877.
2. Pan, A.; Chandler, D. J. Phys. Chem. B 2004, 108, 19681-19686
3. https://sites.google.com/site/aaronskeys/resources/tutorials/transition-path-sampling
4. A Hagberg, D Schult, P Swart, Proceedings of the 7th Python in Science conference (SciPy 2008), G Varoquaux, T Vaught, J Millman (Eds.), pp. 11-15
5. Langville, Amy N., and Carl D. Meyer. SIAM review 47.1 (2005): 135-161.
6. Ulrik Brandes, Social Networks 30 (2008) 136–145.
7. Jian Xu, Thanuka L. Wickramarathne, and Nitesh V. Chawla. Science Advances 2, no. 5 (2016): e1600028.

Results and Discussions

1. Linear regression

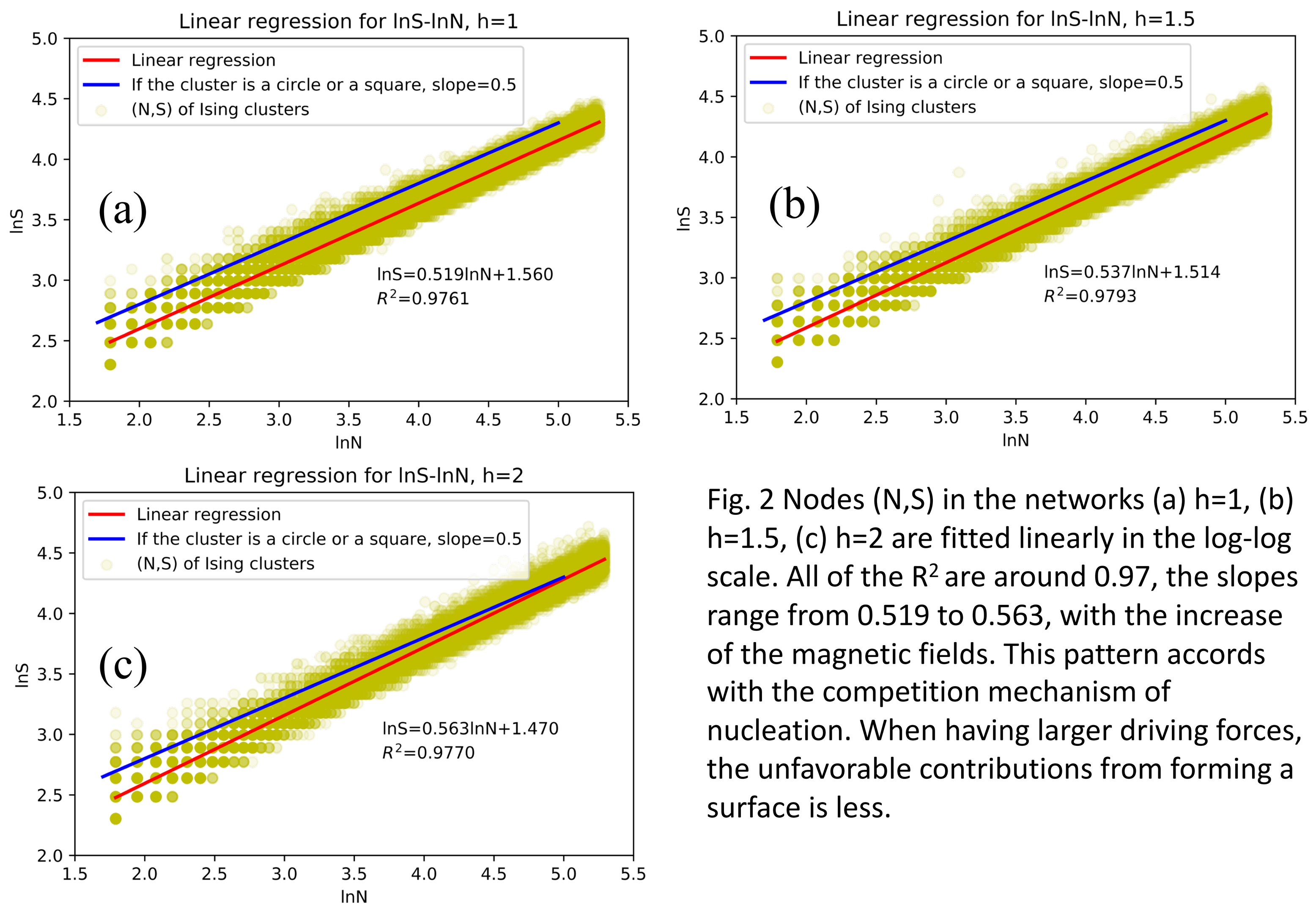
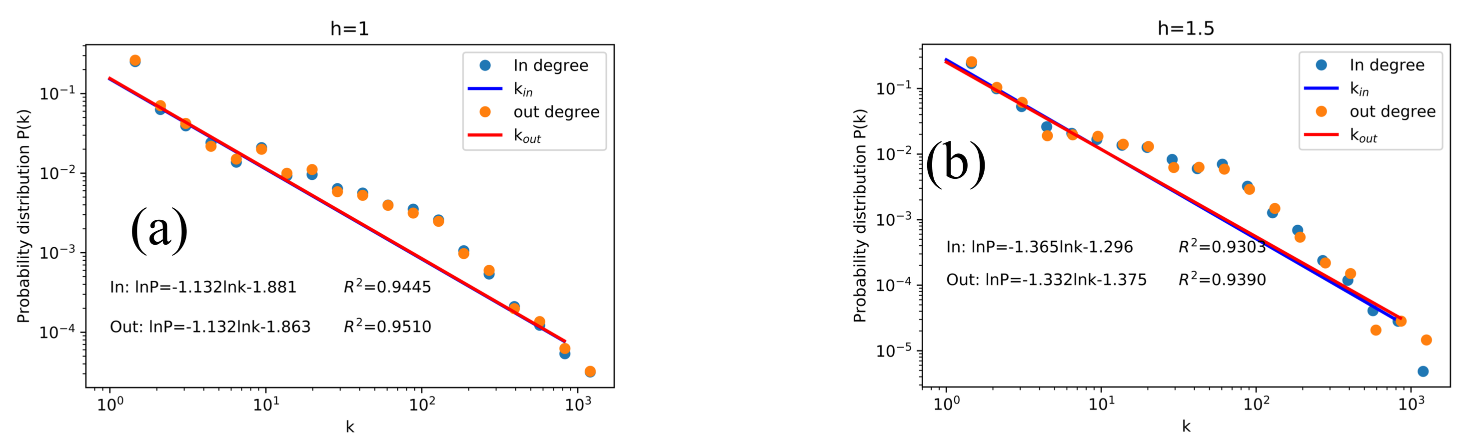


