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Spin models on random graphs with controlled topologies beyond degree constraints

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Abstract

We study Ising spin models on finitely connected random interaction graphs which are drawn from an ensemble in which not only the degree distribution p(k) can be chosen arbitrarily, but which allows for further fine tuning of the topology via preferential attachment of edges on the basis of an arbitrary function Q(k, k') of the degrees of the vertices involved. We solve these models using finite connectivity equilibrium replica theory, within the replica symmetric ansatz. In our ensemble of graphs, phase diagrams of the spin system are found to depend no longer only on the chosen degree distribution, but also on the choice made for Q(k, k'). The increased ability to control interaction topology in solvable models beyond prescribing only the degree distribution of the interaction graph enables a more accurate modeling of realworld interacting particle systems by spin systems on suitably defined random graphs.

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1. Introduction

The study of spin systems on finitely connected random graphs started nearly 30 years ago [1-5], but in the last decade has enjoyed renewed popularity as a result of many successful multi-disciplinary applications of the mathematical tools that it generates. The reason is clear: interacting particle systems in the real world do not have full connectivity, but generally involve an average number of interaction partners per unit that is indeed limited. Moreover, apart from carefully prepared pure samples of magnetic materials or crystalline solids, the graph that represents which elements interact with each other appears in most disciplines

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random in the first approximation, often with features that are remarkably universal across fields, such as a power-law distribution of node degrees. The mathematical techniques used to study such systems are consequently being refined and applied in areas as diverse as spinglass and glass modeling [6–11], error correcting codes [12–16], theoretical computer science [17–23], recurrent neural networks [24–26], 'small-world' networks [27–29], socio-economic modeling [30, 31] and CDMA communication [32–35]. Although the replica route is not the only method available for analyzing finitely connected spin systems, see, e.g. [36], it has the advantages of allowing for arbitrary bond distributions and more general graph statistics, and being fully systematic. Following a first wave of equilibrium studies, based on the finite connectivity replica method, we are now also beginning to acquire mathematical techniques with which to bring the dynamics of spin systems on finitely connected random graphs under control [37–44].

In modeling real-world systems of the above type one places the dynamical variables (e.g. spins) on the vertices of a graph, with edges connecting the variables that interact. The behavior of the model depends strongly on the choice made for the graph; however, this graph has to be drawn randomly to make analytical progress using disordered systems theory. So one tries to define a random graph ensemble with topological characteristics that are as close as possible to those observed in the system to be modeled, while keeping the model solvable. The state of the art in this respect is defining a random graph ensemble where edges are drawn subject to the constraint that all vertex degrees are prescribed. Here the only information on the topology of the system that is effectively carried over from the real world (apart from irrelevant site permutations) is the graph's degree distribution. Since for most degree distributions there is still a large and diverse set of compatible microscopic graph realizations, with possibly distinct macroscopic phenomenology for spin dynamics and statics, one would like to increase the amount of topological information embedded in the random graph ensemble, beyond prescribing just the degree distribution.

In this paper we present a simple class of Ising spin models on finitely connected random graphs, where these graphs are drawn from ensembles in which not only the degree distributions can be chosen arbitrarily and imposed as a constraint, but where in addition the edges are drawn in a way that allows for preferential attachment on the basis of an arbitrary function of the degrees of the two vertices concerned (similar in spirit to the so-called hidden variable ensembles [45–49]). The graphs thus generated are no longer characterized by their degree distribution alone, yet the associated spin models can still be solved in thermal equilibrium using conventional finite connectivity replica techniques. The graphs in the proposed ensemble remain effectively tree-like, and the clustering coefficients of randomly selected vertices are zero with probability one (as in the standard finite connectivity ensembles with prescribed degrees only). We solve our models with the replica symmetry (RS) ansatz, and show which features of the phase diagrams and the degree distribution, and which features depend more specifically on the extra topological information that is included.

2. Definitions

We study a finitely connected and bond-disordered system of N interacting Ising spins $\sigma_i \in \{-1, 1\}$, in thermal equilibrium characterized by the following Hamiltonian:

$$H(\boldsymbol{\sigma}) = -\sum_{i < j} c_{ij} \sigma_i J_{ij} \sigma_j \qquad \boldsymbol{\sigma} = (\sigma_1, \dots, \sigma_N).$$
(1)

The frozen variables $c_{ij} \in \{0, 1\}$ define the connectivity of the system; they define a random graph, with vertices labeled by $i, j \in \{1, ..., N\}$ and with $c_{ij} = 1$ if an only if i and j are connected by a link. We define $c_{ij} = c_{ji}$ and $c_{ii} = 0$ for all (i, j), and abbreviate $\mathbf{c} = \{c_{ij}\}$. The bonds $J_{ij} \in \mathbb{R}$ are drawn randomly and independently from some distribution P(J). To characterize the topology of a graph \mathbf{c} we define for each vertex i the degree $k_i(\mathbf{c}) = \sum_j c_{ij}$ (the number of links to this vertex), and the degree distribution $p(k|\mathbf{c}) = N^{-1} \sum_i \delta_{k,k_i(\mathbf{c})}$. Thus the average connectivity of a graph \mathbf{c} is $\langle k \rangle = \sum_{k \ge 0} kp(k|\mathbf{c})$, which we choose to be finite, even in the limit $N \to \infty$. We draw the graph \mathbf{c} randomly from an ensemble defined by a probability distribution Prob(\mathbf{c}) in which not only the degrees are constrained to take prescribed values $\{k_1, \ldots, k_N\}$, but where the link probabilities are modified further according to some function $Q(\cdot, \cdot)$ of the degrees of the two vertices involved

$$\operatorname{Prob}(\mathbf{c}) = \frac{1}{\mathcal{Z}_N} \prod_{i < j} \left[\frac{\langle k \rangle}{N} Q(k_i, k_j) \delta_{c_{ij}, 1} + \left(1 - \frac{\langle k \rangle}{N} Q(k_i, k_j) \right) \delta_{c_{ij}, 0} \right] \prod_i \delta_{k_i, k_i(\mathbf{c})}$$
(2)

$$\mathcal{Z}_{N} = \sum_{\mathbf{c}} \prod_{i < j} \left[\frac{\langle k \rangle}{N} Q(k_{i}, k_{j}) \delta_{c_{ij}, 1} + \left(1 - \frac{\langle k \rangle}{N} Q(k_{i}, k_{j}) \right) \delta_{c_{ij}, 0} \right] \prod_{i} \delta_{k_{i}, k_{i}(\mathbf{c})}.$$
(3)

The *N* degrees are, in turn, drawn randomly from a prescribed distribution p(k). Clearly we require $Q(k, k') \ge 0$ for all k, k'. In order to ensure furthermore that for large *N* such graphs can actually be found, we need to choose the function $Q(\cdot, \cdot)$ such that in formula (2) the partial measure $\prod_{i < j} [\cdots]$ is consistent with the average connectivity $\langle k \rangle = \sum_{k} kp(k)$ imposed by the constraining factor $\prod_{i} \delta_{k_i,k_i}(c)$. Upon defining Q(k, k') = Q(k', k), this is achieved when $\lim_{N \to \infty} N^{-2} \sum_{i \neq j} Q(k_i, k_j) = 1$, so the function $Q(\cdot, \cdot)$ is to be chosen subject to

$$Q(k,k') \ge 0 \quad \forall k,k' \qquad \text{and} \qquad \sum_{k,k'\ge 0} p(k)p(k')Q(k,k') = 1.$$
 (4)

In the appendix we list and derive several properties of the random graph ensemble (2), and show that Q(k, k') represents the probability that two randomly drawn vertices with degrees k and k' will be connected, divided by the overall probability for two randomly drawn links to be connected (irrespective of their degrees).

Given the above definitions, our objective is to calculate for the system (1) the asymptotic disorder-averaged free energy per spin \overline{f} , in order to find the phase diagrams for spin systems defined on typical graphs in the ensemble (2):

$$\overline{f} = -\lim_{N \to \infty} \frac{1}{\beta N} \overline{\log \sum_{\sigma} e^{-\beta H(\sigma)}} = -\lim_{N \to \infty} \lim_{n \to 0} \frac{1}{\beta n N} \log \left[\sum_{\sigma} e^{-\beta H(\sigma)} \right]^n$$
(5)

in which $\overline{\cdots}$ denotes averaging over the disorder in the problem, namely the randomly drawn graph **c** with statistics (2) and the random bonds $\{J_{ij}\}$. This calculation is done with the finite connectivity replica method, within the replica symmetric (RS) ansatz. We will be particularly interested in the dependence of the phase diagrams on the choice made for $Q(\cdot, \cdot)$. In the absence of the degree constraints, the function $Q(\cdot, \cdot)$ would have controlled the bond probabilities fully, via $\langle c_{ij} \rangle = Q(k_i, k_j) \langle k \rangle / N$. Here, in contrast, its role is to *deform* the measure imposed by the degree constraints, biasing the probabilities in those cases where there exist multiple graphs with the same degree distribution.

A relevant question to be asked at the beginning is whether the ensemble deformation induced by Q(k, k') can have sufficient impact in the thermodynamic limit on macroscopic observables to justify the present calculation. For instance, upon calculating for the ensemble (2) the joint distribution of degrees and clustering coefficients for $N \to \infty$ one finds that, like ensembles with degree constraints only, the clustering coefficients are zero with probability one, see appendix A.2. However, upon reflection it becomes clear that the proposed ensemble deformation will generally affect the system's phase diagram. A quick way to see this is to compare the two choices Q(k, k') = 1 and $Q(k, k') = \delta_{kk'} / \sum_{k''} p^2(k'')$. In the first case we return to the degree-constrained ensemble in [26]. In the second case our ensemble describes graphs that are each composed of disconnected regular sub-graphs, of sizes p(k)Nfor each k with p(k) > 0. The transitions away from the paramagnetic state will now be those corresponding to the sub-graph with the largest degree allowed by p(k); these will only coincide with those of Q(k, k') = 1 when $p(k) = \delta_{k,c}$, i.e. when the degree distribution itself is that of a regular graph.

