NUCLEATION DURING PHASE TRANSITIONS IN RANDOM NETWORKS

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ABSTRACT. We analyze the 3-parameter family of random networks that are uniform on networks with fixed number of edges, triangles, and nodes (between 33 and 66). We find precursors of phase transitions which are known to be present in the asymptotic node regime as the edge and triangle numbers are varied, and focus on one of the discontinuous ones. By use of a natural edge flip dynamics we determine nucleation barriers as a random network crosses the transition, in analogy to the process a material undergoes when frozen or melted, and characterize some of the stochastic properties of the network nucleation.

1. Introduction

When a fluid is frozen to a crystal a disordered array of molecules has to rearrange into an ordered array. In practice molecules have difficulty doing this; careful experiments can easily cool a liquid into a disordered supercooled liquid, well below the freezing temperature, before transforming it into a crystalline solid [1]. The manner in which the difficulty is eventually overcome is traditionally modelled by Classical Nucleation Theory, CNT, some of whose predictions are off by many orders of magnitude [1].

There is no satisfactory solvable toy model that exhibits a fluid/solid phase transition - this is a famous unsolved problem [2, 3] - so we will use a mathematical model of random networks, which has adjustable parameters and exhibits phase transitions with the parameters treated as analogues of thermodynamic parameters. The model is unphysical but may still be useful to determine precisely how a dynamically driven phase transition between incompatible structures is actually obtained.

Our model is a mean-field model, namely the random ‘edge/triangle’ network model popularized by Strauss in 1986 [4]. We first give some background to explain the meaning of the transitions found in these models. We then sketch our results on dynamically driving such a system between phases, exhibiting a form of nucleation as incompatible structures are bridged.

We begin with some notation. Given n abstract labelled nodes, we denote by \( E(G) \) and \( T(G) \) the number of edges and triangles in the simple network \( G \). (Simple means that two nodes can have at most one edge connecting them and there are no loops connecting a node with itself.) Strauss put on the set of all such networks the 2-parameter family of unnormalized probability mass functions:

\[
\exp[s_1 e(G) + s_2 t(G)],
\]
where

\begin{equation}
(2) \quad e(G) = \frac{E(G)}{\binom{n}{2}} \quad \text{and} \quad t(G) = \frac{T(G)}{\binom{n}{3}}
\end{equation}

are the edge and triangle densities in $G$, with value 1 in the complete network. The model parameters $s_1, s_2$ are analogues of $\beta \mu$ and $\beta$ in a grand canonical distribution of statistical mechanics, where $\beta$ is inverse temperature and $\mu$ is chemical potential.

A network $G$ is described by its adjacency matrix $M(G)$. This is a symmetric $n \times n$ matrix whose $(i,j)$ entry is 1 if nodes $i$ and $j$ are connected by an edge, and zero otherwise. The statistical properties of the matrix are independent of the (arbitrary) ordering of the nodes. Permutation-invariant data such as the eigenvalues of $M(G)$ are particularly informative.

As in statistical mechanics, phases in parametric models of random networks require an infinite-system-size limit formalism. Instead of looking at a symmetric 0–1 matrix $M(G)$, one considers a symmetric function $g$ on the unit square $[0,1]^2$ taking values in the interval $[0,1]$. (The points in $[0,1]$ are thought of as representing infinitely many nodes.) Such a graphon $g$ is the kernel of an integral operator $M(g)$ acting on $L^2([0,1])$. In an important series of papers [5, 6, 7, 8, 9], Borgs et al used a certain metric on the space of networks to construct a completion, called the space of (reduced) graphons, with many useful properties. Used together with an important large deviation result [10] of Chatterjee/Varadhan, one may study convergence of distributions to infinite size through optimal-free-energy graphons $g_{s_1,s_2}$. See for instance [11].

These network models are mean-field in the sense that there is no space cutoff limiting the direct influence of variables on one another. For traditional statistical mechanics models with short range forces there is an equivalence of ensembles, connected by Legendre transforms. However, as is common in mean-field models, Legendre transforms are not invertible for these graphon models and lose information contained in the microcanonical ensemble. This is not necessarily a problem when studying a network with a small number of nodes, as is common in social science modelling [12]. However, when studying asymptotically large networks to study phase transitions the loss would be a problem so we must use the microcanonical version of the model [13, 14]. That is, we must specify the parameters $e(G)$ and $t(G)$ and consider the uniform distribution on networks with the fixed values of $e$ and $t$. We then study convergence to infinite size through optimal-entropy graphons, $g_{e,t}$.

For fixed values of $(e,t)$, the graphon formalism allows one to take a limit in the number of nodes, $n \to \infty$, with ‘most’ constrained networks $G$ converging to an entropy-optimal graphon $g_{e,t}$, in the sense that their (suitably normalized) adjacency matrices $M(G)$, viewed as operators on $\mathbb{R}^n$, converge in a weak sense to the compact linear integral operator $M(g_{e,t})$ on $L^2([0,1]^2)$, with the (suitably normalized) ordered sets of eigenvalues of the $M(G)$’s converging to those of $M(g_{e,t})$; see section 11.6 in [15]. In [13, 14, 16, 17, 18, 19, 20, 21, 22] this and similar models have been studied in depth; we describe some results next.

