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PHASE TRANSITIONS IN EXPONENTIAL RANDOM GRAPHS

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We derive the full phase diagram for a large family of 2-parameter exponential random graph models, each containing a first order transition curve ending in a critical point.

1. Introduction. We will treat a class of models of large, 'dense' random graphs, that is, simple graphs on n vertices in which the average number of edges is of order n^2. More specifically we will consider 2-parameter families of exponential random graphs in which dependence between the random edges is defined through certain finite subgraphs H_2, in imitation of the use of potential energy to provide dependence between particle states in a grand canonical ensemble of statistical physics. Intuitively, the two parameters allow one to adjust the density of edges and the density of subgraphs H_2, and analyze the extent to which specific values of these densities 'interfere' with one another. Exponential random graphs have been widely studied (see [3, 4] for a range of recent work) since the pioneering work on the independent case by Erdős and Rényi [2]. We will concentrate on the phenomenon of phase transitions which can emerge for dependent variables: a sharp, unambiguous partition of parameter ranges separating those values in which changes in parameters lead to smooth changes in the two densities, from those special parameter values where the response in the densities is singular. This subject has attracted enormous interest in mathematics, as well as in various applied disciplines (some references may be found, for instance, in Häggström and Jonasson [6]). Analyses using mean-field and other uncontrolled approximations (see for instance [10, 11]) have predicted such partitions, but with some qualitative error which we discuss in the last section. There has recently been important progress by Chatterjee and Diaconis [1], including the first rigorous proof of singular dependence on parameters. We will extend their result both in the class of models and parameter values under control and provide an appropriate formalism of phase structure for such models.

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2. Statement of Results. We consider the class of models in which the probability of the simple graph G_n on n vertices is given by:

$$\mathbb{P}_n^{\beta_1,\beta_2}(G_n) = e^{n^2[\beta_1 t(H_1,G_n)+\beta_2 t(H_2,G_n)-\psi_n]}, \tag{1}$$

where: H_1 is an edge, H_2 is any finite simple graph with $p \geq 2$ edges, $\psi_n = \psi_n(\beta_1,\beta_2)$ is the normalization constant, $t(H,G_n)$ is the density of graph homomorphisms $H \to G_n$:

$$t(H,G_n) = \frac{|\hom(H,G_n)|}{|V(G_n)|^{|V(H)|}}, \tag{2}$$

and $V(\cdot)$ denotes the vertex set. Expectation of a real function of a random graph is denoted $\mathbb{E}_{\beta_1,\beta_2}\{\cdot\}$. Our main results are the following.

THEOREM 2.1. *For any allowed H_2, the pointwise limit*

$$\psi_\infty(\beta_1,\beta_2) = \lim_{n\to\infty} \psi_n(\beta_1,\beta_2) \tag{3}$$

exists and is analytic at all (β_1,β_2) in the upper half-plane ($\beta_2 \geq 0$) except on a certain continuous curve $\beta_2 = q(\beta_1)$ which includes the end point

$$(\beta_1^c,\beta_2^c) = \Big(\frac{1}{2}\log(p-1) - \frac{p}{2(p-1)}, \frac{p^{p-1}}{2(p-1)^p}\Big). \tag{4}$$

The derivatives $\frac{\partial}{\partial\beta_1}\psi_\infty$ and $\frac{\partial}{\partial\beta_2}\psi_\infty$ have (jump) discontinuities across the curve, except at (β_1^c,β_2^c) where, however, all the second derivatives $\frac{\partial^2}{\partial\beta_1^2}\psi_\infty$, $\frac{\partial^2}{\partial\beta_1\partial\beta_2}\psi_\infty$, and $\frac{\partial^2}{\partial\beta_2^2}\psi_\infty$ diverge.

THEOREM 2.2. *If the graph H_2 is a p-star, $p \geq 2$, then the pointwise limit $\psi_\infty(\beta_1,\beta_2)$ exists and is analytic at all (β_1,β_2) in the lower half-plane ($\beta_2 \leq 0$).*

REMARK. *A p-star has p edges meeting at a vertex.*

COROLLARY 2.3. *For any allowed H_2, the parameter space $\{(\beta_1,\beta_2) : \beta_2 \geq 0\}$ consists of a single phase with a first order phase transition across the indicated curve and a second order phase transition at the critical point (β_1^c,β_2^c).*

To explain the language of phase transitions in Corollary 2.3 we first give a superficial introduction to the formalism of classical statistical mechanics within d-dimensional lattice gas models; for more details see for instance [9].

Assume each point in a d-dimensional cube

$$C = \{-n, -(n-1), \cdots 0, \cdots (n-1), n\}^d \subset \mathbb{Z}^d \tag{5}$$

is randomly occupied (by one particle) or not occupied, and assume there is a (many-body) potential energy of fixed value $a \neq 0$ associated with every occupied subset of C congruent to a certain $H_2 \subset C$. The interaction is attractive if $a < 0$ and repulsive if $a > 0$. We define the probability that the occupied sites in C are precisely c by

$$\mathbb{P}_n^{\beta,\mu}(c) = \frac{e^{-\beta[\mu E_1(c) + a E_2(c)]}}{\mathbb{Z}_n}, \tag{6}$$