3. Equilibrium replica analysis

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3.1. Derivation of saddle-point equations

As usual, we calculate (5) upon writing the Kronecker δs of the degree constraints in integral form, using $\delta_{nm} = (2\pi)^{-1} \int_{-\pi}^{\pi} d\omega e^{i\omega(n-m)}$. This gives, after some rearranging of summations, factorization over the disorder variables. We define the short-hands $\sigma_i = (\sigma_i^1, \ldots, \sigma_i^n)$, so that

$$\overline{f} = \lim_{N \to \infty} \lim_{n \to 0} \frac{1}{\beta n N} \left\{ \log \mathcal{Z}_N - \log \sum_{\sigma_1 \dots \sigma_N} \int_{-\pi}^{\pi} \prod_i \left[\frac{\mathrm{d}\omega_i}{2\pi} e^{\mathrm{i}\omega_i k_i} \right] \right. \\ \left. \times \prod_{i < j} \left(1 + \frac{\langle k \rangle}{N} \mathcal{Q}(k_i, k_j) \left[\int \mathrm{d}J P(J) e^{\beta J \sigma_i \cdot \sigma_j - \mathrm{i}(\omega_i + \omega_j)} - 1 \right] \right) \right\} \\ = \lim_{N \to \infty} \lim_{n \to 0} \frac{1}{\beta n N} \left\{ \log \mathcal{Z}_N - \log \sum_{\sigma_1 \dots \sigma_N} \int_{-\pi}^{\pi} \prod_i \left[\frac{\mathrm{d}\omega_i}{2\pi} e^{\mathrm{i}\omega_i k_i} \right] \right. \\ \left. \times \exp \left[\frac{\langle k \rangle}{2N} \sum_{ij} \mathcal{Q}(k_i, k_j) \left[\int \mathrm{d}J P(J) e^{\beta J \sigma_i \cdot \sigma_j - \mathrm{i}(\omega_i + \omega_j)} - 1 \right] + \mathcal{O}(N^0) \right] \right\}.$$
(6)

We proceed toward a steepest descent integration by introducing for $\sigma \in \{-1, 1\}^n$ and $k \in \{0, 1, 2, ...\}$ the functions $D(k, \sigma | \{\sigma_i, \omega_i\}) = N^{-1} \sum_i \delta_{k,k_i} \delta_{\sigma,\sigma_i} e^{-i\omega_i}$. They are introduced via the substitution of integrals over appropriate δ -distributions, written in integral form, namely

$$1 = \int \frac{\mathrm{d}D(k,\sigma)\,\mathrm{d}\hat{D}(k,\sigma)}{2\pi/N}\,\mathrm{e}^{\mathrm{i}N\hat{D}(k,\sigma)[D(k,\sigma)-D(k,\sigma|\{\sigma_i,\omega_i\})]}.\tag{7}$$

Upon using also $N^{-1} \sum_{ij} Q(k_i, k_j) = N + \mathcal{O}(\sqrt{N})$ due to (4), and the short hand $\{dD \, d\hat{D}\} = \prod_{k,\sigma} D(k,\sigma) \, d\hat{D}(k,\sigma)$ we then obtain

$$\overline{f} = \lim_{N \to \infty} \lim_{n \to 0} \frac{1}{\beta n N} \left\{ \log \mathcal{Z}_N - \log \int \{ \mathrm{d}D \, \mathrm{d}\hat{D} \} e^{\mathrm{i}N \sum_{k\sigma} \hat{D}(k,\sigma) D(k,\sigma) - \frac{1}{2}N\langle k \rangle + \mathcal{O}(N^{1/2})} \\ \times \exp\left[\frac{1}{2} \langle k \rangle N \sum_{kk'} Q(k,k') \sum_{\sigma\sigma'} D(k,\sigma) D(k',\sigma') \int \mathrm{d}J P(J) e^{\beta J \sigma \cdot \sigma'} \right] \\ \times \exp\left[N \sum_k p(k) \log \sum_{\sigma} \int_{-\pi}^{\pi} \frac{\mathrm{d}\omega}{2\pi} e^{\mathrm{i}\omega k - \mathrm{i}\hat{D}(k,\sigma) e^{-\mathrm{i}\omega}} \right] \right\}.$$
(8)

We next define $z = \lim_{N \to \infty} N^{-1} \log \mathcal{Z}_N$ (anticipating this limit to exist), which allows us to evaluate \overline{f} by steepest descent and write

$$\overline{f} = \lim_{n \to 0} \frac{1}{n} \operatorname{extr}_{\{D, \hat{D}\}} f_n[\{D, \hat{D}\}]$$

$$f_n[\{D, \hat{D}\}] = -\frac{1}{\beta} \left\{ i \sum_{k\sigma} \hat{D}(k, \sigma) D(k, \sigma) - \frac{1}{2} \langle k \rangle - z + \frac{1}{2} \langle k \rangle \sum_{kk'} Q(k, k') \sum_{\sigma\sigma'} D(k, \sigma) D(k', \sigma') \int dJ P(J) e^{\beta J \sigma \cdot \sigma'} + \sum_{k} p(k) \log \sum_{\sigma} \int_{-\pi}^{\pi} \frac{d\omega}{2\pi} e^{i\omega k - i\hat{D}(k, \sigma)} e^{-i\omega} \right\}.$$

$$(10)$$

The extremization in (9) with respect to $\{D, \hat{D}\}$ gives the following saddle-point equations:

$$\hat{D}(k,\sigma) = i\langle k \rangle \sum_{k'} Q(k,k') \sum_{\sigma'} D(k',\sigma') \int dJ P(J) e^{\beta J \sigma \cdot \sigma'}$$
(11)

$$D(k, \sigma) = \frac{p(k) \int_{-\pi}^{\pi} d\omega \, \mathrm{e}^{\mathrm{i}\omega(k-1)-\mathrm{i}\hat{D}(k,\sigma) \, \mathrm{e}^{-\mathrm{i}\omega}}}{\sum_{\sigma'} \int_{-\pi}^{\pi} d\omega \, \mathrm{e}^{\mathrm{i}\omega k-\mathrm{i}\hat{D}(k,\sigma') \, \mathrm{e}^{-\mathrm{i}\omega}}}.$$
(12)

The second of these equations can be simplified using the identity

$$\int_{-\pi}^{\pi} d\omega \, \mathrm{e}^{\mathrm{i}\omega\ell - \mathrm{i}\hat{D}(k,\sigma)\,\mathrm{e}^{-\mathrm{i}\omega}} = \begin{cases} 2\pi [-\mathrm{i}\hat{D}(k,\sigma)]^{\ell}/\ell! & \text{if } \ell \ge 0\\ 0 & \text{if } \ell < 0. \end{cases}$$
(13)

So, if we also re-define $\hat{D}(k, \sigma) = i\langle k \rangle F(k, \sigma)$, we arrive at

$$F(k,\sigma) = \sum_{k'} Q(k,k') \sum_{\sigma'} D(k',\sigma') \int dJ P(J) e^{\beta J \sigma \cdot \sigma'}$$
(14)

$$D(k, \sigma) = \frac{p(k)k}{\langle k \rangle} \frac{F^{k-1}(k, \sigma)}{\sum_{\sigma'} F^k(k, \sigma')}.$$
(15)

3.2. Simplified expression for free energy per spin

Formula (9) for the disorder-averaged free energy per spin, which is to be evaluated at the relevant solution of the saddle-point equations (14) and (15), still contains the term $z = \lim_{N\to\infty} N^{-1} \log Z_N$, which measures the effective number of graphs in our ensemble (2). Since z is independent of β we can use the identity $\lim_{\beta\to 0} (\beta \overline{f}) = -\log 2$ to find it. With (13), (14) and (15) we first write (9) as

$$\overline{f} = \lim_{n \to 0} \frac{1}{\beta n} \left\{ z + \langle k \rangle - \langle k \rangle \log \langle k \rangle - \sum_{k} p(k) \log \left[\frac{1}{k!} \sum_{\sigma} F^{k}(k, \sigma) \right] \right\}$$
(16)

(with *D* and *F* taken at the relevant saddle point). Working out the saddle-point equations for $\beta \to 0$ shows that there the two-order parameter functions $\{D, F\}$ become independent of σ , namely $D(k, \sigma) = 2^{-n}D(k)$ and $F(k, \sigma) = F(k)$, where the latter obey

$$F(k) = \sum_{k'} \frac{p(k')k'}{\langle k \rangle} Q(k,k') F^{-1}(k'), \qquad D(k) = \frac{p(k)k}{\langle k \rangle} F^{-1}(k).$$
(17)

Insertion into the equation $\lim_{\beta\to 0} (\beta \overline{f}) = -\log 2$, together with (16), then leads us after some further simple manipulations to the following formula, where F(k) is the solution of (17):

$$z = \langle k \rangle \log \langle k \rangle - \langle k \rangle + \sum_{k} p(k) \log \left[\frac{1}{k!} F^{k}(k) \right]$$
(18)

and hence

$$\overline{f} = -\lim_{n \to 0} \frac{1}{\beta n} \sum_{k} p(k) \log \left[\sum_{\sigma} [F(k, \sigma) / F(k)]^{k} \right].$$
(19)

We note that for the non-deformed graph ensemble with degree constraints and finite connectivity statistics only, namely Q(k, k') = 1 for all (k, k'), the solution of (17) would be F(k) = 1 and $D(k) = p(k)k/\langle k \rangle$. If we now define $\pi(k) = e^{-\langle k \rangle} \langle k \rangle^k / k!$, i.e. Poissonnian degree probabilities with average degree $\langle k \rangle$, we see that

$$z = z_{\rm nd} + \sum_{k} p(k)k\log F(k)$$
⁽²⁰⁾

$$z_{\rm nd} = \sum_{k} p(k) \log \pi(k) = -H_p - D(p \| \pi)$$
(21)

with the entropy $H_p = -\sum_k p(k) \log p(k) \ge 0$ of the degree distribution and the Kullback– Leibler distance $D(p||\pi) = \sum_k p(k) \log[p(k)/\pi(k)] \ge 0$ between the actual degree distribution p(k) and the Poissonnian $\pi(k)$. Since *z* measures the effective number of graphs that can be generated from our ensemble, and z_{nd} is its value in the absence of deformation, it follows from (20) that we can define a simple measure Σ_{def} of the graph specificity increase resulting from the introduction of the deformation defined by a function Q(k, k') as follows:

$$\Sigma_{\text{def}} = -\sum_{k} p(k)k \log F(k).$$
⁽²²⁾

3.3. Replica symmetric theory

To take the required limit $n \to 0$ in our formulae we make the ergodic or replica-symmetric (RS) ansatz. The replica order parameter $D(k, \sigma)$ must now be invariant under all replica permutations, and therefore have the following form, with $\int dh D(k, h) = \sum_{\sigma} D(k, \sigma)$:

$$D(k, \sigma) = \int dh D(k, h) \frac{e^{\beta h \sum_{\alpha} \sigma_{\alpha}}}{[2 \cosh(\beta h)]^n}.$$
(23)

We work out the implication of this ansatz for the order parameter $F(k, \sigma)$, using the identity $f(\sigma) = e^{A\sigma}B$, with $A = \frac{1}{2}\log[f(1)/f(-1)]$ and $B = \sqrt{f(1)f(-1)}$ (which holds for $\sigma = \pm 1$), as well as the identity $\frac{1}{2}\log[\cosh(x+y)/\cosh(x-y)] = \operatorname{atanh}[\tanh(x)\tanh(y)]$. This results in

$$F(k, \sigma) = \sum_{k'} Q(k, k') \int dh' dJ D(k', h') P(J) \prod_{\alpha} \frac{\cosh(\beta[J\sigma_{\alpha} + h'])}{\cosh(\beta h')}$$

=
$$\sum_{k'} Q(k, k') \int dh' dJ D(k', h') P(J) G_n(h', J) e^{\frac{1}{2}(\sum_{\alpha} \sigma_{\alpha}) \log[\cosh(\beta[J+h'])/\cosh(\beta[J-h'])]}$$

=
$$\int dh F(k, h) e^{\beta h \sum_{\alpha} \sigma_{\alpha}}$$
(24)

with

$$G_n(h, J) = [\cosh(\beta[h+J])\cosh(\beta[h-J])/\cosh^2(\beta h)]^{n/2}$$
(25)

$$F(k,h) = \sum_{k'} Q(k,k') \int dh' dJ D(k',h') P(J) G_n(h',J)$$

$$\times \delta [h - \beta^{-1} \operatorname{atanh}[\operatorname{tanh}(\beta J) \operatorname{tanh}(\beta h')]].$$
(26)