The optimal-entropy graphons have been shown to have a very simple form. If we break the interval $[0,1]$ into finitely many sub-intervals, called “podes”, and thereby break the square $[0,1]^2$ into finitely many rectangular blocks, then the optimal graphon is constant on each block. As noted above, the interval $[0,1]$ is thought of as representing infinitely many nodes, so we are envisioning a decomposition of the set of nodes into a finite number of collections, called podes, of ‘equivalent’ nodes, equivalent in the sense that two equivalent nodes have
the same probability of connection with any other node. It only takes a few parameters to describe such a “multipodal” graphon, namely the sizes of the sub-intervals and the value of \( g \) on each block; this vast reduction in degrees of freedom is chiefly responsible for the proliferation of results in these models.

By a phase in our network model we mean an open connected region in the space of pairs \( \{(e, t)\} \); at each point of which there is a unique optimal-entropy graphon \( g_{(e,t)} \), whose parameters are smooth functions of \( (e,t) \). At a phase boundary there may be two or more optimal-entropy graphons, typically with qualitatively different structures, in which case we say the phase transition is discontinuous. Alternatively there may be a single optimal-entropy graphon, in which case we say the phase transition is continuous. These are in some sense analogous to first-order and second-order phase transitions in statistical mechanics, but the analogy can only be taken so far, especially since this is a mean-field model. (In particular, the expansion of the entropy as a power series in \( e \) and \( t \) sometimes involves fractional powers.)

In Figure 1 we sketch the phase diagram of the microcanonical edge/triangle model [13]. This model exhibits three infinite families of phases labelled \( A(m,0) \), \( B(m,1) \) and \( C(m,2) \) as well as a singleton \( F(1,1) \). An \( A(m,0) \) graphon (that is, the optimizing graphon in the \( A(m,0) \) phase) has \( m \) podes and is invariant under permutation of these indistinguishable podes; see Figure 2. A \( B(m,1) \) graphon has \( m \) indistinguishable podes and one pode that is different. A \( C(m,2) \) graphon has \( m \) indistinguishable podes and two additional podes that are different from the \( m \) podes but are indistinguishable from each other. The differences between these phases are reflected in the different eigenvectors of the adjacency matrices of generic networks in each phase.

We will be concentrating on the transition between the \( B(1,1) \) and \( A(3,0) \) phases as we go through the point \( (e,t) = (0.67, 0.2596) \) along constant edge density 0.67. This transition is particularly interesting because it has been proven to be discontinuous; the optimizing graphons for \( t \) slightly above 0.2596 are very different from the optimizing graphons for \( t \) slightly below 0.2596. (See Figure 2.)

In switching from an arrangement described by one graphon to an arrangement described by the other, nodes need to rearrange their connections in a process analogous to nucleation in a liquid/crystal transition. Patterns are broken, patterns are formed, and once sufficiently many nodes follow the new pattern, the rest follow suit.

Our study of this transition involved two major challenges. First, we needed to work with finite networks, yet the very notion of phases requires taking infinite-size limits. Although the graphon formalism ensures that systems of large enough size are modelled well by graphons, there is no mechanism in the formalism to determine how large is ‘large enough’. Fortunately, we were able to see unambiguous evidence of the emergence of the \( B(1,1)/A(3,0) \) transition in systems with as few as 30 nodes, well below the 100-or-so nodes that our computers can comfortably handle; we describe this in Section 2. The fact that such transitions can be seen in systems of such low size is significant both for the computer analysis of network transitions and for the modelling of scientific data of such size, and is the first major result of this paper.
Second, we needed to introduce a random dynamics to play the role of cooling or heating a material from an equilibrium state at one set of thermodynamic parameters to an equilibrium state at another set. Our dynamics respects the constraint on the edge density while introducing enough randomness to drive the triangle density across a transition.

![Figure 1. Schematic sketch of 14 of the phases in the edge/triangle model. Continuous phase transitions are shown in red, and discontinuous phase transitions in black. The boundary of the phase space is in blue. The transition point studied in this paper is indicated by a black dot.](https://www.youtube.com/playlist?list=PLZcI2rZdDGQqx3WEY6BXoJXcxqQXF5ZzQ)

The solutions we found are described in Section 3, both for going from $B(1,1)$ to $A(3,0)$ and for going from $A(3,0)$ to $B(1,1)$. Along the way we produced videos, available at [https://www.youtube.com/playlist?list=PLZcI2rZdDGQqx3WEY6BXoJXcxqQXF5ZzQ](https://www.youtube.com/playlist?list=PLZcI2rZdDGQqx3WEY6BXoJXcxqQXF5ZzQ) that literally show nodes rearranging into the pod structure appropriate to prescribed constraints. (The rearrangement is not in physical space, which plays no role in this mean-field...
model. Rather, the podal structure and its changes are seen in the eigenvectors of the adjacency matrix, as noted above.)