Fig. 2 Nodes (N,S) in the networks (a) h=1, (b) h=1.5, (c) h=2 are fitted linearly in the log-log scale. All of the R^2 are around 0.97, the slopes range from 0.519 to 0.563, with the increase of the magnetic fields. This pattern accords with the competition mechanism of nucleation. When having larger driving forces, the unfavorable contributions from forming a surface is less.

2. First-order network

- Degree distribution



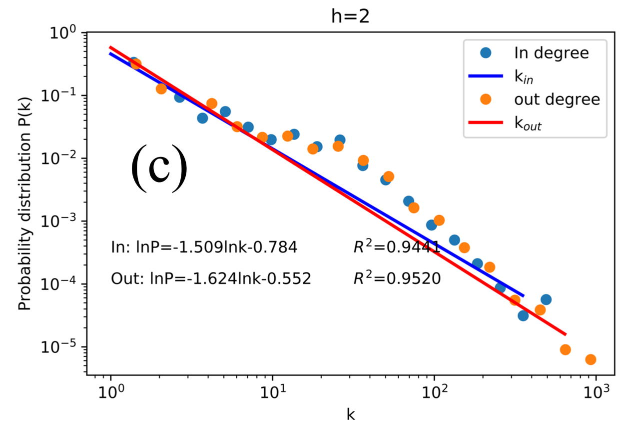


Fig. 3 In and out degree distribution of networks (a) h=1, (b) h=1.5, (c) h=2. They show similar distribution patterns. If viewing them as scale-free networks, γ is between 1.5-2, which is the anomalous regime, meaning the number of hubs has "surpassed" total number of nodes. $k_{in}\approx k_{out}$ in network (a) illustrates an equilibrium process taking place. The nonequilibrium processes displayed in h=1.5 and h=2 are mainly induced by few nodes with big degrees. The identification of the hubs will be discussed in 4. Pagerank and load centrality.