where the parameter $\beta > 0$ is called the inverse temperature, the parameter $\mu \in \mathbb{R}$ is called the chemical potential, the normalization constant $\mathbb{Z}_n(\beta, \mu)$ is called the partition function, H_1 and H_2 are subsets of C with H_1 a singleton and the cardinality $|H_2| \geq 2$, and $E_j(c)$ is the number of copies of H_j in c. (We are using 'free' boundary conditions.) One of the basic features of the formalism is that the free energy density, $F_n(\beta, \mu) = \ln[\mathbb{Z}_n(\beta, \mu)]/n^d$, contains all ways to interact with or influence the system, so that 'all' physically significant quantities can be obtained by differentiating it with respect to β and μ. For instance

$$\frac{\partial}{\partial \mu} F_n(\beta, \mu) = -\beta \mathbb{E}_{\beta,\mu}\Big\{\frac{E_1}{n^d}\Big\}, \tag{7}$$

the (average) particle density. To model materials in thermal equilibrium, calculations in this formalism normally require that the system size be sufficiently large, and in practice one often resorts to using $n \to \infty$. With this as motivation we tentatively define a 'phase' as a set of states (i.e. probability distributions) corresponding to a connected region of the (β, μ) parameter space, which is maximal for the condition that $\lim_{n\to\infty} \frac{\partial^{j+k}}{\partial \beta^j \partial \mu^k} F_n(\beta, \mu)$ are analytic in β and μ for all j, k. One associates a 'phase transition' with singularities which develop in some of these quantities as the system size diverges. Such singularities are sometimes detected in simulations through the variances $\sigma_1^2(n)$, $\sigma_2^2(n)$ of the particle and energy densities, E_1/n^d, E_2/n^d, respectively. It is easy to check for instance that

$$\frac{\partial^2}{\partial \mu^2} F_n(\beta, \mu) = \beta^2 n^d \ \sigma_1^2(n), \tag{8}$$

and therefore a finite limit for $\frac{\partial^2}{\partial\mu^2}F_n(\beta,\mu)$ as $n\to\infty$ implies $\sigma_1^2(n)\to 0$ at least as fast as $1/n^d$, while the divergence of $\frac{\partial^2}{\partial\mu^2}F_n(\beta,\mu)$ more slowly than n^d as $n\to\infty$ implies $\sigma_1^2(n)\to 0$ more slowly than $1/n^d$, and a jump discontinuity in $\frac{\partial}{\partial\mu}F_n(\beta,\mu)$ as $n\to\infty$ implies $\sigma_1^2(n)$ does not go to 0 as $n\to\infty$. An important simplification was proven by Yang and Lee [12] who showed that the limiting free energy density $F_\infty(\beta,\mu)=\lim_{n\to\infty}F_n(\beta,\mu)$ always exists and that certain limits commute:

$$\lim_{n\to\infty}\frac{\partial^{j+k}}{\partial\beta^j\partial\mu^k}F_n(\beta,\mu)=\frac{\partial^{j+k}}{\partial\beta^j\partial\mu^k}\lim_{n\to\infty}F_n(\beta,\mu)=\frac{\partial^{j+k}}{\partial\beta^j\partial\mu^k}F_\infty(\beta,\mu). \tag{9}$$

This implies that phases and phase transitions can be determined from the limiting free energy density, and so a phase is commonly defined (see for instance [5]) as a connected region of the (β,μ) parameter space maximal for the condition that $F_\infty(\beta,\mu)$ is analytic.

Using the obvious analogues for random graphs, with β_1 playing the role of $-\beta\mu$ and β_2 the role of $-\beta a$ (and therefore positive if and only if the model is 'attractive'), $\psi_n=\psi_n(\beta_1,\beta_2)$ plays the key role of the free energy density $F_n(\beta,\mu)$. We will show in Theorems 3.9 and 3.10 below that the limiting free energy density $\psi_\infty(\beta_1,\beta_2)$ exists, and the proof of Theorem 2 by Yang and Lee [12], on the commutation of limits, then goes through without any difficulty in this setting, so we can again define phases and phase transitions through the limiting free energy density, as follows.

Definition 2.4. *A phase is a connected region, of the parameter space $\{(\beta_1,\beta_2)\}$, maximal for the condition that the limiting free energy density, $\psi_\infty(\beta_1,\beta_2)$, is analytic. There is a jth-order transition at a boundary point of a phase if at least one j^{th}-order partial derivative of $\psi_\infty(\beta_1,\beta_2)$ is discontinuous there, while all lower order derivatives are continuous.*

Theorems 2.1 and 2.2 thereby justify our interpretation in Corollary 2.3 that each of our models consists of a single phase with a first order phase transition across the indicated curve except at the end (or 'critical') point (β_1^c,β_2^c), where the transition is second order, superficially similar to the transition between liquid and gas in equilibrium materials.

3. Proofs. Chatterjee and Diaconis have proven that the main object of interest, $\psi_\infty(\beta_1,\beta_2)$, exists for all β_1 and nonnegative β_2 and is the solution of a certain optimization problem:

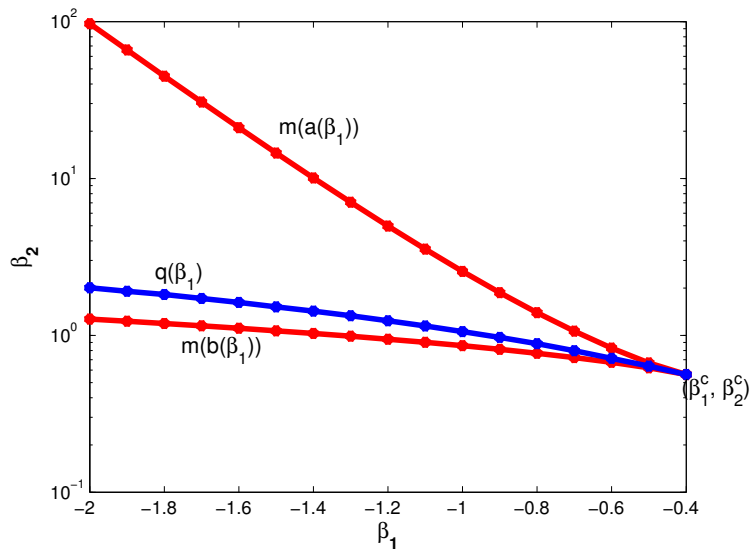

FIG 1. *The V-shaped region (with phase transition curve inside) in the* (β_1, β_2) *plane. Graph drawn for* $p = 3$.