Figure 2. Transition between phases $B(1, 1)$ and $A(3, 0)$ at edge density 0.670. Triangle densities of the two graphons: 0.25979, 0.25907. Triangle density at transition: 0.25963868.
Understanding this process is the **second major result** of this paper. In each direction, the evolution from one phase structure to the other occurs in three distinct stages. The first stage is very quick and brings the density $t$ of triangles to its desired value. The second stage is a factor of 10–100 slower and results in a structure that can be viewed as “new phase plus defects”, e.g. with podes that are slightly too big or too small. The third phase is a factor of 1000–10,000 slower than the first and achieves true equilibrium.

Finally, the time required for crystal nucleation in physical systems is random, as are other features of the process. We have begun an statistical analysis of the time required for each of the three stages of network nucleation (both for $A(3,0) \to B(1,1)$ and for $B(1,1) \to A(3,0)$), with details in Section 3.

### 2. Equilibrium in finite systems

Our goal is to understand how a network changes from the structure of one phase to that of another, under an appropriate dynamics. Before we can do this, we must understand the structure of the two phases. We begin with the entropy-maximizing graphons that describe infinite (or sufficiently large) random networks, and then consider finite-size effects. For more about these graphons and the precise transition between them, see [13].

In the $A(3,0)$ phase, an optimizing graphon $g_{e,t}$ is shown in the bottom of Figure 2. If we denote the value of the graphon along the diagonal by $a$ and the off-diagonal value by $b$, then this describes an infinite network with the following properties.

1. The nodes group into three classes or “podes” of equal size, which we might imagine as red, blue, and green nodes.
2. The edges within each pode, e.g. connecting two red nodes, appear with probability $a$.
3. The edges between different podes appear with probability $b > a$.
4. The corresponding integral operator $M(g_{e,t})$ has rank three. Its nonzero eigenvalues are $(a + 2b)/3$ with multiplicity 1 and $(a - b)/3$ with multiplicity 2.
5. The positive eigenvalue $(a + 2b)/3$ is the overall edge density, and the corresponding eigenfunction is constant.
6. The triangle density is

$$t = \frac{1}{9}a^3 + \frac{2}{3}ab^2 + \frac{2}{9}b^3 = e^3 + 2\left(\frac{a - b}{3}\right)^2,$$

which is the trace of the cube of the integral operator. Given $e$ and $t$, it is easy to compute $a$ and $b$, the eigenvalues and eigenfunctions of $M(g_{e,t})$, and the densities of all subnetworks.

7. The eigenspace corresponding to the negative eigenvalue $(a - b)/3$ consists of functions that are constant on each pode and integrate to zero. If we pick an orthonormal basis $\{\xi_1(x), \xi_2(x)\}$ for this eigenspace and pick a random point $x \in [0,1]$, the ordered pair $(\xi_1(x), \xi_2(x))$ can lie at three possible points in $\mathbb{R}^2$, and these points form the vertices of an equilateral triangle centered at the origin. A change of basis only serves to rotate the triangle.
If we pick a network \( G \) with \( n \) nodes whose adjacency matrix \( M(G) \) is close to this graphon (which necessarily requires \( n \) large), then \( M(G) \) will have two large negative eigenvalues of approximate size \( n(a-b)/3 \) and one large positive eigenvalue of approximate size \( n(a+2b)/3 \). The eigenfunctions for the negative eigenvalues will be approximately constant on each pode, so that if we plot the values \( \{(\xi_1(v_i),\xi_2(v_i))\} \) for the \( n \) nodes \( \{v_i\} \), we will get (with high probability) three clusters of roughly equal size, centered at the vertices of an equilateral triangle. Moreover, the second largest negative eigenvalue \( \lambda_2 \) will be nearly as large as the largest negative eigenvalue \( \lambda_1 \), while all other negative eigenvalues will be of order \( \sqrt{n} \).

We now turn to the \( B(1,1) \) phase, with an optimal graphon shown at the top of Figure 2. The corresponding integral operator has rank two, and in particular only has one negative eigenvalue, whose eigenfunction is constant on each pode. If we pick a large random network that is close to this structure, then the most negative eigenvalue \( \lambda_1 \) of the adjacency matrix will be \( O(n) \), and the values of \( \xi_1(v) \) will distinguish the two podes, but the second most negative eigenvalue \( \lambda_2 \) will only be \( O(\sqrt{n}) \). \( \xi_2 \) will be essentially zero on the smaller pode and random on the larger pode. A scatter plot of \( \{(\xi_1(v_i),\xi_2(v_i))\} \) will then give a tight cluster of points corresponding to the small pode and a vertical bar corresponding to the large pode.