We will now have two new saddle-point equations, written in terms of the RS kernels F and D. The first equation is (26). The second follows upon inserting (23) and (24) into (15)

$$\int dh D(k,h) \frac{e^{\beta h \sum_{\alpha} \sigma_{\alpha}}}{[2\cosh(\beta h)]^{n}} = \frac{p(k)k}{\langle k \rangle} \frac{\int \prod_{\ell \leqslant k-1} [dh_{\ell} F(k,h_{\ell})] e^{\beta \sum_{\alpha} \sigma_{\alpha} \sum_{\ell \leqslant k-1} h_{\ell}}}{\int \prod_{\ell \leqslant k} [dh_{\ell} F(k,h_{\ell})] [2\cosh(\beta \sum_{\ell \leqslant k} h_{\ell})]^{n}}$$
$$= \frac{p(k)k}{\langle k \rangle} \int dh e^{\beta h \sum_{\alpha} \sigma_{\alpha}}$$
$$\times \frac{\int \prod_{\ell \leqslant k-1} [dh_{\ell} F(k,h_{\ell})] \delta[h - \sum_{\ell \leqslant k-1} h_{\ell}]}{\int \prod_{\ell \leqslant k} [dh_{\ell} F(k,h_{\ell})] [2\cosh(\beta \sum_{\ell \leqslant k} h_{\ell})]^{n}}.$$
(27)

From this result we can read off the second-order parameter equation. Upon taking the limit $n \rightarrow 0$ in the latter result and our first equation (26), we arrive at the transparent expressions

$$F(k,h) = \sum_{k'} Q(k,k') \int dh' \, dJ D(k',h') P(J) \delta\left[h - \frac{1}{\beta} \operatorname{atanh}[\tanh(\beta J) \tanh(\beta h')]\right]$$
(28)

$$D(k,h) = \frac{p(k)k}{\langle k \rangle} \frac{\int \prod_{\ell \leqslant k-1} [dh_{\ell} F(k,h_{\ell})] \delta[h - \sum_{\ell \leqslant k-1} h_{\ell}]}{\left[\int dh' F(k,h')\right]^{k}}.$$
(29)

Upon defining finally $D(k) = \int dh D(k, h)$ and $F(k) = \int dh F(k, h)$, we discover that these last two integrals are exactly the quantities in (17), since upon integrating over h in both equations (28) and (29) they reduce precisely to (17). This does not seem to be a trivial result, since (17) was derived from the properties of the random graph ensemble alone. Given these relations one is prompted automatically to define D(k, h) = D(h|k)D(k) and F(k, h) = F(h|k)F(k), where now $\int dh D(h|k) = \int dh F(h|k) = 1$. Our RS order parameter equations thereby take the form

$$F(h|k) = \sum_{k'} \frac{Q(k,k')p(k')k'}{\langle k \rangle F(k)F(k')} \int dh' dJ D(h'|k')P(J) \\ \times \delta \left[h - \frac{1}{\beta} \operatorname{atanh}[\operatorname{tanh}(\beta J) \operatorname{tanh}(\beta h')] \right]$$
(30)

$$D(h|k) = \int \prod_{\ell < k} [dh_{\ell} F(h_{\ell}|k)] \delta \left[h - \sum_{\ell < k} h_{\ell} \right]$$
(31)

$$F(k) = \langle k \rangle^{-1} \sum_{k'} p(k')k'Q(k,k')F^{-1}(k'),$$
(32)

where D(k) subsequently follows from the second identity in (17), and where (32) automatically ensures that the solutions of (30) and (31) are normalized. If we write the free energy (19) for our present RS solution in terms of the quantities in (30), (31) and (32)

and take the limit $n \to 0$, using relations such as $\sum_k D(k)F(k) = 1$, we find in a similar manner the remarkably simple result

$$\overline{f}_{\rm RS} = -\frac{1}{\beta} \log 2 - \frac{1}{\beta} \sum_{k} p(k) \int \prod_{\ell \leqslant k} [dh_\ell F(h_\ell | k)] \log \cosh\left(\beta \sum_{\ell \leqslant k} h_\ell\right).$$
(33)

3.4. Physical observables

To find formulae for observables like $m = \lim_{N \to \infty} N^{-1} \sum_{i} \overline{\langle \sigma_i \rangle}$ and $q = \lim_{N \to \infty} N^{-1} \sum_{i} \overline{\langle \sigma_i \rangle^2}$, it will be convenient to calculate for an *n*-replica system where $\sigma_i = (\sigma_i^1, \ldots, \sigma_i^n)$, i.e. before the limit $n \to 0$, the expectation value $P(k, \sigma) = \lim_{N \to \infty} N^{-1} \sum_{i} \overline{\langle \delta_{k,k_i} \delta_{\sigma,\sigma_i} \rangle}$. We can calculate $P(k, \sigma)$ using steps similar to those taken in the evaluation of the free energy, using (10)

$$P(k, \sigma) = \lim_{N \to \infty} N^{-1} \sum_{i} \left[\frac{\sum_{\sigma_{1}...\sigma_{N}} \delta_{k,k_{i}} \delta_{\sigma,\sigma_{i}} e^{-\beta \sum_{\alpha} H(\sigma^{\alpha})}}{\sum_{\sigma_{1}...\sigma_{N}} e^{-\beta \sum_{\alpha} H(\sigma^{\alpha})}} \right]$$
$$= \lim_{n' \to -n} \lim_{N \to \infty} \frac{1}{N} \sum_{i} \delta_{k,k_{i}} \overline{\sum_{\sigma^{1}...\sigma^{n+n'}} \delta_{(\sigma_{1}...,\sigma_{n}),(\sigma_{i}^{1}...,\sigma_{i}^{n})} e^{-\beta \sum_{\alpha=1}^{n+n'} H(\sigma^{\alpha})}}$$
$$= \lim_{n' \to -n} \lim_{N \to \infty} \frac{1}{N} \sum_{i} \delta_{k,k_{i}} \int \{dD \ d\hat{D}\} e^{-\beta N f_{n+n'}[\{D,\hat{D}\}]}$$
$$\times \left[\frac{\sum_{\sigma_{n+1},...,\sigma_{n+n'}} \int d\omega \ e^{i\omega k - i\hat{D}(k,\sigma_{1},...,\sigma_{n+n'}) \ e^{-i\omega}}}{\sum_{\sigma_{1}',...\sigma_{n+n'}'} \int d\omega \ e^{i\omega k - i\hat{D}(k,\sigma_{1}'...,\sigma_{n+n'}') \ e^{-i\omega}}} \right]$$
$$= \lim_{n' \to -n} p(k) \left[\frac{\sum_{\sigma_{n+1},...,\sigma_{n+n'}} \int d\omega \ e^{i\omega k + \langle k \rangle F(k,\sigma_{1},...,\sigma_{n+n'}) \ e^{-i\omega}}}{\sum_{\sigma_{1}',...\sigma_{n+n'}'} \int d\omega \ e^{i\omega k + \langle k \rangle F(k,\sigma_{1}'...,\sigma_{n+n'}') \ e^{-i\omega}}} \right],$$
(34)

where in the last line we now have to take $F(k, \sigma_1, \ldots, \sigma_{n+n'})$ at the saddle point of $f_{n+n'}[\cdots]$, with $\hat{D}[\cdots] = i\langle k \rangle F[\cdots]$, and where we have used $\lim_{n\to 0} \operatorname{extr}_{\{D,\hat{D}\}} f_n[\{D, \hat{D}\}] = 0$. Once more we can carry out the ω -integrations and find

$$P(k, \sigma) = \lim_{n' \to -n} p(k) \left[\frac{\sum_{\sigma_{n+1}, \dots, \sigma_{n+n'}} F^k(k, \sigma_1, \dots, \sigma_{n+n'})}{\sum_{\sigma'_1, \dots, \sigma'_{n+n'}} F^k(k, \sigma'_1, \dots, \sigma'_{n+n'})} \right].$$
 (35)

In replica symmetric states, where $F(k, \sigma) = \int dh F(k) F(h|k) e^{\beta h \sum_{\alpha} \sigma_{\alpha}}$, we can carry out the remaining spin summations, giving

$$P_{\text{RS}}(k,\sigma) = \lim_{n' \to -n} p(k) \left[\frac{\int \prod_{\ell \leqslant k} [dh_{\ell} F(h_{\ell}|k)] [2 \cosh\left(\beta \sum_{\ell \leqslant k} h_{\ell}\right)]^{n'} e^{\beta(\sum_{\ell \leqslant k} h_{\ell})(\sum_{\alpha \leqslant n} \sigma_{\alpha})}}{\int \prod_{\ell \leqslant k} [dh_{\ell} F(h_{\ell}|k)] [2 \cosh\left(\beta \sum_{\ell \leqslant k} h_{\ell}\right)]^{n+n'}} \right]$$
$$= p(k) \int \prod_{\ell \leqslant k} [dh_{\ell} F(h_{\ell}|k)] \frac{e^{\beta(\sum_{\ell \leqslant k} h_{\ell})(\sum_{\alpha \leqslant n} \sigma_{\alpha})}}{[2 \cosh\left(\beta \sum_{\ell \leqslant k} h_{\ell}\right)]^{n}}$$
$$= p(k) \int dh W(h|k) \frac{e^{\beta h \sum_{\alpha \leqslant n} \sigma_{\alpha}}}{[2 \cosh(\beta h)]^{n}}$$
(36)

with the degree-conditioned effective field distribution

$$W(h|k) = \int \prod_{\ell \leqslant k} [\mathrm{d}h_{\ell} F(h_{\ell}|k)] \delta \bigg[h - \sum_{\ell \leqslant k} h_{\ell} \bigg].$$
(37)

The order parameters m and q can now be written in their usual form

$$m = \int dh W(h) \tanh(\beta h), \qquad q = \int dh W(h) \tanh^2(\beta h)$$
(38)

$$W(h) = \sum_{k} p(k)W(h|k)$$
(39)

and the free energy formula (33) becomes simply

$$\overline{f}_{\rm RS} = -\frac{1}{\beta} \log 2 - \frac{1}{\beta} \int dh W(h) \log \cosh(\beta h).$$
(40)

3.5. Simple solutions for special cases

The simplest limit is $\beta \to 0$, where we expect a paramagnetic state. Setting $\beta = 0$ in our order parameter equations (30), (31) and (32) indeed gives $F(h|k) = D(h|k) = \delta(h)$, and $\lim_{\beta\to 0} (\beta \overline{f}) = -\log 2$ as well as m = q = 0. As always in such systems one notes that $F(h|k) = D(h|k) = \delta(h)$ is in fact always a solution of (30), (31) and (32), at any temperature.