THEOREM 3.1 (Part of Theorem 4.1 in [1]). *Fix one of our models and assume* H_2 *has* $p \geq 2$ *edges. Then for all* (β_1, β_2) *in the upper half-plane* $(\beta_2 > 0)$*, the pointwise limit* $\psi_\infty(\beta_1, \beta_2) = \lim_{n\to\infty} \psi_n(\beta_1, \beta_2)$ *exists and:*

$$\psi_\infty(\beta_1, \beta_2) = \sup_{u\in[0,1]} \Big(\beta_1 u + \beta_2 u^p - \frac{1}{2} u \log u - \frac{1}{2}(1-u)\log(1-u)\Big). \tag{10}$$

The following detailed analysis of this maximization problem is therefore fundamental to understanding the phase structure of our models, and we now address it.

PROPOSITION 3.2. *Fix an integer* $p \geq 2$*. Consider the maximization problem for*

$$l(u; \beta_1, \beta_2) = \beta_1 u + \beta_2 u^p - \frac{1}{2} u \log u - \frac{1}{2}(1-u)\log(1-u) \tag{11}$$

on the interval $[0, 1]$*, where* $-\infty < \beta_1 < \infty$ *and* $-\infty < \beta_2 < \infty$ *are parameters. Then there is a V-shaped region in the* (β_1, β_2) *plane with corner point* (β_1^c, β_2^c) *such that outside this region,* $l(u)$ *has a unique local maximizer (hence global maximizer)* u^**; whereas inside this region,* $l(u)$ *always has exactly two local maximizers* u_1^* *and* u_2^**. Moreover, for every* β_1 *inside this*

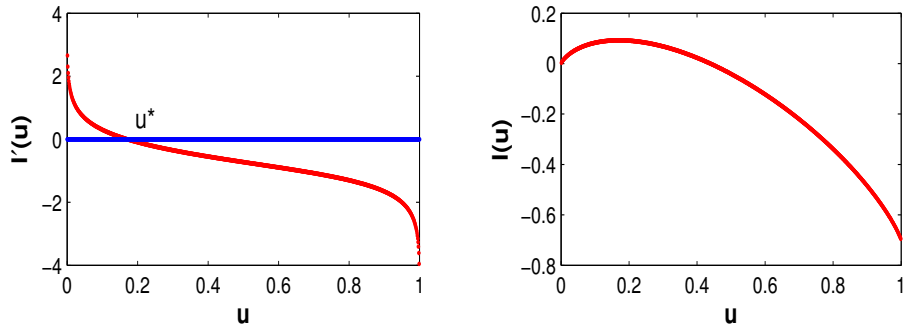

FIG 2. *Outside the V-shaped region, $l(u)$ has a unique local maximizer (hence global maximizer) u^*. Graph drawn for $\beta_1 = -0.8$, $\beta_2 = 0.1$, and $p = 3$.*

V-shaped region ($\beta_1 < \beta_1^c$), there is a unique $\beta_2 = q(\beta_1)$ such that the two local maximizers of $l(u; \beta_1, q(\beta_1))$ are both global maximizers. Furthermore q is a continuous and decreasing function of β_1.

REMARK. *By the Lebesgue Differentiation Theorem, q being monotone guarantees that it is differentiable almost everywhere.*

PROOF. The location of maximizers of $l(u)$ on the interval $[0, 1]$ are closely related to properties of its derivatives $l'(u)$ and $l''(u)$:

$$l'(u) = \beta_1 + p\beta_2 u^{p-1} - \frac{1}{2}\log\frac{u}{1-u}, \tag{12}$$

$$l''(u) = p(p-1)\beta_2 u^{p-2} - \frac{1}{2u(1-u)}. \tag{13}$$

We first analyze properties of $l''(u)$ on the interval $[0, 1]$. Consider instead the function

$$m(u) = \frac{1}{2p(p-1)u^{p-1}(1-u)}. \tag{14}$$

Simple optimization shows

$$0 \le (p-1)u^{p-1}(1-u) \le \left(\frac{p-1}{p}\right)^p, \tag{15}$$

and the equality holds if and only if $u = \frac{p-1}{p}$. Thus

$$\frac{p^{p-1}}{2(p-1)^p} \le m(u) < \infty, \tag{16}$$

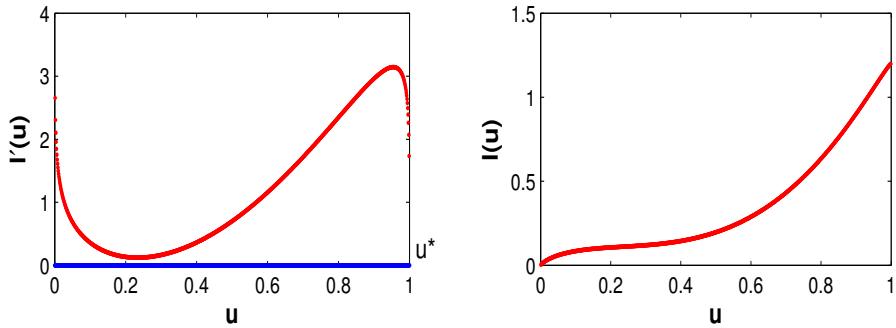

FIG 3. *Outside the V-shaped region, $l(u)$ has a unique local maximizer (hence global maximizer) u^*. Graph drawn for $\beta_1 = -0.8$, $\beta_2 = 2$, and $p = 3$.*