The upshot is that both the size of \( \lambda_2 \) and the distribution of \( (\xi_1(v),\xi_2(v)) \) are strong indicators of the phase we are in. Another indicator is the size of the podes themselves, as indicated by the size of the clusters in the \( (\xi_1,\xi_2) \) plot. In the \( A(3,0) \) phase, there are three podes of equal size. In \( B(1,1) \), there are two podes with a roughly 60-40 split between the larger and the smaller pode.

The left side of Figure 3 shows the distribution of \( (\xi_1(v),\xi_2(v)) \) for a typical graph with \( n = 54, e = 0.67 \) and \( t = 0.24 \). Grouping nodes, we then generate a tripodal graphon by simply counting the number of edges that blue-blue, blue-green, etc. Figure 4 is similar, only for a sample graph at \( t = 0.26 \), which is in the \( B(1,1) \) phase. In the plot of Figure 4, we attempt to segregate the nodes into three podes, as before, but there is no clear dividing line between the reddish triangles and squares. We prefer to treat such graphs as in the second plot, where the entire vertical bar is considered a single pode.

Of course, the uniform ensemble of networks of a fixed node number \( n \) and fixed numbers of edges and triangles are only proven to look like the optimal graphons in the \( n \rightarrow \infty \) limit. We need a procedure to generate the ensemble for finite \( n \). To do this, we implement a dynamics on the space of networks with given \( e \), described in Subsection 2.1, which has as limit set the subset of those with given \( t \). (The dynamics then plays the role of an adjustable heat bath.) We then run the dynamics ‘sufficiently long’ to obtain samples of this limit set. We next examine the histogram of values of \( \lambda_2 \) we obtained this way.

The histograms for \( n = 54, e = 0.67 \) and equal jumps of \( t \) from 0.24 to 0.26 are shown in Figure 5. When \( t = 0.248 \) or \( t = 0.250 \) the variance in \( \lambda_2 \) is large, but when \( t > 0.250 \) or \( t < 0.248 \) the variance is much smaller. We interpret this as meaning that for the higher \( t \) the networks represent one phase and for lower \( t \) they represent a different phase, and where the variance is large we have some sort of transition. Note that \( \lambda_2 \) is much more negative for values of \( t \) below the transition than above, which is what we would expect from a \( B(1,1)/A(3,0) \) transition. The behavior of the eigenfunctions is harder to quantify but easy to spot. As noted earlier, Figures 3 and 4 show the distributions of \( (\xi_1(v),\xi_2(v)) \)
Figure 3. \((\xi_1(v), \xi_2(v))\) plot and best-fit tripodal graphon for a typical graph with 54 nodes and triangle density \(t = 0.24\). Each mark on the left corresponds to a node in the graph. Using spatial clustering on the left-hand plot, these nodes were divided into three podes (denoted by different colors and shapes in the left-hand plot). The plot on the right shows the empirical graphon corresponding to this division into three: the division of the axes represents the three podes, and the color of a region represents the density of edges between the corresponding podes.

Figure 4. \((\xi_1(v), \xi_2(v))\) plot and best fit tri- and bipodal graphons for a typical graph with 54 nodes and triangle density \(t = 0.26\). See Figure 3 for a thorough description.
for two representative sample networks, one substantially below and one substantially above the transition.

\[ n = 54 \]

\[ t = 0.26 \]  \hspace{1cm} \lambda_2 \hspace{1cm} t = 0.248 \\
\[ t = 0.258 \]  \hspace{1cm} \lambda_2 \hspace{1cm} t = 0.246 \\
\[ t = 0.256 \]  \hspace{1cm} \lambda_2 \hspace{1cm} t = 0.244 \\
\[ t = 0.254 \]  \hspace{1cm} \lambda_2 \hspace{1cm} t = 0.242 \\
\[ t = 0.252 \]  \hspace{1cm} \lambda_2 \hspace{1cm} t = 0.24 \\
\[ t = 0.25 \]  \hspace{1cm} \lambda_2 \hspace{1cm} t \]

**Figure 5.** Density plots showing the distribution of the second most negative eigenvalue \( \lambda_2 \), for graphs with 54 nodes, edge density 0.67, and various triangle densities \( t \).

Figure 6 shows what happens when \( n = 30, 48 \) or 66. Qualitatively, the picture is the same as for \( n = 54 \). Quantitatively, there are some small differences. The transition is sharper when \( n \) is larger, but is still visible when \( n \) is as small as 30. The specific location of the transition varies somewhat in \( n \). As \( n \) increases, the transition point approaches from below the known location of the \( B(1, 1)/A(3, 0) \) phase transition for infinite \( n \), namely \( t = 0.2596 \).