A less trivial special case is the choice Q(k, k') = 1 for all (k, k') (non-deformed graph ensemble), where we should be able to connect the present theory to earlier results in the literature. Here one has F(k) = 1 and $D(k) = p(k)k/\langle k \rangle$, and F(h|k) is no longer dependent on k. We may thus simply write F(h|k) = F(h) (not to be confused with F(k)), so that upon eliminating D(h|k) from (30) via (31), we are left with the order parameter equation

$$F(h) = \sum_{k} \frac{p(k)k}{\langle k \rangle} \int dJ P(J) \int \prod_{\ell < k} [dh_{\ell} F(h_{\ell})] \\ \times \delta \left[h - \frac{1}{\beta} \operatorname{atanh} \left[\tanh(\beta J) \tanh\left(\beta \sum_{\ell < k} h_{\ell}\right) \right] \right].$$
(41)

To establish the connection with earlier results for the Ising system on graphs taken from the non-deformed ensemble we define a new field distribution $\tilde{W}(h)$

$$\tilde{W}(h) = \sum_{k} \frac{p(k)k}{\langle k \rangle} \int \prod_{\ell < k} [\mathrm{d}h_{\ell} F(h_{\ell})] \delta \bigg[h - \sum_{\ell < k} h_{\ell} \bigg].$$
(42)

According to (37), the latter cavity field distribution $\tilde{W}(h)$ is expressed in terms of the degreeconditioned effective field distributions W(h|k) via $\tilde{W}(h) = \sum_{k} p(k)k\langle k \rangle^{-1}W(h|k-1)$. Equation (41) now tells us that

$$F(h) = \int dJ \, dh' P(J) \tilde{W}(h') \delta\left[h - \frac{1}{\beta} \operatorname{atanh}[\tanh(\beta J) \tanh(\beta h')]\right]$$
(43)

and hence we find the following RS order parameter equation in terms of $\tilde{W}(h)$, which we recognize from earlier studies on Ising systems with random graph ensembles that are given prescribed degree distributions

$$\tilde{W}(h) = \sum_{k} \frac{p(k)k}{\langle k \rangle} \int \prod_{\ell < k} [\mathrm{d}J_{\ell} \mathrm{d}h_{\ell} P(J_{\ell}) \tilde{W}(h_{\ell})] \delta \left[h - \frac{1}{\beta} \sum_{\ell < k} \mathrm{atanh}[\mathrm{tanh}(\beta J_{\ell}) \mathrm{tanh}(\beta h_{\ell})] \right].$$
(44)

Similarly we can write the free energy (33) for non-deformed ensembles in terms of $\tilde{W}(h)$

$$\overline{f}_{RS} = -\frac{1}{\beta} \log 2 - \frac{1}{\beta} \sum_{k} p(k) \int \prod_{\ell \leqslant k} [dh_{\ell} dJ_{\ell} P(J_{\ell}) \tilde{W}(h_{\ell})] \\ \times \log \cosh \left(\sum_{\ell \leqslant k} \operatorname{atanh}[\tanh(\beta J_{\ell}) \tanh(\beta h_{\ell})] \right).$$
(45)

We should emphasize that the two field distributions $W(h) = \sum_{k} p(k)W(h|k)$ and $\tilde{W}(h) = \sum_{k} p(k+1)(k+1)\langle k \rangle^{-1}W(h|k)$ are generally different. The obvious exceptions are Poissonnian degree distributions, where $p(k+1)(k+1)\langle k \rangle^{-1} = p(k)$, and systems where W(h|k) does not vary with the degree k.

4. Continuous phase transitions

4.1. Bifurcations away from the paramagnetic state

Continuous bifurcations away from the paramagnetic (P) state $F(h|k) = \delta(h)$ are found in the usual manner, by expansion in moments of F(h|k). We assume the existence of a small parameter ϵ with $0 < |\epsilon| \ll 1$ such that $\int dh h^{\ell} F(h|k) = \mathcal{O}(\epsilon^{\ell})$. Let us first define $\epsilon_k = \int dh h F(h|k)$. Multiplication of (30) and (31) by *h*, followed by integration over *h* gives the lowest nontrivial order

$$\epsilon_{k} = \frac{1}{\beta} \sum_{k'} \frac{Q(k, k') p(k')k'}{\langle k \rangle F(k) F(k')} \int dJ P(J) \int \prod_{\ell < k'} [dh_{\ell} F(h_{\ell} | k')] \\ \times \operatorname{atanh} \left[\operatorname{tanh}(\beta J) \operatorname{tanh} \left(\beta \sum_{\ell < k'} h_{\ell} \right) \right] \\ = \int dJ P(J) \operatorname{tanh}(\beta J) \sum_{k'} \frac{Q(k, k') p(k')k'(k'-1)}{\langle k \rangle F(k) F(k')} \epsilon_{k'} + \mathcal{O}(\epsilon^{2}).$$
(46)

Thus a continuous transition to a ferromagnetic (F) state occurs when the matrix with entries $M_{kk'} \int dJ P(J) \tanh(\beta J)$ has an eigenvalue one, where $k, k' \in \{0, 1, 2, ...\}$ and where

$$M_{kk'} = \frac{Q(k,k')p(k')k'(k'-1)}{\langle k \rangle F(k)F(k')}.$$
(47)

In a ferromagnetic state one will have a nonzero magnetization $m = \beta \sum_{k} p(k)k\epsilon_{k} + \mathcal{O}(\epsilon^{2})$. Similarly we can check what happens if $\int dh h F(h|k) = 0$ for all k, so m = 0, and the first nontrivial order to bifurcate is ϵ^{2} . This corresponds to a transition from a paramagnetic to a spin-glass (SG) state. Now we define $\epsilon_{k} = \int dh h^{2} F(h|k) = \mathcal{O}(\epsilon^{2})$. Multiplication of (30) and (31) by h^{2} , followed by integration over h now gives

$$\epsilon_{k} = \int dJ P(J) \tanh^{2}(\beta J) \sum_{k'} \frac{Q(k, k') p(k')k'}{\langle k \rangle F(k) F(k')} \int \prod_{\ell < k'} [dh_{\ell} F(h_{\ell}|k')] \sum_{\ell, \ell' < k'} h_{\ell} h_{\ell'} + \mathcal{O}(\epsilon^{3})$$
$$= \int dJ P(J) \tanh^{2}(\beta J) \sum_{k'} \frac{Q(k, k') p(k')k'(k'-1)}{\langle k \rangle F(k) F(k')} \epsilon_{k'} + \mathcal{O}(\epsilon^{3})$$
(48)

(where we have used $\int dh h F(h|k) = 0$ to eliminate terms with $\ell \neq \ell'$). Thus a continuous transition to a spin-glass (SG) state occurs when the matrix with entries $M_{kk'} \int dJ P(J) \tanh^2(\beta J)$ has an eigenvalue one. The previous $P \rightarrow F$ transitions mark bifurcations away from (m, q) = (0, 0) to states with $(m \neq 0, q \neq 0)$, and the $P \rightarrow SG$ transitions mark bifurcations away from (m, q) = (0, 0) to states with $(m = 0, q \neq 0)$

$$P \to F$$
: $\sum_{k'} M_{kk'} \epsilon_{k'} = \Lambda_F \epsilon_k \qquad \Lambda_F^{-1} = \int dJ P(J) \tanh(\beta J)$ (49)

$$P \to SG: \sum_{k'} M_{kk'} \epsilon_{k'} = \Lambda_{SG} \epsilon_k \qquad \Lambda_{SG}^{-1} = \int dJ P(J) \tanh^2(\beta J)$$
 (50)

with the matrix elements $M_{kk'}$ as given in (47) and with F(k) to be solved from (32)

$$F(k) = \langle k \rangle^{-1} \sum_{k'} p(k')k'Q(k,k')F^{-1}(k').$$
(51)

The physical transition occurs at the largest eigenvalue of the matrix *M*. It will be of the type $P \rightarrow F$ if $\int dJ P(J) \tanh(\beta J) > \int dJ P(J) \tanh^2(\beta J)$, and otherwise it will be $P \rightarrow SG$. If for the bond distribution we choose the binary form $P(J) = \frac{1}{2}(1+\eta)\delta(J-J_0) + \frac{1}{2}(1-\eta)\delta(J+J_0)$, we can already deduce that the triple point (where the phases P, F and SG come together) is found along the line $\eta = \tanh(\beta J_0)$, with the $P \rightarrow F$ transition being the physical one for $\eta > \tanh(\beta J_0)$ and $P \rightarrow SG$ transition being the physical one for $\eta < \tanh(\beta J_0)$. This will be true irrespective of the choice made for the ensemble deformation function Q(k, k').

4.2. Analysis of the eigenvalue problems

We will now analyze the bifurcation eigenvalue problem for the matrix (47), to be solved in conjunction with (51), for a number of graph ensembles, which in this paper are characterized by an ensemble deformation function Q(k, k') and a degree distribution p(k). The deformation function must always obey $Q(k, k') \ge 0$, Q(k, k') = Q(k', k) and $\sum_{kk'} p(k)p(k')Q(k, k') = 1$. Upon writing the largest eigenvalue of the matrix (47) as $\lambda_{\max}(Q, p)$, the continuous bifurcations away from the paramagnetic state occur for

$$P \to F: \quad 1 = \lambda_{\max}(Q, p) \int dJ P(J) \tanh(\beta J)$$
 (52)

$$P \rightarrow SG: \quad 1 = \lambda_{\max}(Q, p) \int dJ P(J) \tanh^2(\beta J).$$
 (53)

4.2.1. Type I: Separable deformation functions. The simplest family of deformation functions are of the separable form $Q(k, k') = g(k)g(k')/\langle g \rangle^2$, with $g(k) \ge 0$ for all k, and $\langle g \rangle = \sum_k p(k)g(k) > 0$. The special choice g(k) = 1 gives the ensemble without deformation. For this family it follows immediately from (51) that $F(k) = g(k)/\langle g \rangle$, and (47) reduces to

$$M_{kk'} = p(k')k'(k'-1)/\langle k \rangle.$$
(54)

There is just one eigenvector, namely $\epsilon_k = 1$ for all k, with eigenvalue $\lambda = \langle k^2 \rangle / \langle k \rangle - 1$. Hence the continuous transition lines are

$$\mathbf{P} \to \mathbf{F}: \quad \mathbf{1} = \left[\langle k^2 \rangle / \langle k \rangle - 1 \right] \int \mathrm{d}J P(J) \tanh(\beta J) \tag{55}$$

$$P \to SG: \quad 1 = [\langle k^2 \rangle / \langle k \rangle - 1] \int dJ P(J) \tanh^2(\beta J).$$
(56)

The function g(k) has dropped out of our equations, so the transition lines will be identical to those of the non-deformed ensemble, i.e. to those found when Q(k, k') = 1. For a Poissonian degree distribution one has $\langle k^2 \rangle = \langle k \rangle^2 + \langle k \rangle$, so $\lambda = \langle k \rangle$ and we recover the standard results for Erdös–Rényi graphs. Moreover, the solution $F(k) = g(k)/\langle g \rangle$ of (51) gives Q(k, k')/F(k)F(k') = 1 for all (k, k'), which implies that g(k) also drops out of the order parameter equations (30) and (31). It follows that for separable deformation functions *Q* not only the transition lines, but the complete solution of the model, including the values of the physical observables anywhere in the phase diagram, is independent of g(k) and therefore identical to that of the ensemble with degree constraints only. This is true for any degree distribution, and has a simple explanation: upon substituting $Q(k, k') = g(k)g(k')/\langle g \rangle^2$ into the graph probabilities (A.2) one obtains

$$Prob(\mathbf{c}) = \frac{e^{N\{\frac{1}{2}\langle k \rangle \log[\langle k \rangle / \langle g \rangle^2 N] + N^{-1} \sum_i k_i(\mathbf{c}) \log g(k_i(\mathbf{c})) + \mathcal{O}(N^{-1})\}} \prod_i \delta_{k_i, k_i(\mathbf{c})}}{\sum_{\mathbf{c}'} e^{N(\frac{1}{2}\langle k \rangle \log[\langle k \rangle / \langle g \rangle^2 N] + N^{-1} \sum_i k_i(\mathbf{c}') \log g(k_i(\mathbf{c}')) + \mathcal{O}(N^{-1})\}} \prod_i \delta_{k_i, k_i(\mathbf{c}')}} = \frac{e^{\mathcal{O}(N^0)} \prod_i \delta_{k_i, k_i(\mathbf{c})}}{\sum_{\mathbf{c}'} e^{\mathcal{O}(N^0)} \prod_i \delta_{k_i, k_i(\mathbf{c}')}}.$$
(57)

For $Q(k, k') = g(k)g(k')/\langle g \rangle^2$ the Q-dependent factors in Prob(c) depend in leading order on c via the degrees $k_i(c)$ only. Since the degrees are constrained, these factors drop out, leaving only subdominant terms with a vanishing impact on the thermodynamics in the limit $N \to \infty$.