with the lower bound achieved only at $u = \frac{p-1}{p}$, and $m(u)$ decreases before this minimum and increases after it. This implies that for $\beta_2 \leq \frac{p^{p-1}}{2(p-1)^p}$, $l''(u) \leq 0$ on the whole interval $[0,1]$; whereas for $\beta_2 > \frac{p^{p-1}}{2(p-1)^p}$, $l''(u)$ will take on both positive and negative values, and we denote the transition points by u_1 and u_2 ($u_1 < \frac{p-1}{p} < u_2$).

Based on properties of $l''(u)$, we next analyze properties of $l'(u)$ on the interval $[0,1]$. For $\beta_2 \leq \frac{p^{p-1}}{2(p-1)^p}$, $l'(u)$ is monotonically decreasing. For $\beta_2 > \frac{p^{p-1}}{2(p-1)^p}$, $l'(u)$ is decreasing from 0 to u_1, increasing from u_1 to u_2, then decreasing again from u_2 to 1.

Based on properties of $l'(u)$ and $l''(u)$, we analyze properties of $l(u)$ on the interval $[0,1]$. Independent of the choice of parameters β_1 and β_2, $l(u)$ is a bounded continuous function, $l'(0) = \infty$, and $l'(1) = -\infty$, so $l(u)$ can not be maximized at 0 or 1. For $\beta_2 \leq \frac{p^{p-1}}{2(p-1)^p}$, $l'(u)$ crosses the u-axis only once, going from positive to negative. Thus $l(u)$ has a unique local maximizer ((hence global maximizer) u^*. For $\beta_2 > \frac{p^{p-1}}{2(p-1)^p}$, the situation is more complicated and deserves a careful analysis. If $l'(u_1) \geq 0$ (resp. $l'(u_2) \leq 0$), $l(u)$ has a unique local maximizer (hence global maximizer) at a point $u^* > u_2$ (resp. $u^* < u_1$). If $l'(u_1) < 0 < l'(u_2)$, then $l(u)$ has two local maximizers u_1^* and u_2^*, with $u_1^* < u_1 < \frac{p-1}{p} < u_2 < u_2^*$.

Notice that u_1 and u_2 are solely determined by the choice of parameter $\beta_2 > \frac{p^{p-1}}{2(p-1)^p}$, and vice versa. By (14),

$$l'(u_1) = \beta_1 + \frac{1}{2(p-1)(1-u_1)} - \frac{1}{2}\log\frac{u_1}{1-u_1}, \tag{17}$$

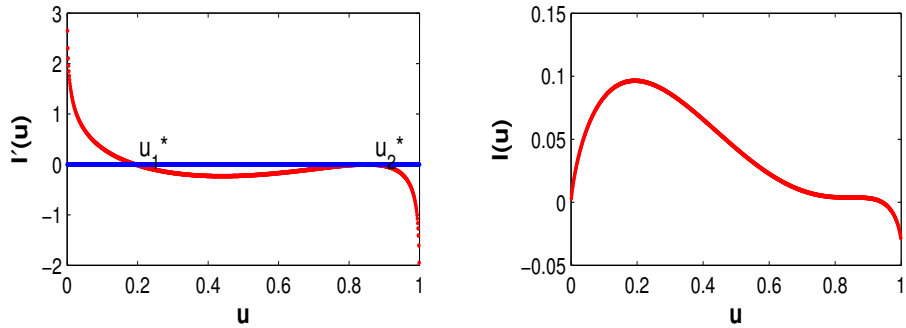

FIG 4. *Along the lower bounding curve of the V-shaped region, $l'(u)$ has two zeros u_1^* and u_2^*, but only u_1^* is the global maximizer for $l(u)$. Graph drawn for $\beta_1 = -0.8$, $\beta_2 = 0.769$, and $p = 3$.*

$$l'(u_2) = \beta_1 + \frac{1}{2(p-1)(1-u_2)} - \frac{1}{2}\log\frac{u_2}{1-u_2}. \tag{18}$$

Consider the function

$$n(u) = \frac{1}{2(p-1)(1-u)} - \frac{1}{2}\log\frac{u}{1-u}. \tag{19}$$

It is not hard to see that $n(0) = \infty$, $n(1) = \infty$, $n(u)$ is decreasing from 0 to $\frac{p-1}{p}$, then increasing from $\frac{p-1}{p}$ to 1, and the global minimum value is

$$n\Big(\frac{p-1}{p}\Big) = \frac{p}{2(p-1)} - \frac{1}{2}\log(p-1). \tag{20}$$

This implies in particular that $l'(u_1) \geq 0$ for $\beta_1 \geq \frac{1}{2}\log(p-1) - \frac{p}{2(p-1)}$. The only possible region in the (β_1, β_2) plane where $l'(u_1) < 0 < l'(u_2)$ is thus bounded by $\beta_1 < \frac{1}{2}\log(p-1) - \frac{p}{2(p-1)}$ and $\beta_2 > \frac{p^{p-1}}{2(p-1)^p}$.