The dependence of the transition \( t \) on \( n \) is particularly intriguing. There is a lower limit to the value of \( t \) achievable by a bipodal network in which each pode has an Erdős-Rényi structure. For the range of values of \( n \) considered in this paper (30 to 66), the transition actually occurs below this point! The networks just above the transition have a clear division into “red” and “blue” nodes, but the number of red-red-red triangles is significantly less than one would expect from an Erdős-Rényi graph with the given number of red-red edges. That is, in this range of \( t \)-values the red pode has some sort of \( n \)-dependent internal structure that we do not yet understand. This phenomenon is the subject of continuing research.

Finally, we examine whether our results are sensitive to changes in the edge density \( e = 0.67 \). They are not. Figure 7 shows the mean value of \( \lambda_2 \) as a function of \( (e, t) \). There is a sharp transition for all values of \( e \). All that changes with \( e \) is the specific value of \( t \) at which it occurs.

Having established that the phenomena we are investigating are insensitive to changes in \( e \) or \( n \), we will henceforth restrict attention to \( n = 54, e = 0.67 \).
Figure 6. Density plots showing the distribution of the second most negative eigenvalue $\lambda_2$ for $n = 30$, 48 and 66 nodes, edge density 0.67, and various triangle densities $t$.

2.1. Sampling from equilibrium. We use Markov Chain Monte Carlo (MCMC) to (approximately) uniformly sample graphs with specific numbers of edges and triangles. In order to ensure that our results are not sensitive to the sampling procedure, we carry this out in several different ways, all of which follow the same general procedure: given fixed number $n$ of vertices, and given fixed edge and triangle counts $E$ and $T$, we define the following three objects:

1. a constraint set $\Omega$ which contains all graphs on $n$ vertices with $E$ edges and $T$ triangles,
2. a function $d_\Omega$ measuring the “distance” from a graph to $\Omega$, and
3. for each graph $G$, a probability measure $Q_G$ on graphs with $n$ nodes (the “proposal distribution”).

We use this data to define a Metropolis-Hastings Markov chain with the following update rule: given the current state $G$ (a graph on $n$ nodes), we draw the graph $G'$ from $Q_G$. If $G' \in \Omega$, it becomes the next state of the Markov chain. If $G' \notin \Omega$ but $d_\Omega(G') \leq d_\Omega(G)$, $G'$ becomes the next state of the Markov chain. Otherwise, the Markov chain remains at $G$.

The Markov chain defined above is reversible, and the uniform measure on $\Omega$ is a stationary measure (and if $\Omega$ is connected under the proposal distributions, this stationary measure is unique). Finally, we generate a random graph by running the Markov chain for a long time.
The second-most-negative eigenvalue $\lambda_2$ of a typical 54-node graph, as a function of edge density $e$ and triangle density $t$. The phase transition is clearly visible as a curve along which $\lambda_2$ changes rapidly as a function of $e$ and $t$.

(for most of the empirical results presented here, $10^9$ accepted steps were sufficient) and accepting the final graph if it had exactly $E$ edges and $T$ triangles.

All of the results presented here were checked with the following three choices of $\Omega$, $d_\Omega$, and $Q$:

1. $\Omega$ is the set of graphs with exactly $E$ edges and at most $T$ triangles; $d_\Omega(G) = \max\{0, T(G) - T\}$; and $Q_G$ is the random graph obtained from $G$ by deleting an edge at random and adding an edge at random.
2. $\Omega$ and $d_\Omega$ are as above; $Q_G$ is the random graph obtained from $G$ by choosing a vertex at random, then deleting an incident edge at random and adding an incident edge at random.
3. $\Omega$ is the set of graphs with $|E(G) - E| \leq C$ and $|T(G) - T| \leq C$ for some constant $C$; $d_\Omega(G) = \max\{0, |E(G) - E| + |T(G) - T| - 2C\}$; and $Q_G$ is the random graph obtained from $G$ by either deleting a random edge, adding a random edge, or deleting a random edge and adding a random edge.

The figures and numbers that we present in the main body of this work are all for the first choice of dynamics. The other two choices of dynamics showed the same qualitative behavior but mixed more slowly; the third choice of dynamics in particular has a tendency to “get stuck” for long periods, since after deleting an edge it sometimes struggles to find another move that respects the triangle constraints.

2.1.1. Evaluating convergence. Since we are not able to prove bounds on the mixing time of any of the Markov chains above, we validated the convergence of our Markov chains
by verifying that the distribution of certain statistics of interest (for example, the second-smallest eigenvalue of the resulting graphs) were independent of the Markov chains’ initial states. Specifically, we initialized our various Markov chains from three different initial distributions:

1. a uniformly random graph with exactly $E$ edges,
2. a graph drawn from a $B(1, 1)$ graphon, and
3. a graph drawn from an $A(3, 0)$ graphon.

Note that these three distributions have very different spectral properties. After running the Markov chains above, however, we verified that the spectral statistics of the outputs did not depend on which of the three initializations we chose.