4.2.2. Type II: Additive deformation functions. The second class of deformation functions we will study is $Q(k, k') = [g(k) + g(k')]/2\langle g \rangle$, with $g(k) \ge 0$ for all k and $\langle g \rangle > 0$. Again the simplest choice g(k) = 1 gives the non-deformed graph ensemble. Now it follows from (51) that F(k) = Ag(k) + B, with

$$A = \frac{1}{2\langle k \rangle \langle g \rangle} \left\langle \frac{k}{Ag(k) + B} \right\rangle \qquad B = \frac{1}{2\langle k \rangle \langle g \rangle} \left\langle \frac{kg(k)}{Ag(k) + B} \right\rangle.$$
(58)

We can rewrite B to get a simple relation between A and B

$$AB = \frac{1}{2\langle k \rangle \langle g \rangle} \left\langle \frac{Akg(k)}{Ag(k) + B} \right\rangle = \frac{1}{2\langle k \rangle \langle g \rangle} \left\langle k - \frac{Bk}{Ag(k) + B} \right\rangle = \frac{1}{2\langle g \rangle} - AB.$$
(59)

Thus $AB = 1/4\langle g \rangle$, i.e. $B = 1/4A\langle g \rangle$. Upon eliminating B from our equations and upon defining $A = x/\langle g \rangle$ with $x \ge 0$, we then find that x is to be solved from $\mathcal{F}(x) = 1$, where

$$\mathcal{F}(x) = \frac{2}{\langle k \rangle} \left\langle \frac{k}{1 + 4x^2 g(k) / \langle g \rangle} \right\rangle.$$
(60)

We note that $d\mathcal{F}(x)/dx \leq 0$ for $x \geq 0$, with $\mathcal{F}(0) = 2$ and $\mathcal{F}(\infty) = 0$, so there is indeed a unique and well-defined solution $x \geq 0$ of $\mathcal{F}(x) = 1$. For the trivial case g(k) = 1 (i.e. Q(k, k') = 1, no ensemble deformation) we obtain $\mathcal{F}(x) = 2/(1 + 4x^2)$, giving $x = \frac{1}{2}$ and the correct simple solution F(k) = 1 encountered earlier.

We proceed with the analysis of nontrivial choices for g(k). Let us define the short-hand $G(k) = g(k)/\langle g \rangle$, so $\langle G(k) \rangle = 1$, $Q(k, k') = \frac{1}{2}[G(k) + G(k')]$ and F(k) = xG(k) + 1/4x. The matrix (47) to be diagonalized then takes the following form:

$$M_{kk'} = \frac{8x^2}{\langle k \rangle} \frac{[G(k) + G(k')]p(k')k'(k'-1)}{[4x^2G(k) + 1][4x^2G(k') + 1]}.$$
(61)

Its eigenvalue equation becomes (with brackets denoting averages over the degree distribution)

$$\lambda \epsilon_k = \frac{8x^2 G(k)}{\langle k \rangle [4x^2 G(k) + 1]} \left\langle \frac{k'(k'-1)\epsilon_{k'}}{4x^2 G(k') + 1} \right\rangle + \frac{8x^2}{\langle k \rangle [4x^2 G(k) + 1]} \left\langle \frac{G(k')k'(k'-1)\epsilon_{k'}}{4x^2 G(k') + 1} \right\rangle.$$
(62)

We see that the components ϵ_k of any eigenvector must always be of the form

$$\epsilon_k = \frac{\cos(\phi)G(k) + \sin(\phi)}{4x^2G(k) + 1},\tag{63}$$

where

$$\lambda \cos(\phi) = \frac{8x^2}{\langle k \rangle} \left\langle \frac{k(k-1)[\cos(\phi)G(k) + \sin(\phi)]}{[4x^2G(k) + 1]^2} \right\rangle$$
(64)

$$\lambda \sin(\phi) = \frac{8x^2}{\langle k \rangle} \left\langle \frac{G(k)k(k-1)[\cos(\phi)G(k) + \sin(\phi)]}{[4x^2G(k) + 1]^2} \right\rangle$$
(65)

or, in the matrix form

$$\lambda \begin{pmatrix} \cos(\phi) \\ \sin(\phi) \end{pmatrix} = \frac{8x^2}{\langle k \rangle} \begin{pmatrix} \frac{k(k-1)G(k)}{[4x^2G(k)+1]^2} & \frac{k(k-1)}{[4x^2G(k)+1]^2} \\ \frac{k(k-1)G^2(k)}{[4x^2G(k)+1]^2} & \frac{k(k-1)G(k)}{[4x^2G(k)+1]^2} \end{pmatrix} \begin{pmatrix} \cos(\phi) \\ \sin(\phi) \end{pmatrix}.$$
(66)

The two eigenvalues are now calculated easily. We need the largest one, giving us the following expression for $\lambda_{\max}(Q, p)$ for the present family of graph ensembles, with $y = 4x^2/\langle g \rangle$:

$$\lambda_{\max}(Q, p) = \frac{2y}{\langle k \rangle} \left\{ \left\langle \frac{k(k-1)g(k)}{[yg(k)+1]^2} \right\rangle + \sqrt{\left\langle \frac{k(k-1)}{[yg(k)+1]^2} \right\rangle \left\langle \frac{k(k-1)g^2(k)}{[yg(k)+1]^2} \right\rangle} \right\}$$
(67)

where *y* is the solution of

$$\left\langle \frac{k}{yg(k)+1} \right\rangle = \frac{1}{2} \langle k \rangle. \tag{68}$$

It is a trivial matter to check that for the simple choice g(k) = 1, where y = 1, one indeed recovers from (67) the correct eigenvalue $\langle k^2 \rangle / \langle k \rangle - 1$ of the non-deformed ensembles. It will also be clear from (67) that for the present non-separable family of ensemble deformation functions Q(k, k'), the phase diagram will generally indeed be affected by the deformation.

4.2.3. Type III: Simple binary deformation functions. Our third class of deformation functions are those where Q(k, k') takes only two values. Here the deformation can even strictly forbid links that otherwise would have been allowed. We will focus on the simple example $Q(k, k') = \gamma_0 + \gamma \delta_{kk'}$, where $\gamma_0 = 1 - \gamma \sum_k p^2(k)$ and $0 \le |\gamma| \le \left[\sum_k p^2(k)\right]^{-1}$. The problem (51) now reduces to a quadratic equation for F(k), of which the nonnegative solution is

$$F(k) = \frac{1}{2}y + \frac{1}{2}\sqrt{y^2 + 4\gamma p(k)k/\langle k\rangle}$$
(69)

$$y = \frac{1 - \gamma \langle p(k) \rangle}{\langle k \rangle} \left\langle \frac{2k}{y + \sqrt{y^2 + 4\gamma p(k)k/\langle k \rangle}} \right\rangle.$$
(70)

The right-hand side of (70) decreases monotonically from $[1 - \gamma \langle p(k) \rangle] \langle \sqrt{k/p(k)} \rangle / \sqrt{\gamma \langle k \rangle}$ at y = 0 to zero as $y \to \infty$, so (70) always has a unique non-negative solution y. One also quite easily established the useful bounds

$$\sqrt{1 - \gamma \langle p(k) \rangle} \left\langle \frac{k/\langle k \rangle}{\sqrt{1 + 4\gamma p(k)k/[\langle k \rangle [1 - \gamma \langle p(k) \rangle]]}} \right\rangle \leqslant y \leqslant \sqrt{1 - \gamma \langle p(k) \rangle}$$
(71)

(which are seen to become tight both for $\gamma \to 0$, where y = 1, and for $\gamma \to \langle p(k) \rangle^{-1}$, where y = 0). The matrix (47) will always have an eigenvalue $\lambda = 0$, corresponding to the eigenspace $\epsilon_k = 0$ for all k > 1. The eigenvectors of (47) with nonzero eigenvalue λ are seen to be

$$\epsilon_k = \frac{1}{\lambda F(k) - \gamma p(k)k(k-1)/\langle k \rangle F(k)},\tag{72}$$

where λ then follows upon solving

$$1 = \left[1 - \gamma \langle p(k) \rangle\right] \left\{ \frac{k(k-1)}{\lambda F^2(k) \langle k \rangle - \gamma p(k)k(k-1)} \right\}.$$
(73)

Upon inserting (69) this equation takes the following explicit form, with y (which is itself not a function of λ) to be solved from (70)

$$1 = \left[1 - \gamma \langle p(k) \rangle\right] \left\langle \frac{4k(k-1)}{\lambda \langle k \rangle \left[y + \sqrt{y^2 + 4\gamma p(k)k/\langle k \rangle}\right]^2 - 4\gamma p(k)k(k-1)} \right\rangle.$$
(74)

The right-hand side diverges to $-\infty$ for $\lambda \downarrow 0$ and decays to zero for $\lambda \rightarrow \infty$. Furthermore, provided there exists k > 1 with p(k) > 0, it has singularities for each k with p(k) > 0 at the special values $\lambda = \lambda_c(k)$, where

$$\lambda_c(k) = \frac{4\gamma p(k)k(k-1)}{\langle k \rangle [y + \sqrt{y^2 + 4\gamma p(k)k/\langle k \rangle}]^2} \ge 0.$$
(75)

Let us define $\max_{k,p(k)>0} \lambda_c(k) = \lambda_c(k^*)$. We know that the right-hand side of (74) decreases monotonically on the interval $[\lambda_c(k^*), \infty)$ from ∞ down to zero. Hence there is always a positive solution λ of (74), and the largest solution $\lambda_{\max}(Q, p)$ lies in $[\lambda_c(k^*), \infty)$. Furthermore,

$$\lambda_{\max}(Q, P) \ge \max_{k} \lambda_c(k) = \max_{k} \frac{4\gamma p(k)k(k-1)}{\langle k \rangle [y + \sqrt{y^2 + 4\gamma p(k)k/\langle k \rangle}]^2}.$$
(76)