We now analyze the behavior of $l'(u_1)$ and $l'(u_2)$ more closely when β_1 and β_2 are chosen from this region. Recall that by construction, $u_1 < \frac{p-1}{p} < u_2$. By monotonicity of $n(u)$ on the intervals $(0, \frac{p-1}{p})$ and $(\frac{p-1}{p}, 1)$, there exist continuous functions $a(\beta_1)$ and $b(\beta_1)$ of β_1, such that $l'(u_1) < 0$ for $u_1 > a(\beta_1)$ and $l'(u_2) > 0$ for $u_2 > b(\beta_1)$. $a(\beta_1)$ is an increasing function of β_1, whereas $b(\beta_1)$ is a decreasing function, and they satisfy

$$n(a(\beta_1)) = n(b(\beta_1)) = -\beta_1. \tag{21}$$

Also, as $\beta_1 \to -\infty$, $a(\beta_1) \to 0$ and $b(\beta_1) \to 1$. By (14), the restrictions on u_1 and u_2 yield restrictions on β_2. We have $l'(u_1) < 0$ for $\beta_2 < m(a(\beta_1))$ and

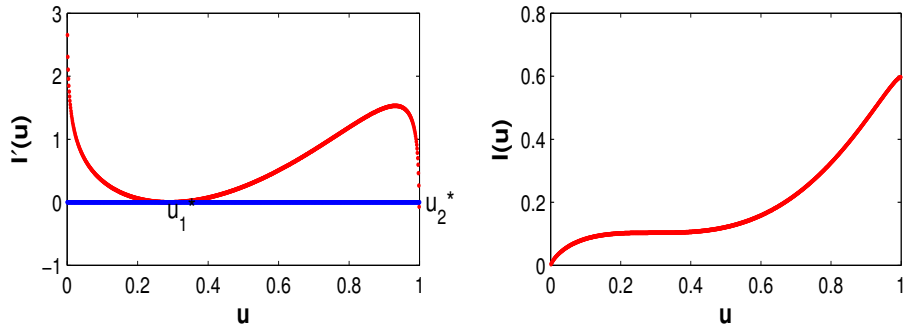

FIG 5. *Along the upper bounding curve of the V-shaped region, $l'(u)$ has two zeros u_1^* and u_2^*, but only u_2^* is the global maximizer for $l(u)$. Graph drawn for $\beta_1 = -0.8$, $\beta_2 = 1.396$, and $p = 3$.*

$l'(u_2) > 0$ for $\beta_2 > m(b(\beta_1))$. Notice that $m(a(\beta_1))$ and $m(b(\beta_1))$ are both decreasing functions of β_1, and as $\beta_1 \to -\infty$, they both grow unbounded. By construction, for every parameter value (β_1, β_2), $l'(u_2) > l'(u_1)$. Also, for fixed β_1, $m(a(\beta_1))$ is the value of β_2 for which $l'(u_1) = 0$, and $m(b(\beta_1))$ is the value for which $l'(u_2) = 0$. Thus the curve $m(b(\beta_1))$ must lie below the curve $m(a(\beta_1))$. And together they generate the bounding curves of the V-shaped region in the (β_1, β_2) plane where two local maximizers exist for $l(u)$. It is not hard to see that the corner point is given by $(\beta_1^c, \beta_2^c) = \left(\frac{1}{2}\log(p-1) - \frac{p}{2(p-1)}, \frac{p^{p-1}}{2(p-1)^p}\right)$. (See Figures 1–6.)

Fixing an arbitrary $\beta_1 < \beta_1^c$, we examine the effect of varying β_2 on the graph of $l'(u)$. It is clear from (12) that $l'(u)$ shifts upward as β_2 increases. As a result, as β_2 gets large, the positive area bounded by the curve $l'(u)$ increases, whereas the negative area decreases. By the fundamental theorem of calculus, the difference between the positive and negative areas is the difference between $l(u_2^*)$ and $l(u_1^*)$, which goes from negative ($l'(u_2) = 0$, u_1^* is the global maximizer) to positive ($l'(u_1) = 0$, u_2^* is the global maximizer) as β_2 goes from $m(b(\beta_1))$ to $m(a(\beta_1))$. Thus there must be a unique β_2 : $m(b(\beta_1)) < \beta_2 < m(a(\beta_1))$ such that u_1^* and u_2^* are both global maximizers. We denote this β_2 by $q(\beta_1)$; see Figures 1 and 6.

By analyzing the graph of $l'(u)$, we see that the parameter values of $(\beta_1, q(\beta_1))$ are exactly the ones for which positive and negative areas bounded by $l'(u)$ equal each other. An increase in β_1 will induce an upward shift of $l'(u)$, which must be balanced by a decrease in $\beta_2 = q(\beta_1)$. Similarly, a decrease in β_1 will induce a downward shift of $l'(u)$, which must be balanced by an increase in $\beta_2 = q(\beta_1)$. This justifies that q is monotonically decreasing