- Edge weights distribution

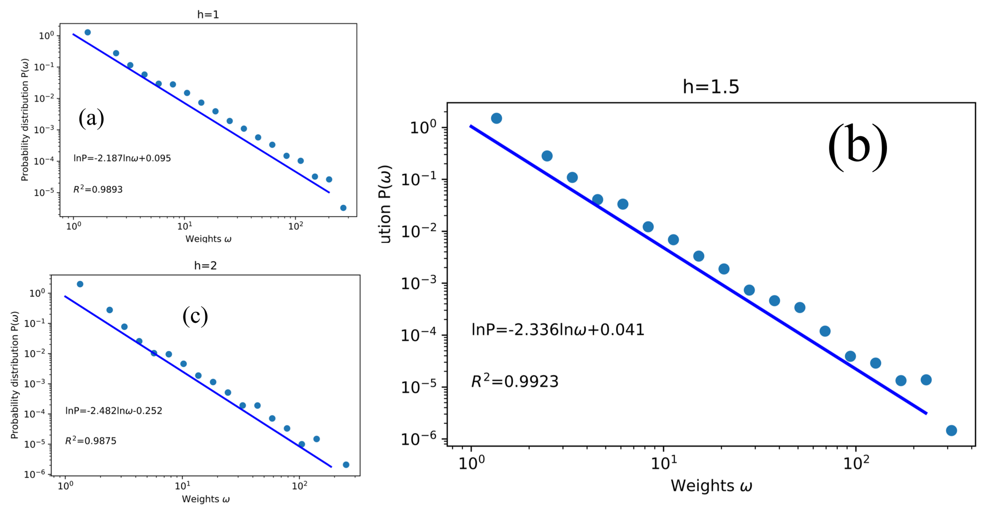


Fig. 4 Edge weights distribution of networks (a) h=1, (b) h=1.5, (c) h=2. Scale-free property is shown in the edge weights distribution.

Table 1 The summary of network

h	1	1.5	2
Number of nodes	506	555	650
Number of edges	8861	8375	7580
Slope	-1.227	-1.261	-1.434
R^2	0.9397	0.9829	0.9563
Shannon entropy of edge weights	8.10	8.06	8.20
Entropy of pagerank (high order)	*4.50*	*4.17*	*3.66*
Entropy of load centrality	*5.08*	*5.30*	*5.77*