A second simple but effective bound on solutions $\lambda > 0$ is established easily

$$\lambda = \frac{1 - \gamma \langle p(k) \rangle}{\langle k \rangle} \left\langle \frac{4k(k-1)}{[y + \sqrt{y^2 + 4\gamma p(k)k/\langle k \rangle}]^2 - 4\gamma p(k)k(k-1)/\lambda\langle k \rangle} \right\rangle$$
$$\geq \frac{1 - \gamma \langle p(k) \rangle}{\langle k \rangle} \left\langle \frac{4k(k-1)}{[y + \sqrt{y^2 + 4\gamma p(k)k/\langle k \rangle}]^2} \right\rangle \geq \frac{1 - \gamma \langle p(k) \rangle}{\langle k \rangle} \left\langle \frac{k(k-1)}{y^2 + 4\gamma p(k)k/\langle k \rangle} \right\rangle$$

and hence

$$\lambda_{\max}(Q, P) \ge [1 - \gamma \langle p(k) \rangle] \left\langle \frac{k(k-1)}{y^2 \langle k \rangle + 4\gamma p(k)k} \right\rangle.$$
(77)

For the trivial choice $\gamma = 0$, where Q(k, k') = 1, we recover the correct results for the non-deformed ensemble, namely F(k) = 1 and $\lim_{\gamma \to 0} \lambda_{\max}(Q, p) = \langle k^2 \rangle / \langle k \rangle - 1$. Here the second bound (77) is satisfied with equality. In the opposite limit $\gamma \to \langle p(k) \rangle^{-1}$, where $Q(k, k') \to \delta_{kk'} / \langle p(k) \rangle$, we obtain $F(k) = \sqrt{p(k)k} / \sqrt{\langle p(k) \rangle \langle k \rangle} + \mathcal{O}(\epsilon)$ and $y = \epsilon \langle \sqrt{k/p(k)} \rangle / \sqrt{\langle k \rangle / \langle p(k) \rangle} + \mathcal{O}(\epsilon^2)$, with $\epsilon = 1 - \gamma \langle p(k) \rangle$. Our equation for λ thereby becomes

$$1 = \left\langle \frac{k(k-1)\langle p(k) \rangle}{p(k)k(\lambda-k+1)/\epsilon + \lambda\sqrt{p(k)k}\langle p(k) \rangle \langle \sqrt{k/p(k)} \rangle - p(k)k(\lambda-k+1) + \mathcal{O}(\epsilon^2)} \right\rangle.$$
(78)

It follows that for $\gamma \to \langle p(k) \rangle^{-1}$ all nonzero eigenvalues are of the form $\lambda = k^* - 1 + \mathcal{O}(1 - \gamma \langle p(k) \rangle)$ with $k^* \in \{1, 2, ...\}$ such that $p(k^*) > 0$. The largest such eigenvalue corresponds to the largest k^* with $p(k^*) > 0$, so $\lim_{\gamma \to \langle p(k) \rangle^{-1}} \lambda_{\max}(Q, p) = k^* - 1$. Thus in the latter limit we obtain the transition lines corresponding to a regular random graph with degree k^* , which is consistent with our earlier observation that for $Q(k, k') = \delta_{kk'}/\langle p(k) \rangle$ our graphs decompose into a collection of disconnected regular graphs, one for each degree *k* that is allowed by p(k). Here we find that the first bound (76) is satisfied with equality.

4.3. Phase diagrams

Our order parameter equations apply in principle to arbitrary choices of the bond distribution P(J), the degree distribution p(k) and the ensemble deformation function Q(k, k'). Here we will limit ourselves for brevity to the deformation functions analyzed in the previous section, and to the binary bond distribution $P(J) = \frac{1}{2}(1 + \eta)\delta(J - J_0) + \frac{1}{2}(1 - \eta)\delta(J + J_0)$, with $\eta \in [-1, 1]$ and $J_0 > 0$. Equations (52) and (53) can now be written as

$$P \to F: \quad T_F/J_0 = 2/\log\left[\frac{\eta \lambda_{\max}(Q, p) + 1}{\eta \lambda_{\max}(Q, p) - 1}\right]$$
(79)

$$P \to SG: \quad T_{SG}/J_0 = 2/\log\left[\frac{\sqrt{\lambda_{\max}(Q, p)} + 1}{\sqrt{\lambda_{\max}(Q, p)} - 1}\right]. \tag{80}$$

The P \rightarrow F transition is the physical one for $\eta > \tanh(\beta J_0)$ and the P \rightarrow SG transition is the physical one for $\eta < \tanh(\beta J_0)$, with a triple point at $\eta = \tanh(\beta J_0)$. We will consider only two types of degree distributions, both with average connectivity $\langle k \rangle = c$

Poissonnian:
$$p(k) = c^k e^{-c} / k!, \qquad \langle k^2 \rangle / c = c + 1$$
 (81)

power law:
$$p(k) = \left(1 - \frac{c\zeta(3+\alpha)}{\zeta(2+\alpha)}\right)\delta_{k0} + (1-\delta_{k0})\frac{ck^{-3-\alpha}}{\zeta(2+\alpha)}, \qquad \langle k^2 \rangle/c = \frac{\zeta(1+\alpha)}{\zeta(2+\alpha)}.$$
(82)

Here $\zeta(x)$ denotes the Riemann zeta function $\zeta(x) = \sum_{k>0} k^{-x}$ [50], and we take $\alpha \in [0, 1]$ to ensure that $c = \langle k \rangle$ exists (limiting ourselves to $c \leq \zeta(2+\alpha)/\zeta(3+\alpha)$, so that $p(0) \geq 0$, which means that c will remain modest), but with the possibility to take the scale-free limit $\alpha \to 0$. In practice, however, in calculating averages over p(k) numerically one has to truncate the values of k; here we used $k \leq k_{\text{max}} = 10^8$. For Poissonnian p(k) this has no noticeable implications, but for power law p(k) the slow divergence of $\sum_k k^{-1} \approx \log k_{\max}$ manifests itself in transition temperatures for $\alpha \to 0$ that should have been infinite but are finite. On the other hand, in any finite real system or simulation one will have k < N, so one expects also to see there the same effects of bounded degrees (e.g. finite transition temperatures). The 'ideal' situation of unbounded degrees and truly scale-free graphs is never realized in practice. The power-law distribution (82) has the property $p(k)|_c = cp(k)_{c=1}$ for k > 0. Hence for any function $\psi(k)$ with $\psi(0) = 0$ one will have $\langle \psi(k) \rangle = c \langle \psi(k) \rangle_{c=1}$. As a consequence one finds immediately upon checking the various formulae of the previous section that the bifurcation lines for type I and type II ensemble deformations are completely independent of the connectivity c for power-law distributed degrees. For type III deformations this is not the case. Note, finally, that there is no point in choosing regular graphs $p(k) = \delta_{kc}$, since there the function Q(k, k')is always equal to one due to the normalization requirement $\sum_{kk'} p(k)p(k')Q(k,k') = 1$.

We will compare phase diagrams for the previously analyzed families of deformation functions Q(k, k'), namely the separable ones, the additive ones, and the binary ones. In the separable case (type I), where one always has the simple eigenvalue $\lambda_{\max}(Q, p) = \langle k^2 \rangle / \langle k \rangle - 1$, we have fully explicit expressions for the transition lines that are identical to those describing non-deformed ensembles with degree constraints only

Poissonnian
$$p(k)$$
: $T_{\rm F}/J_0 = 2/\log\left[\frac{\eta c+1}{\eta c-1}\right], \qquad T_{\rm SG}/J_0 = 2/\log\left[\frac{\sqrt{c}+1}{\sqrt{c}-1}\right]$ (83)

power law
$$p(k)$$
: $T_{\rm F}/J_0 = 2/\log\left[\frac{\eta\zeta(1+\alpha) + (1-\eta)\zeta(2+\alpha)}{\eta\zeta(1+\alpha) - (1+\eta)\zeta(2+\alpha)}\right],$ (84)



Figure 1. Continuous bifurcation lines for $P \rightarrow SG$ (dotted) and $P \rightarrow F$ (solid, with $\eta \in \{0.25, 0.5, 0.75, 1\}$ from bottom to top), for type II deformed ensembles (with $Q(k, k') = [g(k) + g(k')]/2\langle g(k) \rangle$), $P(J) = \frac{1}{2}(1 + \eta)\delta(J - J_0) + \frac{1}{2}(1 - \eta)\delta(J + J_0)$, and Poissonnian degree distributions $p(k) = c^k e^{-c}/k!$. Left to right: $g(k) \in \{1, k, k^2\}$. The left picture represents the non-deformed ensemble, to serve as a reference. The effect of a deformation with $Q(k, k') = [k^m + (k')^m]/2\langle k^m \rangle$ in graphs with Poissonnian p(k) is seen to be a slight reduction of all critical temperatures with increasing *m*.

$$T_{\rm SG}/J_0 = 2/\log\left[\frac{\sqrt{\zeta(1+\alpha) - \zeta(2+\alpha)} + \sqrt{\zeta(2+\alpha)}}{\sqrt{\zeta(1+\alpha) - \zeta(2+\alpha)} - \sqrt{\zeta(2+\alpha)}}\right]$$
(85)

(in non-deformed graphs of the type considered here, the transition temperatures for powerlaw distributed degree distributions are independent of the average connectivity). Clearly, in non-deformed Poissonnian graphs we can only have an SG phase if c > 1 and an *F* phase if $c > 1/\eta$, whereas in non-deformed power-law graphs we can only have an SG phase if $\zeta(1+\alpha)/\zeta(2+\alpha) > 2$ (giving $\alpha < \alpha_c \approx 0.479$) and an *F* phase if $\zeta(1+\alpha)/\zeta(2+\alpha) > 1+1/\eta$. We will not show these lines describing the non-deformed ensembles in a separate figure, but will include them as a benchmark when showing data for the type II and type III deformations, since in type II models the non-deformed ensemble is recovered for the special choice g(k) = 1whereas in the type III models it corresponds to $\gamma = 0$.

For the additive functions Q(k, k') (type II) the eigenvalue $\lambda_{\max}(Q, p)$ depends in a nontrivial way on Q(k, k') and p(k), and must be solved from (67) and (68) numerically. Here we will choose either g(k) = k or $g(k) = k^2$ in the function Q(k, k'). For Poissonnian distributed degrees this gives G(k) = k/c and $G(k) = k^2/c(c+1)$, respectively. For the power-law distributed degrees one finds G(k) = k/c and $G(k) = k^2\zeta(2+\alpha)/c\zeta(1+\alpha)$, respectively. Upon solving (67) and (68) numerically for Poissonnian graphs, we obtain the bifurcation lines as shown in figure 1. We also show the lines for the non-deformed case g(k) = 1, as a benchmark. The deformation causes only minor changes to the phase diagram, mainly a slight reduction of all transition temperatures for small values of the connectivity c. When applied to graphs with power-law degrees, in contrast, the impact of the deformation is much more drastic, as shown in figure 2. This can be understood mathematically on the basis of equations (67) and (68). If we consider the case $\alpha \to 0$ we only need to inspect what happens to the divergent sums over k: one finds for both g(k) = k and $g(k) = k^2$ that $\lambda_{\max}(Q, p) \sim \sqrt{\log k_{\max}}$ as $\alpha \to 0^+$ (rather than $\lambda_{\max}(Q, p) \sim \log k_{\max}$, as was the case for the non-deformed ensemble).