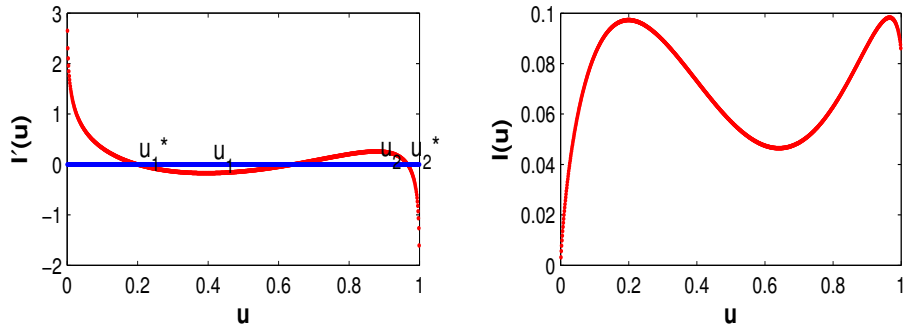

FIG 6. *Along the phase transition curve, $l(u)$ has two local maximizers u_1^* and u_2^*, and both are global maximizers. Graph drawn for $\beta_1 = -0.8$, $\beta_2 = 0.884$, and $p = 3$.*

in β_1. Furthermore, the continuity of $l'(u)$ as a function of β_1 and β_2 implies the continuity of q as a function of β_1. □

COROLLARY 3.3. *The transition curve $\beta_2 = q(\beta_1)$ displays a universal asymptotic behavior as $\beta_1 \to -\infty$:*

$$\lim_{\beta_1 \to -\infty} |q(\beta_1) + \beta_1| = 0. \tag{22}$$

PROOF. Assume $\beta_1 = \beta = -\beta_2 + \delta$ where $|\delta| \neq 0$, and define $F(u, \beta) = \beta(u - u^p)$, $I(u) = -(1/2)u \log u - (1/2)(1-u)\log(1-u)$, and $G(u) = \delta u^p + I(u)$. Then $\ell(u; \beta_1, \beta_2) = \ell(u, \beta) = F(u, \beta) + G(u)$. We will show, for sufficiently negative β, that if $\delta > 0$ the global maximum u^* of $\ell(u, \beta)$ equals u_2^*, while if $\delta < 0$ u^* equals u_1^*. This implies, for these β, that $-\beta - |\delta| < q(\beta) < -\beta + |\delta|$, which will prove the desired limit.

From the continuity of $G(u)$ there exists $\eta \in (0, 1/p)$, such that $|G(u) - G(u_0)| < |\delta|/2$ for all $|u - u_0| < \eta$, for both $u_0 = 0$ and $u_0 = 1$. Recall that $u_1^* < u_1 < \frac{p-1}{p} < u_2 < u_2^*$. Since $u - u^p = u(1 - u^{p-1}) > 0$ on $(0, 1)$, there exists $B < 0$ such that for all $\beta < B$ and $u \in [\eta, 1 - \eta]$, $F(u, \beta) < -1 - |\delta|$ and therefore $\ell(u, \beta) < 0 = \ell(0, \beta)$, so $u^* \in [0, \eta) \cup (1 - \eta, 1]$. Using that $F(u, \beta) \leq 0$ for all $\beta < 0$ and all $u \in [0, 1]$, if $\delta > 0$ and $u < \eta < 1/p \leq (p-1)/p$ then $\ell(u, \beta) < \delta/2 < \delta = \ell(1, \beta)$ so $u^* = u_2^*$, while if $\delta < 0$ and $u > 1 - \eta > (p-1)/p$ then $\ell(u, \beta) < -|\delta|/2 < 0 = \ell(0, \beta)$ and therefore $u^* = u_1^*$.

□

So far we have used results from [1] but have avoided specific reference to the framework of graph limits, developed by Lovász et al, which was used

to prove those results. We now need to refer directly to graph limits; for the notation and an introduction to this material see for instance [8] or [1].

THEOREM 3.4. *Let G_n be a random graph on n vertices in one of our models. For parameter values of (β_1, β_2) in the upper half-plane $\beta_2 > -\frac{2}{p(p-1)}$, the behavior of G_n in the large n limit is as follows:*

$$\min_{u \in U} \delta_\square(\tilde{G}_n, \tilde{u}) \to 0 \text{ in probability as } n \to \infty, \tag{23}$$

where U is the set of maximizers of (11).

PROOF. The assumptions of Theorems 4.2 or 6.1 in [1] are satisfied for parameter values $\beta_2 > -\frac{2}{p(p-1)}$. By Proposition 3.2, along the curve $(\beta_1, q(\beta_1))$, the maximization problem (11) is solved at two values u_1^* and u_2^*; whereas off this curve, it is solved at a unique value u^*. Thus in the large n limit, along the curve $(\beta_1, q(\beta_1))$, G_n behaves like an Erdős-Rényi graph $G(n, u)$ (u picked by some distribution from u_1^* and u_2^*); whereas off this curve, G_n is indistinguishable from the Erdős-Rényi graph $G(n, u^*)$. □

COROLLARY 3.5. *Fix any $\beta_2 > \beta_2^c$. Let H be an edge, so $t(H, G_n)$ is the edge density of G_n. Then there exists a continuous and decreasing function $q^{-1}(\beta_2)$ such that*

$$\lim_{n \to \infty} \mathbb{P}_n^{\beta_1, \beta_2}(t(H, G_n) > u_2) = 1 \text{ if } \beta_1 > q^{-1}(\beta_2) \tag{24}$$

and

$$\lim_{n \to \infty} \mathbb{P}_n^{\beta_1, \beta_2}(t(H, G_n) < u_1) = 1 \text{ if } \beta_1 < q^{-1}(\beta_2). \tag{25}$$

Here u_1 and u_2 are defined as in the proof of Proposition 3.2: $m(u_1) = m(u_2) = \beta_2$.