3. Structural rearrangement under change of phase

We now turn to the central question of this paper. We have seen that for $t = t_{\text{low}} = 0.24$, the ensemble is dominated by $A(3, 0)$ networks, as evidenced by $\lambda_2$ being very negative, and by $(\xi_1, \xi_2)$ being clustered around three points, with equal numbers of nodes near each point. When $t = t_{\text{high}} = 0.26$, the ensemble is dominated by networks with $\lambda_2$ much smaller, with the $(\xi_1, \xi_2)$ plot being a vertical bar (representing 60% of the nodes) and a separate cluster (40%). But how does the network change from one kind of network to the other under our dynamics, described in Section 2?

The supplementary material contains several animations that show the evolution of $(\xi_1, \xi_2)$ and various other statistics across the three stages. In this section, we do our best to summarize the main features using figures and text. However, we highly recommend viewing the actual animations. A picture is worth a thousand words, and a movie is worth a thousand pictures.

3.1. Increasing $t$. We display 100 short runs of 10,000 steps in Figure 8 and two long runs of 1,000,000 steps in Figure 9. Both figures show $\lambda_2$ as a function of time. Figure 9 also shows the number of embedded “two ear” graphs, where a “two ear” is two triangles sharing a common edge, or equivalently a tetrahedron with one edge missing. The data in Figure 9 has been smoothed, with both $\lambda_2$ and the 2-ear count averaged over 1000 successive times. The data in Figure 8 has not been smoothed.

A typical transition occurs in three dynamical stages. The first two are visible in Figure 8 and the third is visible in Figure 9. In the first stage, which only takes about 50 steps, the network retains its $A(3, 0)$ structure as $t$ increases from $t_{\text{low}}$ to $t_{\text{high}}$. In this stage $\lambda_2$ increases somewhat as the parameters $a$ and $b$ change, but the distribution of $(\xi_1, \xi_2)$ does not significantly change. This stage is visible in Figure 8 as a sudden, but modest, increase in $\lambda_2$ at the very beginning of each plot.

In the second stage, which usually takes between 1000-6000 steps, the network loses its $A(3, 0)$ structure as two of the clusters merge. This stage is marked by an increase in $\lambda_2$ and a dramatic change in the distribution of $(\xi_1, \xi_2)$. At the end of this stage, we have a structure that is very similar to the optimal $B(1, 1)$ graphon, except that the podes do not have the optimal sizes, being closer to 2 : 1 than to 60:40. This stage is visible in Figure 8, and accounts for most of the visible change in $\lambda_2$. In the last stage, which takes hundreds of
thousands of steps, the relative sizes of the podes adjust back and forth among a number of possibilities with nearly equal entropies, resulting in fluctuations in $\lambda_2$ and the 2-ear count over very long time scales. The beginning of this stage can be seen in Figure 8 as the point at which $\lambda_2$ becomes approximately constant over time. In order to actually see the pode sizes changing, one has to view the trajectories at the larger time-scale shown in Figure 9.

The first stage is driven entirely by entropy. Since all networks are well below the target number of triangles, all swaps of one edge for another are allowed. This results in edges simply moving from where they are concentrated to where they are not. Since $a < b$, $a$ gets bigger and $b$ gets smaller, but (aside from random noise) the graphon remains piecewise constant, with the three podes remaining indistinguishable. This is reflected in the fact that plots of $(\xi_1, \xi_2)$ basically do not change. Since $\lambda_2$ is proportional to $a - b$, $\lambda_2$ increases somewhat. For $n = 54$, it goes from a little below $-16$ to around $-14.5$.

In the second stage, the network explores the available phase space for $t = t_{\text{high}}$ starting from an $A(3,0)$ structure. Within each cluster, the variances in $\xi_1$ and $\xi_2$ increase, and an occasional vertex may move from one cluster to another. In a typical run, there is a latency period during which $\lambda_2$ gradually increases from around $-14.5$ to around $-11$, after which two of the clusters join and $\lambda_2$ rises quickly to around $-7$. During the merger, all three clusters spread out, and sometimes the third cluster gains or loses a vertex or two. Figure 10 shows the evolution of $\xi_1$ and $\xi_2$ during this second stage.

The third stage involves punctuated equilibrium. Most of the time, both $\lambda_2$ and the 2-ear density fluctuate in a range, and the distribution of $(\xi_1, \xi_2)$ does not change qualitatively. Once in a while, a node moves from one pode to another, triggering sudden changes in both
Figure 9. Two different random trajectories of $\lambda_2$ (in blue), and the number of embedded “two ear” graphs (in red) as a function of time, as the triangle count is increased from 0.24 to 0.26 over $10^6$ steps. The data is smoothed by averaging over windows of 1000 steps.