Finally, we have solved numerically equations (70) and (74) for the case of the binary functions Q(k, k') (type III), for $\gamma \langle p(k) \rangle \in \{0, 0.4, 0.8\}$ (with the first value $\gamma = 0$, the non-deformed case, serving as a benchmark) and c = 1. Positive values of γ imply increased connections between links with identical degree, which favors especially the formation of



Figure 2. Continuous bifurcation lines for $P \rightarrow SG$ (dotted) and $P \rightarrow F$ (solid, with $\eta \in \{0.25, 0.5, 0.75, 1\}$ from bottom to top), for type II deformed ensembles (with $Q(k, k') = [g(k) + g(k')]/2\langle g(k) \rangle$), $P(J) = \frac{1}{2}(1 + \eta)\delta(J - J_0) + \frac{1}{2}(1 - \eta)\delta(J + J_0)$, and power-law degree distributions $p(k) \sim k^{-3-\alpha}$. Left to right: $g(k) \in \{1, k, k^2\}$. The left picture represents the non-deformed ensemble, to serve as a reference. The effect of a deformation with $Q(k, k') = [k^m + (k')^m]/2\langle k^m \rangle$ in graphs with power law p(k) is now seen to be a dramatic reduction of all critical temperatures with increasing *m*.



Figure 3. Continuous bifurcation lines for $P \rightarrow SG$ (dotted) and $P \rightarrow F$ (solid, with $\eta \in \{0.25, 0.5, 0.75, 1\}$ from bottom to top), for type III deformed ensembles (with $Q(k, k') = \gamma_0 + \gamma \delta_{kk'}$), $P(J) = \frac{1}{2}(1+\eta)\delta(J-J_0) + \frac{1}{2}(1-\eta)\delta(J+J_0)$, and Poissonnian degree distributions $p(k) = c^k e^{-c}/k!$. Left to right: $\gamma \langle p(k) \rangle \in \{0, 0.4, 0.8\}$. The left picture represents the non-deformed ensemble, to serve as a reference. The effect of a deformation with $Q(k, k') = \gamma_0 + \gamma \delta_{kk'}$ in graphs with Poissonnian p(k) is seen to be a significant increase of all critical temperatures with increasing γ .

regular graphs with large values of k. Here we always observe a significant increase of all critical temperatures, both for Poissonnian and for power-law distributed graphs, see figure 4. The effect becomes stronger as c increases. Choosing negative values of γ , i.e. discouraging the formation of links between nodes with identical degree, is found to decrease all transition temperatures. Note that without the degree cut-off $k_{\text{max}} = 10^8$, one would have diverging critical temperatures at all c > 0 and all $\alpha \ge 0$ in the limit $\gamma \langle p(k) \rangle \rightarrow 1$.

5. Discussion

The rationale behind studying interacting particle models on complex *random* graphs is that the latter can be used as solvable proxies for models on *specific* graphs of a topology for which either no exact solution is available (e.g. spin models on cubic lattices), or on which we



Figure 4. Continuous bifurcation lines for $P \rightarrow SG$ (dotted) and $P \rightarrow F$ (solid, with $\eta \in \{0.25, 0.5, 0.75, 1\}$ from bottom to top), for type III deformed ensembles (with $Q(k, k') = \gamma_0 + \gamma \delta_{kk'}$), $P(J) = \frac{1}{2}(1 + \eta)\delta(J - J_0) + \frac{1}{2}(1 - \eta)\delta(J + J_0)$, and power-law degree distributions $p(k) \sim k^{-3-\alpha}$ with c = 1. Left to right: $\gamma \langle p(k) \rangle \in \{0, 0.4, 0.8\}$. The left picture represents the non-deformed ensemble, to serve as a reference. The effect of a deformation with $Q(k, k') = \gamma_0 + \gamma \delta_{kk'}$ in graphs with power law p(k) is now seen to be a dramatic increase of all critical temperatures with increasing γ .

lack precise information (e.g. proteomic networks). We then have to choose an appropriate ensemble of random graphs, which is sufficiently simple to allow for analytical progress, while incorporating as much as possible the topology of the specific system one aims to understand. Specifying just the degree distribution p(k) of a complex connectivity graph for an interacting spin system will clearly not yet permit reliable predictions on the system's phase diagram. For instance, the critical temperature of the D-dimensional Ising model on a cubic lattice, where $p(k) = \delta_{k,2D}$, is different from that of a regular random graph with $p(k) = \delta_{k,2D}$.⁴ The question is then which further topological information on a graph beyond p(k) could be added to reduce the entropy of the underlying graph ensemble and make more specific and more accurate predictions of phase transitions, while at the same time maintaining the vital property that the resulting spin models can be solved analytically. In this paper we have established that the proposed deformation of random graph ensembles can be a useful step in this direction: it generally allows us to differentiate between models with the same p(k) (which can be chosen freely) but different microscopic realizations of these degree statistics, the resulting models are still solvable, and its impact on the transition lines can be non-negligible⁵. In practice, when seeking to model a complicated real system with some specific given interaction graph \mathbf{c}^{\star} (and hence a known set of degree $\{k_1^{\star}, \ldots, k_N^{\star}\}$ and a known degree distribution p(k)) by a solvable system on a random graph, we could now incorporate at least some of the extra topological information by using our ensemble (2) with constrained degrees $k_i = k_i^*$ for all *i*, and with a function Q(k, k') that is tailored to the graph c^* . This can be done by maximizing the log-likelihood of \mathbf{c}^{\star} for the ensemble (2), i.e. by minimizing over Q (subject to $\sum_{kk'} p(k)p(k')Q(k,k') = 1$) the quantity

$$\Omega[Q] = \frac{1}{N} \log \mathcal{Z}_N - \frac{1}{N} \sum_{i < j} \log \left[\frac{\langle k \rangle}{N} Q(k_i^\star, k_j^\star) \delta_{c_{ij}^\star, 1} + \left(1 - \frac{\langle k \rangle}{N} Q(k_i^\star, k_j^\star) \right) \delta_{c_{ij}^\star, 0} \right]$$

⁴ For a ferromagnetic Ising model on a square lattice in D = 2 one has Onsager's famous result $T_c/J_0 = 4/\log[(\sqrt{2} + 1)/(\sqrt{2} - 1)] \approx 2.26919$, whereas $T_c/J_0 = 2/\log 2 \approx 2.88539$ in the degree-4 regular random graph. Yet both models have the same degree distribution $p(k) = \delta_{k,4}$. ⁵ The only graphs where ensemble deformation is not possible are the regular graphs, with $p(k) = \delta_{kc}$, where the

The only graphs where ensemble deformation is not possible are the regular graphs, with $p(k) = \delta_{kc}$, where the constraint $\sum_{kk'} p(k)Q(k,k')p(k') = 1$ leaves only the trivial choice Q(k,k') = 1.

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$$= z + \frac{1}{2} \langle k \rangle - \frac{1}{2} \langle k \rangle \log[\langle k \rangle / N] - \frac{1}{N} \sum_{i < j} c_{ij}^{\star} \log Q(k_i^{\star}, k_j^{\star}) + \mathcal{O}(N^{-1})$$

= const + $\sum_k p(k) k \log F(k|Q) - \frac{1}{N} \sum_{i < j} c_{ij}^{\star} \log Q(k_i^{\star}, k_j^{\star}) + \mathcal{O}(N^{-1}),$ (86)

where F(k|Q) is the solution of

$$F(k) = \langle k \rangle^{-1} \sum_{k'} p(k')k'Q(k,k')F^{-1}(k').$$
(87)

This will be the subject of a subsequent study. In addition one would like to study certain technical aspects of the present model in more detail, such as the precise physical meaning of the function F(k), and the impact of possible replica symmetry breaking (RSB). In the present type of model RSB does not change the locations of the P \rightarrow F or P \rightarrow SG transition lines, but will alter the nature of the solution in the ordered phases and the location of the F \rightarrow SG transition line.

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Appendix. Statistical properties of the random graph ensemble

A.1. Interpretation

We note that an alternative but mathematically equivalent way to write the graph probabilities is obtained by applying to (2) the general identity

$$\prod_{i< j} [A_{ij}\delta_{c_{ij},1} + B_{ij}\delta_{c_{ij},0}] = \left(\prod_{i< j} B_{ij}\right) e^{\sum_{i< j} c_{ij}[\log A_{ij} - \log B_{ij}]}$$
(A.1)

which gives

$$\operatorname{Prob}(\mathbf{c}) = \frac{1}{\mathcal{Z}_N} e^{\sum_{i < j} c_{ij} \{ \log[\langle k \rangle \mathcal{Q}(k_i, k_j) / N] - \log[1 - \langle k \rangle \mathcal{Q}(k_i, k_j) / N] \}} \prod_i \delta_{k_i, k_i(\mathbf{c})}$$
(A.2)

$$\mathcal{Z}_{N} = \sum_{\mathbf{c}} e^{\sum_{i < j} c_{ij} \{\log[\langle k \rangle \mathcal{Q}(k_{i}, k_{j})/N] - \log[1 - \langle k \rangle \mathcal{Q}(k_{i}, k_{j})/N]\}} \prod_{i} \delta_{k_{i}, k_{i}(\mathbf{c})}.$$
 (A.3)

To see the connection with ensembles considered in previous studies we note that the latter factor \mathcal{Z}_N is identical to the graph partition function $Z_1 = \sum_{\mathbf{c}} \exp\left[\sum_{i < j} h_{ij} c_{ij}\right] \prod_i \delta_{k_i,k_i(\mathbf{c})}$ in, e.g. [51] (rewritten in our present notation), but with a specific choice for the fields h_{ij} , namely

$$h_{ij} = \log[\langle k \rangle Q(k_i, k_j)/N] - \log[1 - \langle k \rangle Q(k_i, k_j)/N].$$
(A.4)

Moreover, in studies such as [51] h_{ij} are only allowed infinitesimal values and serve solely to generate observables in the 'unperturbed' ensemble characterized by $Z = \sum_{\mathbf{c}} \prod_i \delta_{k_i,k_i(\mathbf{c})}$. In contrast, the present study is focused explicitly on *finite* deformations of the graph statistics.