REMARK. *As $\beta_2 \to \infty$, $u_1 \to 0$ and $u_2 \to 1$ and the jump is noticeable even for relatively small values of β_2.*

PROOF. As $q(\beta_1)$ is a continuous and decreasing function of β_1, the inverse function $q^{-1}(\beta_2)$ exists and is also continuous and decreasing. We examine the effect of varying β_1 on the graph of $l'(u)$ (and hence on the global maximizers of $l(u)$). First note that varying β_1 does not change the shape of $l'(u)$. Inside the V-shaped region, there are three cases. Recall that $u_1^* < u_1 < \frac{p-1}{p} < u_2 < u_2^*$. For $\beta_1 = q^{-1}(\beta_2)$, positive and negative areas

bounded by $l'(u)$ equal each other, thus u_1^* and u_2^* are both global maximizers. For $\beta_1 < q^{-1}(\beta_2)$, the graph of $l'(u)$ shifts downward, negative area exceeds positive area, thus u_1^* is the global maximizer. For $\beta_1 > q^{-1}(\beta_2)$, the graph of $l'(u)$ shifts upward, positive area exceeds negative area, thus u_2^* is the global maximizer. Outside the V-shaped region, there are two cases. Below the lower bounding curve, $l'(u)$ has a unique local maximizer $u^* < u_1$. Above the upper bounding curve, $l'(u)$ has a unique local maximizer $u^* > u_2$. Our conclusion then follows from Theorem 3.4. □

THEOREM 3.6. *Assume that in one of our models H_2 is a p-star ($p \geq 2$). For all parameter values (β_1, β_2), the behavior of G_n in the large n limit is as follows:*

$$\min_{u \in U} \delta_\square(\tilde{G}_n, \tilde{u}) \to 0 \text{ in probability as } n \to \infty, \tag{26}$$

where U is the set of maximizers of (11).

PROOF. This follows from related results in [1]. We separate the parameter plane $\{(\beta_1, \beta_2)\}$ into upper and lower half-planes. The upper half-plane ($\beta_2 \geq 0$) satisfies the assumptions of Theorem 4.2, and the lower half-plane ($\beta_2 \leq 0$) satisfies the assumptions of Theorem 6.4. By similar reasoning as in Theorem 3.4, the rest of the proof follows. □

The following is a straightforward application of the standard analytic implicit function theorem, which can be found for instance in the text of Krantz and Parks [7], so we omit the proof.

PROPOSITION 3.7. *Off the end point (β_1^c, β_2^c), the local maximizer u^* for $l(u; \beta_1, \beta_2)$ (u_1^* and u_2^* if inside the V-shaped region) is an analytic function of the parameters β_1 and β_2.*

PROPOSITION 3.8. *Off the phase transition curve, $l(u^*) = \max l(u; \beta_1, \beta_2)$ ($l(u_1^*)$ or $l(u_2^*)$ if inside the V-shaped region) is an analytic function of the parameters β_1 and β_2.*

PROOF. It is clear that $l(u; \beta_1, \beta_2)$ is analytic for $u \in (0, 1)$, $\beta_1 \in (-\infty, \infty)$, and $\beta_2 \in (-\infty, \infty)$. Outside the V-shaped region, $l(u)$ has a unique local maximizer u^* in $(0, 1)$, which is analytic in β_1 and β_2 by Proposition 3.7. Inside the V-shaped region, $l(u)$ has two local maximizers u_1^* and u_2^*, both have values in $(0, 1)$ and are analytic in β_1 and β_2 by Proposition 3.7. Below the

phase transition curve, $\max l(u)$ is given by $l(u_1^*)$, which coincides with $l(u^*)$ along the lower bounding curve. Above the phase transition curve, $\max l(u)$ is given by $l(u_2^*)$, which coincides with $l(u^*)$ along the upper bounding curve. Our claim follows by realizing that compositions of analytic functions are analytic as long as the domains and ranges match up. □

THEOREM 3.9. *Let G_n be a random graph on n vertices in one of our models. The limiting free energy density $\psi_\infty = \lim_{n\to\infty} \psi_n$ is an analytic function of the parameters β_1 and β_2 off the phase transition curve in the upper half-plane $\beta_2 > -\frac{2}{p(p-1)}$.*

PROOF. The assumptions of Theorems 4.1 and 6.1 in [1] are satisfied for parameter values $\beta_2 > -\frac{2}{p(p-1)}$. Our claim then follows from Proposition 3.8. □

THEOREM 3.10. *Assume that in one of our models H_2 is a p-star ($p \geq 2$). The limiting free energy density $\psi_\infty = \lim_{n\to\infty} \psi_n$ is an analytic function of the parameters β_1 and β_2 off the phase transition curve.*

PROOF. The assumptions of Theorems 4.1 or 6.4 in [1] are satisfied. Our claim again follows from Proposition 3.8. □

LEMMA 3.11 (Lovász-Szegedy [8]). *Let $U, W : [0,1]^2 \to [0,1]$ be two symmetric integrable functions. Then for every finite simple graph F,*

$$|t(F,U) - t(F,W)| \leq |E(F)| \cdot \delta_\square(\tilde{U}, \tilde{W}). \tag{27}$$

Proof of Theorems 2.1 and 2.2. The stated analyticity is proven in Theorems 3.9 and 3.10, so we only need to examine the situation along the phase transition curve. We know from Theorems 3.4 and 3.6 that $\tilde{G}_n$ converges in probability to u^*, off the curve. By Lemma 3.11, $t(H_1, G_n)$ then converges in probability to $t(H_1, u^*)$. As $t(H_1, G_n)$ is uniformly bounded in n, this implies that

$$\mathbb{E}_{\beta_1,\beta_2}\{|t(H_1, G_n) - t(H_1, u^*)|\} \to 0 \text{ as } n \to \infty. \tag{28}$$