Figure 10. Snapshots of $(\xi_1, \xi_2)$ after 500, 800, and 1500 steps during an upward trajectory. Each dot corresponds to a vertex $v$; the coordinates of the dot are given by $\xi_1(v)$ and $\xi_2(v)$. The transition can also be viewed in the animations.
λ₂ and the two-ear count. When the new ratio of pode sizes is close to the optimal ratio, the system can stabilize in the new state for almost 100,000 steps. If the new ratio of pode sizes is far from optimal, however, entropy drives them to change back more quickly, usually within 10,000 steps. Such an extreme excursion is visible at time 150,000 in the first run, where the smaller pode grows to 24 nodes and remains there for about 10,000 steps before eventually making its way back to 21 nodes at time 170,000. On its way back, the size of the smaller pode briefly (for about 10,000 steps) stabilizes at 23, corresponding to the two-ear count stabilizing at around 111,150.

The end of stage 1 and the beginning of stage 2 is easy to define. This is when \( t \) first hits its target value, after which the constraint on \( t \) begins to affect which edge swaps are allowed. This consistently takes between 45 and 60 steps, with an average of 50.

The end of stage 2 / beginning of stage 3 is harder to define. To do this, we did a least-squares fit of the first 10,000 steps, minus stage 1, via a line of arbitrary slope followed by a horizontal line. These best fit lines are shown in Figure 8. We interpret the domain of the sloped line as stage 2 and the domain of the horizontal line as stage 3.

The evolution of \( \lambda₂ \) (smoothed over 100 steps) in runs 17, 23 and 65 is shown in more detail in Figure 11. In a run with a long latency, such as run 65, the sloped line tracks the gradual increase during the latency period, and the subsequent rapid rise shows up as a discontinuity between the lines. In runs with short latencies, such as run 23, the entire increase from \(-14.5\) to \(-7\) is captured by the sloped line, so there is no discontinuity. In a few runs, such as run 17, the latency period involves some false starts, where \( \lambda₂ \) first increases and then decreases, and the fit to a sloped line is not good at all. However, even in these exceptional cases, the beginning of the horizontal line provides a credible measure of the beginning of stage 3.

We have plotted the distribution of the length of stage 2 in Figure 12. The shape of this histogram is modeled well by a Gamma distribution with \( \alpha = 7.5 \) and \( \theta = 430 \) (i.e. the function \( x^{6.5}e^{-x/430} \)), which we have superimposed on the histogram.

3.2. Decreasing \( t \). As with increasing \( t \), the trajectories for decreasing \( t \) exhibit three stages of increasing length. We present the data, much as before, in Figures 13, 14, 16, and 17. These show 100 trajectories for 5,000 steps, two trajectories for 1,000,000 steps, close-ups of three of the short downwards trajectories, and a histogram of the lengths of stage 2, respectively. The long runs show both \( \lambda₂ \) and the 2-ear count, while the short runs only show \( \lambda₂ \). The short runs illustrate what happens in stages 1 and 2, while the long runs explore stage 3.

However, there are some important differences between the dynamics for decreasing \( t \) and the dynamics for increasing \( t \). First, because the entropy at \( t = t_{low} \) is substantially lower than the entropy at \( t = t_{high} \), the high-to-low transition has to be forced. As long as \( t \) is above the target value, the dynamics only allow edge swaps that decrease the number of triangles, or at worst keep the number constant. The initial stage of the transition, rather than being an entropy-driven relaxation, is essentially a greedy algorithm for decreasing \( t \). This stage is a little slower than the first stage of the upward transitions, taking around 180 steps instead of about 50.
Figure 11. Close-ups of the 17th, 23rd, and 65th trajectories from Figure 8, smoothed over 100 steps. These three trajectories can also be seen in the animations.
**Figure 12.** The histogram of the length of stage 2 for upwards trajectories, and a best-fit Gamma function with $(\alpha = 7.5$ and $\theta = 430)$

**Figure 13.** 100 repetitions showing the trajectory of $\lambda_2$ as a function of time, as the triangle density is decreased from 0.26 to 0.24 over 5000 steps. The red and green lines show the least-squares best fit of the trajectory by a linear function (the red line) followed by a constant function (the green line). The trajectories are smoothed over 100 timesteps.
Second, the qualitative form of the graph cannot stay the same throughout stage 1. Below $t = 0.26$, it is mathematically impossible to achieve the desired number of triangles with two podes and with Erdős-Rényi structure within each pode. Instead, as noted above, the system has to develop additional structure within the larger pode. As $t$ drops, vertices in this pode start to segregate into two sub-podes, with edges being more likely between sub-podes than within a sub-pode. When we reach $t_{\text{low}}$, this segregation is still not complete, but the vertical bar in the $(\xi_1, \xi_2)$ plot has become more like a dumbbell, with most points near one end or the other, as can be seen in Figure 15. At this point, $\lambda_2$ has dropped to around $-13$.