3. High-order network-memory issue

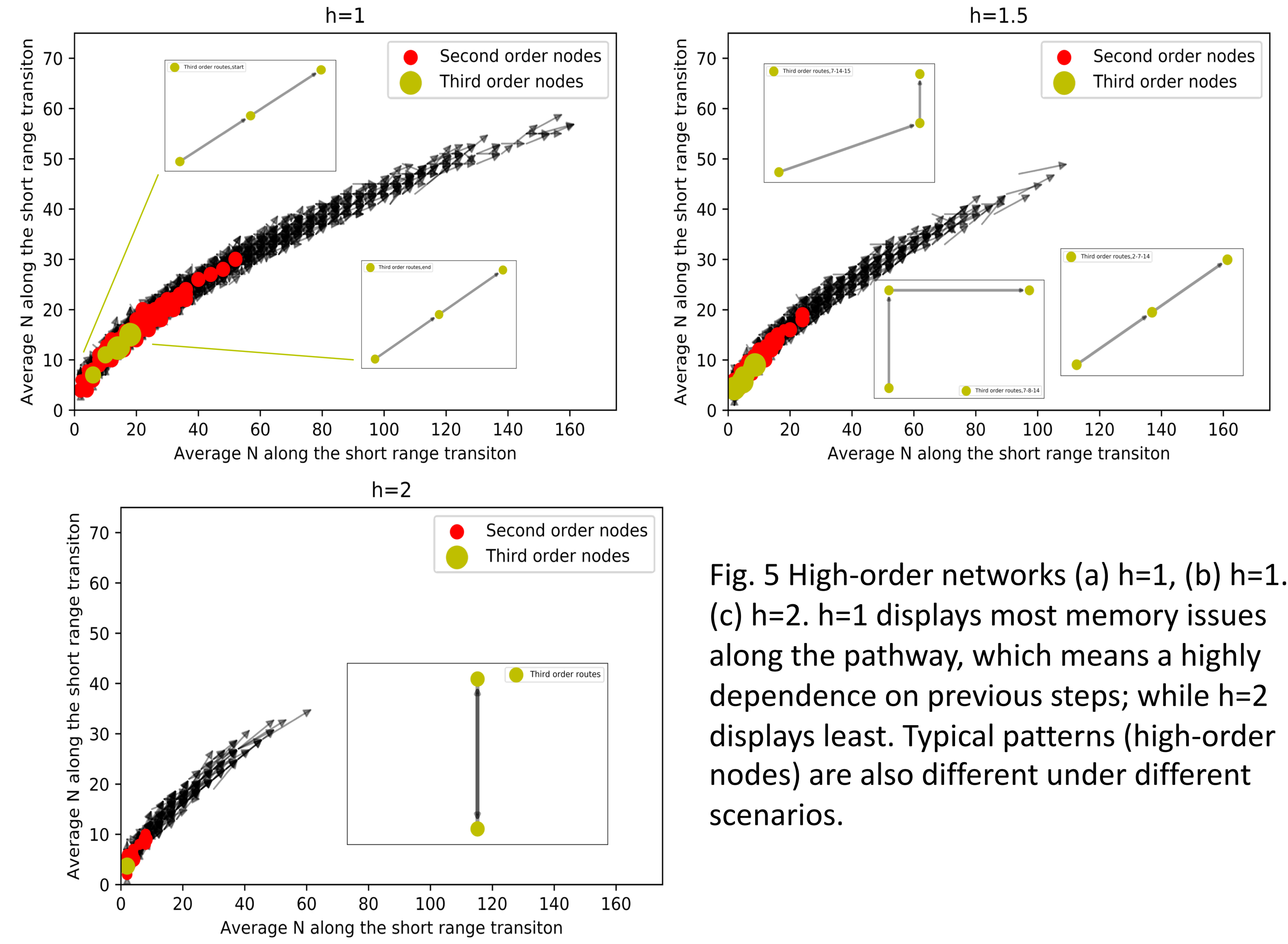


Fig. 5 High-order networks (a) h=1, (b) h=1.5, (c) h=2. h=1 displays most memory issues along the pathway, which means a highly dependence on previous steps; while h=2 displays least. Typical patterns (high-order nodes) are also different under different scenarios.