Therefore

$$\begin{aligned} \mathbb{E}_{\beta_1,\beta_2}\{t(H_1, G_n)\} &\to \mathbb{E}_{\beta_1,\beta_2}\{t(H_1, u^*)\} \\ &= u^*(\beta_1, \beta_2) = \frac{\partial}{\partial \beta_1}\psi_\infty(\beta_1, \beta_2) \text{ as } n \to \infty. \end{aligned} \tag{29}$$

Similarly,

$$\mathbb{E}_{\beta_1,\beta_2}\{t(H_2,G_n)\} \to \mathbb{E}_{\beta_1,\beta_2}\{t(H_2,u^*)\} \tag{30}$$
$$= (u^*(\beta_1,\beta_2))^p = \frac{\partial}{\partial\beta_2}\psi_\infty(\beta_1,\beta_2) \text{ as } n\to\infty.$$

By Corollary 3.5, these two first derivatives $\frac{\partial}{\partial\beta_1}\psi_\infty$ and $\frac{\partial}{\partial\beta_2}\psi_\infty$ are discontinuous across the curve (except at the end point). Let us now take a closer look at the behavior of ψ_∞ at the critical point. Recall that $l'(u;\beta_1^c,\beta_2^c)$ is monotonically decreasing on $[0,1]$, and the unique zero is achieved at $\frac{p-1}{p}$. Take any $0<\epsilon<\frac{1}{p}$. Set $\delta=\min\{l'(\frac{p-1}{p}-\epsilon),-l'(\frac{p-1}{p}+\epsilon)\}$. Consider (β_1,β_2) so close to (β_1^c,β_2^c) such that $|\beta_1-\beta_1^c|+p|\beta_2-\beta_2^c|<\delta$. For every u in $[0,1]$, we then have $|l'(u;\beta_1,\beta_2)-l'(u;\beta_1^c,\beta_2^c)|<\delta$. It follows that the zeros $u^*(\beta_1,\beta_2)$ (u_1^* and u_2^* if inside the V-shaped region) must satisfy $\left|u^*-\frac{p-1}{p}\right|<\epsilon$, which easily implies the continuity of $\frac{\partial}{\partial\beta_1}\psi_\infty$ and $\frac{\partial}{\partial\beta_2}\psi_\infty$ at (β_1^c,β_2^c). To see that the transition at the critical point is second-order, we check the second derivatives of ψ_∞ in its neighborhood. Off the phase transition curve,

$$\lim_{n\to\infty}\frac{\partial^2}{\partial\beta_1^2}\psi_n = \frac{\partial^2}{\partial\beta_1^2}\psi_\infty = \frac{\partial}{\partial\beta_1}u^* = -\frac{1}{l''(u^*)}, \tag{31}$$

$$\lim_{n\to\infty}\frac{\partial^2}{\partial\beta_1\partial\beta_2}\psi_n = \frac{\partial^2}{\partial\beta_1\partial\beta_2}\psi_\infty = \frac{\partial}{\partial\beta_1}(u^*)^p = -\frac{p(u^*)^{p-1}}{l''(u^*)}, \tag{32}$$

$$\lim_{n\to\infty}\frac{\partial^2}{\partial\beta_2^2}\psi_n = \frac{\partial^2}{\partial\beta_2^2}\psi_\infty = \frac{\partial}{\partial\beta_2}(u^*)^p = -\frac{(p(u^*)^{p-1})^2}{l''(u^*)}. \tag{33}$$

But as was explained in the proof of Proposition 3.2, $l''(u^*)$ converges to zero as (β_1,β_2) approaches (β_1^c,β_2^c); the desired singularity is thus justified. □

4. Summary. Much of the literature on phase transitions in exponential random graph models uses techniques, such as mean-field approximations, which are mathematically uncontrolled. As such they have been useful in discovering interesting behavior but they can be misleading in detail. For instance, although phase transitions have been discovered in this way for the two-star (H_2 a two-star) [10] and edge-triangle (H_2 a triangle) models [11], the approximation leads to an error in the qualitative nature of the transition, attributing phase coexistence to the full V-shaped region of Figure 1

rather than just the curve $\beta_2 = q(\beta_1)$; in other words it does not distinguish the local maxima in the region from the global maxima.

Chatterjee and Diaconis [1] gave the first rigorous proof of singular behavior in an exponential random graph model, the edge-triangle model. Our paper is an extension of this important first step; besides extending the models and parameters under control we have provided a mathematical framework of 'phases' which we hope will be useful in motivating future mathematical work in this subject. Our results show that all models with 'attraction' ($\beta_2 > 0$) exhibit a transition qualitatively like the gas/liquid transition: a first order transition corresponding to a discontinuity in density, with a second order criticial point. In Theorem 7.1 of [1] Chatterjee and Diaconis suggest that, quite generally, models with repulsion exhibit a transition qualitatively like the solid/fluid transition, in which one phase has nontrivial structure, as distinguished from the 'disordered' Erdős-Rényi graphs, which have independent edges. We have not yet been able to extend our results to this regime, except for p-star models with 'repulsion' ($\beta_2 < 0$) which we prove do not exhibit a transition. It is an important open problem to determine the qualitative behavior of models based on an H_2 with chromatic number above 2 .

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