Once we reach $t_{\text{low}}$, the dynamics no longer force us to decrease $t$. The second stage is shorter than for increasing $t$, and lasts on the order of 1000 edge swaps. In this stage, $\lambda_2$ continues to drop to a value near $-15$ as the two sub-podes become better defined. (The division of the original large cluster is not always exactly even, and this affects the resulting
Figure 15. Snapshots of \((\xi_1, \xi_2)\) after 10, 100, and 200 steps during an downward trajectory. Each dot corresponds to a vertex \(v\); the coordinates of the dot are given by \(\xi_1(v)\) and \(\xi_2(v)\). The podes are not actually changing size. Rather, values of \((\xi_1, \xi_2)\) are becoming so closely positioned that multiple nodes only show up as a single dot. This transition can also be seen in the animations.

values of \(\lambda_2\).) However, the decrease in \(\lambda_2\) is not as rapid as in stage 1 and is no longer monotonic. Indeed, the onset of this stage can be viewed not only as the point where \(t\) reaches the target value, but also as the point where the plot of \(\lambda_2\) versus time starts to become noisy. This is clearly seen in Figure 16, where the data has not been smoothed. At the end of the second stage, our networks now involve two (more-or-less) identical clusters, each a subset of the original large pode, and a third cluster that is different, with no evidence of any internal structure within these three new podes.

There is considerable variation in the length of stage 2, as can be seen in Figure 13. As before, we define this length by doing a fit of the data after the end of stage 1, and until the 10,000th step, by a slanted line followed by a horizontal line. Three such fits (cut off after the 5000th step) are shown in Figure 16. In most cases, such as run 9 with a long stage 2 and run 46 with a very short stage 2, the lines fit together clearly, with little discontinuity. In a few cases, such as run 99, \(\lambda_2\) overshoes the mark and rebounds, or shows other behavior that does not really fit a linear model, making it difficult to pinpoint the end of stage 2. The distribution of the length of stage 2 is shown in Figure 17, together with a best-fit Gamma functions, with parameters \(\alpha = 2.25\) and \(\theta = 660\). Compared to the similar histogram for the upwards trajectory, the value of \(\alpha\) is much smaller, and the fit is not as good, perhaps because of outliers such as run 99.

The third stage is much more stable than for increasing \(t\). There are still frequent excursions, where a node attempts to leave its pode and usually comes back. These appear as short upwards spikes in \(\lambda_2\), with simultaneous downward spikes in the 2-ear count. Successful migrations are much less common. For instance, in the first plot of Figure 14, the first clear migration only occurs after about 180,000 steps. There is another one after 480,000 steps, and a third at about 700,000 steps, plus less clear events at about 790,000, 830,000, and 960,000 steps. The lowest values of \(\lambda_2\), around \(-16.3\), are associated with the most symmetric configurations, with 18 nodes in each pode, while higher plateaus around \(-15.7\) and \(-15.2\) represent 19-18-17 or 20-17-17 or 19-19-16 splits.

4. Conclusion

In this paper we considered analogues, for constrained random networks, of the nucleation of phase transitions in molecular systems as normally treated statistically, in particular
Figure 16. Close-ups of the 9th, 46th, and 99th trajectories in Figure 13, not smoothed. These three trajectories can also be viewed in the animations.
the melting/freezing transition between neighboring fluid and solid phases, which has been difficult to analyze analytically [2, 3].

Statistical mechanics produces phase diagrams representing states which have settled (after ‘infinite time’) into thermal equilibrium. The states are of macroscopic molecular systems, which means that one is taking an infinite time limit followed by an infinite volume limit (to get well-defined transitions), and the results are applicable to real systems if sufficient care is taken. The ‘transitions’ one sees in a phase diagram could be understood to represent results taken through incremental changes of constraints with ample time allowed for the system to reequilibrate between steps, so-called ‘quasistatic’ changes.

At fixed pressure, a fluid material when cooled can remain fluid far beyond its freezing point unless it is disturbed by complicating inhomogenities. This phenomenon is studied through ‘nucleation theory’, which models the manner by which a supercooled fluid stochastically produces microscale crystalline clusters which, if large enough, grow to macroscopic crystals. This phenomenon is understood as resulting from the improbability for a typical fluid/disordered cluster of molecules to randomly rearrange into a large enough (‘critical size’) crystal cluster.

In this paper we analyzed one of the phase transitions found in constrained random networks to see if there are similar barriers for a network in one phase to rearrange structure to another phase. Our results, detailed in Section 3, show distinct barriers in both directions. We have included our first attempts to analyze these phenomena statistically.

The current standard for modelling nucleation for molecular systems is called classical nucleation theory. It is still too crude, with some predictions wrong by a large factor [1]. It is hard to improve the theory because one cannot follow nucleation experimentally: it occurs
in very small but unpredictable regions of space, over a very small time [1]. But versions of ‘nucleation’ can occur in systems other than molecular matter, and theory can make use of this. Recently nucleation has been found in physical experiments of cyclically sheared ‘sand’ [23, 24], which may prove easier to model accurately since the system is macroscopic. Likewise the nucleation in networks reported here, which was in fact motivated by our work in [23, 24], may also contribute to the general subject. Specifically, as discussed in Section 3 we find that various stages in the rearrangement of the network structure have well defined probability distributions, different in the two directions. Understanding these should be useful for a deeper nucleation theory.

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