4. Pagerank and load centrality

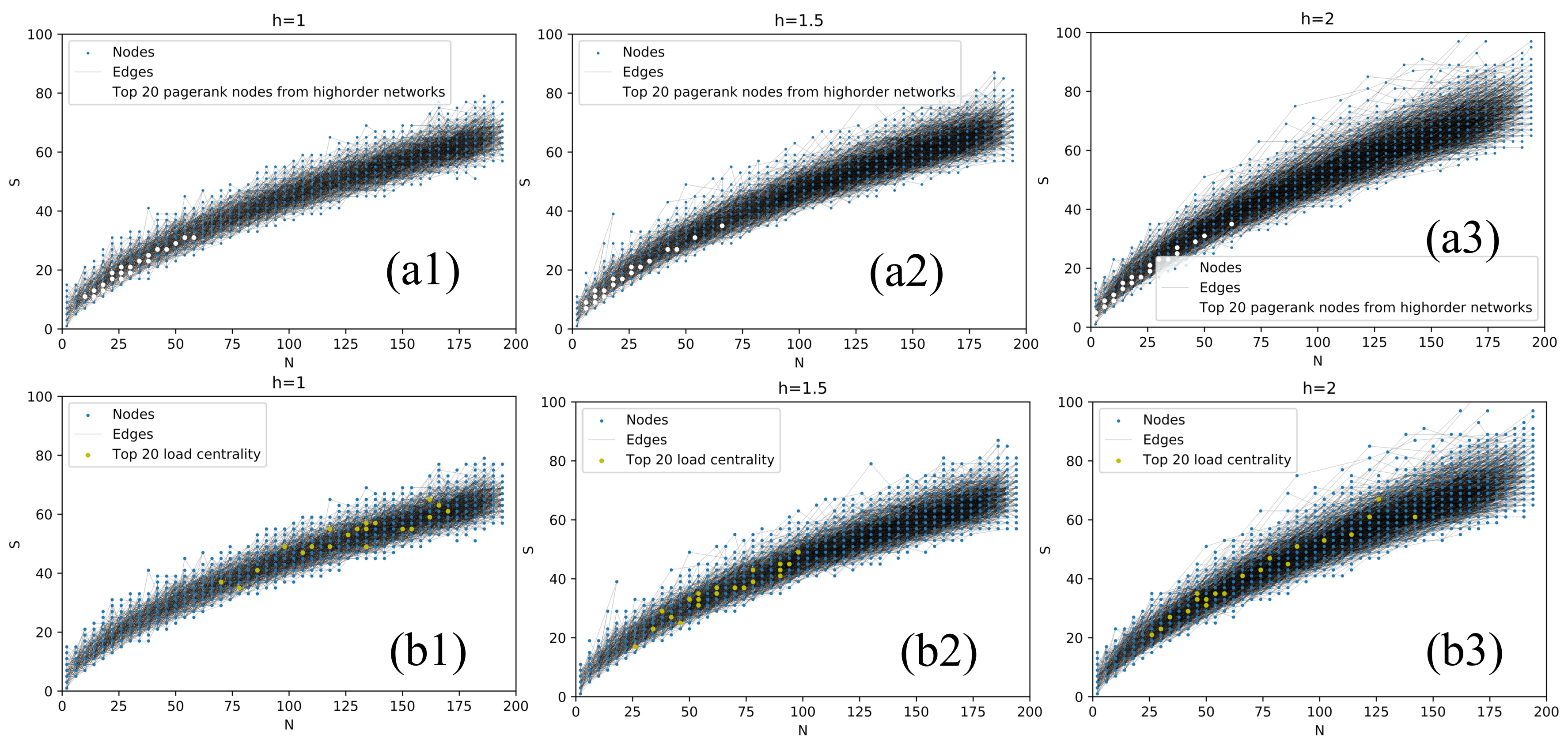


Fig. 6 Pagerank and load centrality of networks (a) h=1, (b) h=1.5, (c) h=2. Top 20 pagerank (from high-order network) and load centrality nodes are highlighted in the plots. For pagerank, different magnetic fields provide similar occupations of sites, which highlights a typical pathway. However, the entropy of pagerank shows a decrease trend, which means with higher magnetic field, nucleation tends to follow the typical path more. For load centrality, it tells where the "bridges" are and thus which nodes have the most degrees, showing different occupations and entropy trend with the pagerank. This entropy indicates the freedom of choosing the next site. Overall, the two entropies don't contradict to each other. It tells us once the magnetic field is big enough, the nucleation process has more freedom to choose the next configuration, but it will favor the typical path at the beginning of the nucleation.

Conclusions

1. A favorable stable phase wins against the unfavorable surface energy in strong magnetic field.
2. Nucleation tends to be a nonequilibrium process with the increase of the magnetic field (external driving force). The underlying reason is the small fraction nodes with big k that has: $k_{out}>k_{in}$.
3. The whole process can be broken down into two parts: the initial clustering and the development. The initial clustering is the key factor of nucleation, for the weak field regime, it highly depends on the old memories. Once the memory starts to disappear, the flexibility of the nodes to chose next step will increase.