In the ensemble (2) all degrees are fully constrained, and the probability for any two randomly drawn vertices to be connected is $\mathcal{P}[\text{conn}] = c/N$. The physical meaning of

Q(k, k') follows from calculating the conditional probability $\mathcal{P}[\operatorname{conn}|k, k']$ that two randomly drawn links with degrees k and k' are connected

$$\mathcal{P}[\operatorname{conn}|k,k'] = \frac{\sum_{\mathbf{c}} \operatorname{Prob}(\mathbf{c}) \sum_{i < j} c_{ij} \delta_{k,k_i}(\mathbf{c}) \delta_{k',k_j}(\mathbf{c})}{\sum_{\mathbf{c}} \operatorname{Prob}(\mathbf{c}) \sum_{i < j} \delta_{k,k_i}(\mathbf{c}) \delta_{k',k_j}(\mathbf{c})}$$
$$= \frac{\sum_{i < j} \delta_{k,k_i} \delta_{k',k_j} \sum_{\mathbf{c}} \operatorname{Prob}(\mathbf{c}) c_{ij}}{\sum_{i < j} \delta_{k,k_i} \delta_{k',k_j}}$$
$$= \frac{\sum_{i < j} \delta_{k,k_i} \delta_{k',k_j} c Q(k,k')/N}{\sum_{i < j} \delta_{k,k_i} \delta_{k',k_j}} = \frac{c}{N} Q(k,k').$$
(A.5)

Hence

$$Q(k,k') = \frac{\mathcal{P}[\operatorname{conn}|k,k']}{\mathcal{P}[\operatorname{conn}]},\tag{A.6}$$

i.e. Q(k, k') is the probability for two randomly drawn vertices with degrees k and k' to be connected, divided by the overall probability of two randomly drawn vertices to be connected (irrespective of their degrees).

A.2. Joint distributions of degree and clustering coefficients

To characterize a graph's local topology we can define for each vertex *i* the degree $k_i(\mathbf{c}) = \sum_j c_{ij}$ (the number of links to this vertex) and the number of length-three loops going through this vertex, as measured by $r_i(\mathbf{c}) = \sum_{jk} c_{ij} c_{jk} c_{ki}$. The clustering coefficient C_i is then given by $C_i = r_i/k_i(k_i - 1)$. We write their joint distribution as $P(k, r|\mathbf{c}) = N^{-1} \sum_i \delta_{k,k_i(\mathbf{c})} \delta_{r,r_i(\mathbf{c})}$, and the asymptotic expectation value of this distribution over the ensemble (2) as

$$P(k,r) = \lim_{N \to \infty} \frac{1}{N} \sum_{i} \sum_{\mathbf{c}} \operatorname{Prob}(\mathbf{c}) \,\delta_{k,k_i(\mathbf{c})} \delta_{r,r_i(\mathbf{c})} = \int \frac{\mathrm{d}\psi}{2\pi} \,\mathrm{e}^{\mathrm{i}\psi r} \lim_{N \to \infty} \frac{1}{N} \sum_{i} \delta_{k,k_i} \hat{P}_i(\psi) \quad (A.7)$$

with

$$\hat{P}_{i}(\psi) = \sum_{\mathbf{c}} \operatorname{Prob}(\mathbf{c}) e^{-i\psi \sum_{j\ell} c_{ij} c_{j\ell} c_{\ell i}}.$$
(A.8)

It will turn out that here we have to expand to higher orders in *N* than in previous calculations. We now re-name all links to/from site *i* as $s_j = c_{ij} \in \{0, 1\}$, while writing all those that do not involve site *i* as $\tau_{j\ell} \in \{0, 1\}$, where $j, \ell \in \{1, ..., i - 1, i + 1, ..., N\}$. This gives

$$\begin{split} \hat{P}_{i}(\psi) &= \frac{1}{\mathcal{Z}_{N}} \sum_{s\tau} e^{-i\psi \sum_{j\ell \neq i} s_{j}\tau_{j\ell}s_{\ell}} \prod_{j \neq i} \left[\frac{\langle k \rangle}{N} \mathcal{Q}(k_{i},k_{j}) \delta_{s_{j},1} + \left(1 - \frac{\langle k \rangle}{N} \mathcal{Q}(k_{i},k_{j}) \right) \delta_{s_{j},0} \right] \delta_{k_{i},\sum_{j \neq i} s_{j}} \\ & \times \prod_{\ell < j \mid \ell, j \neq i} \left[\frac{\langle k \rangle}{N} \mathcal{Q}(k_{\ell},k_{j}) \delta_{\tau_{\ell j},1} + \left(1 - \frac{\langle k \rangle}{N} \mathcal{Q}(k_{\ell},k_{j}) \right) \delta_{\tau_{\ell j},0} \right] \prod_{\ell \neq i} \delta_{k_{\ell},\sum_{j \neq i,\ell} \tau_{\ell j}} \\ &= \frac{1}{\mathcal{Z}_{N}} \sum_{s} \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{i\phi k_{i}} \prod_{j \neq i} \left[\frac{\langle k \rangle}{N} \mathcal{Q}(k_{i},k_{j}) \delta_{s_{j},1} + \left(1 - \frac{\langle k \rangle}{N} \mathcal{Q}(k_{i},k_{j}) \right) \delta_{s_{j},0} \right] e^{-i\phi \sum_{j \neq i} s_{j}} \\ & \times \int_{-\pi}^{\pi} \prod_{\ell \neq i} \left[\frac{d\phi_{\ell}}{2\pi} e^{i\phi_{\ell}k_{\ell}} \right] e^{\frac{\langle k \rangle}{2N} \sum_{\ell j (\neq i)} \mathcal{Q}(k_{\ell},k_{j}) [e^{-i(2\psi s_{\ell} s_{j} + \phi_{\ell} + \phi_{j})} - 1] + \mathcal{O}(N^{-1})} \\ & \times e^{-\frac{\langle k \rangle^{2}}{4N^{2}} \sum_{\ell j (\neq i)} \mathcal{Q}^{2}(k_{\ell},k_{j}) [e^{-i(2\psi s_{\ell} s_{j} + \phi_{\ell} + \phi_{j})} - 1]^{2} - \frac{\langle k \rangle}{2N} \sum_{j \neq i} \mathcal{Q}(k_{j},k_{j}) [e^{-2i(\psi s_{j}^{2} + \phi_{j})} - 1]}. \end{split}$$
(A.9)

At this point we are led to the introduction of the observables

$$W_{sk}(\phi) = \frac{1}{N-1} \sum_{j \neq i} \delta_{ss_j} \delta_{kk_j} \delta(\phi - \phi_j).$$
(A.10)

Clearly $\sum_{s \in \{0,1\}} \sum_{k \ge 0} \int d\phi W_{sk}(\phi) = 1$. We also introduce the short-hand $p_k = N^{-1} \sum_i \delta_{k,k_i}$ (namely the empirical degree frequencies, which will only be identical to p(k) for $N \to \infty$). Upon introducing $W_{sk}(\phi)$ in the usual manner via suitable δ -functions we can then write

W

$$\Psi(W, \hat{W}, \psi) = i \sum_{sk} \int_{-\pi}^{\pi} d\phi \, \hat{W}_{sk}(\phi) \, W_{sk}(\phi) + \sum_{k} p_k \log \int_{-\pi}^{\pi} \frac{d\phi}{2\pi} e^{i[\phi k - \hat{W}_{0k}(\phi)]} + \frac{1}{2} \langle k \rangle \sum_{sks'k'} \int d\phi \, d\phi' \, W_{sk}(\phi) \, W_{s'k'}(\phi') \, Q(k, k') [e^{-i(2\psi ss' + \phi + \phi')} - 1]$$
(A.12)

$$\Phi(W, \hat{W}, \psi) = -\langle k \rangle \sum_{sks'k'} \int d\phi \, d\phi' W_{sk}(\phi) W_{s'k'}(\phi') Q(k, k') [e^{-i(2\psi ss' + \phi + \phi')} - 1] - \frac{1}{4} \langle k \rangle^2 \sum_{sks'k'} \int d\phi \, d\phi' W_{sk}(\phi) W_{s'k'}(\phi') Q^2(k, k') [e^{-i(2\psi ss' + \phi + \phi')} - 1]^2 - \frac{1}{2} \langle k \rangle \sum_{sk} \int d\phi W_{sk}(\phi) Q(k, k) [e^{-2i(\psi s + \phi)} - 1] - i \sum_{sk} \int d\phi \hat{W}_{sk}(\phi) W_{sk}(\phi)$$
(A.13)

$$\Omega(\hat{W}, k_i, \phi) = \langle k \rangle \sum_{k} p_k Q(k_i, k) \left[\frac{\int_{-\pi}^{\pi} d\phi' e^{i[\phi'k - \hat{W}_{0k}(\phi') - \phi]}}{\int_{-\pi}^{\pi} d\phi' e^{i[\phi'k - \hat{W}_{0k}(\phi')]}} - 1 \right] - \log \int_{-\pi}^{\pi} \frac{d\phi'}{2\pi} e^{i[\phi'k_i - \hat{W}_{0k_i}(\phi')]}.$$
(A.14)

Using the normalization identity $\hat{P}_i(0) = 1$ we may then also write

$$\hat{P}_{i}(\psi) = \frac{\int_{-\pi}^{\pi} d\phi \, e^{i\phi k_{i}} \int \{dW \, d\hat{W}\} e^{N\Psi(W,\hat{W},\psi) + \Phi(W,\hat{W},\psi) + \Omega(\hat{W},k_{i},\phi) + \mathcal{O}(N^{-1})}}{\int_{-\pi}^{\pi} d\phi \, e^{i\phi k_{i}} \int \{dW \, d\hat{W}\} e^{N\Psi(W,\hat{W},0) + \Phi(W,\hat{W},0) + \Omega(\hat{W},k_{i},\phi) + \mathcal{O}(N^{-1})}}$$
(A.15)

and, upon defining $P(r|k) = P(k, r)/p_k$

$$P(r|k) = \int_{-\pi}^{\pi} \frac{\mathrm{d}\psi}{2\pi} \,\mathrm{e}^{\mathrm{i}\psi r} L_k(\psi) \tag{A.16}$$

$$L_{k}(\psi) = \lim_{N \to \infty} \frac{\int \{ dW \, d\hat{W} \} e^{N\Psi(W, \hat{W}, \psi) + \Phi(W, \hat{W}, \psi)} \int_{-\pi}^{\pi} d\phi \, e^{i\phi k + \Omega(\hat{W}, k, \phi)}}{\int \{ dW \, d\hat{W} \} e^{N\Psi(W, \hat{W}, 0) + \Phi(W, \hat{W}, 0)} \int_{-\pi}^{\pi} d\phi \, e^{i\phi k + \Omega(\hat{W}, k, \phi)}}.$$
(A.17)

We next need to find the saddle point(s) of the function (A.12), by variation of $\{W, \hat{W}\}$. Functional differentiation with respect to W and \hat{W} gives the following equations, respectively:

$$i\hat{W}_{sk}(\phi) = -\langle k \rangle \sum_{s'k'} \int d\phi' W_{s'k'}(\phi') Q(k,k') [e^{-i(2\psi_{ss'} + \phi + \phi')} - 1]$$
(A.18)

$$W_{sk}(\phi) = \delta_{s0} p_k \frac{\mathrm{e}^{\mathrm{i}[\phi k - W_{0k}(\phi)]}}{\int_{-\pi}^{\pi} \mathrm{d}\phi' \,\mathrm{e}^{\mathrm{i}[\phi' k - \hat{W}_{0k}(\phi')]}}.$$
(A.19)

Upon eliminating \hat{W} and defining $W_{sk}(\phi) = \delta_{s0} p_k \chi_k(\phi)$, we obtain an equation for $\chi_k(\phi)$ only

$$\chi_k(\phi) = \frac{\mathrm{e}^{\mathrm{i}\phi k + \langle k \rangle \sum_{k'} p_{k'} \mathcal{Q}(k,k') \, \mathrm{e}^{-\mathrm{i}\phi} \int \mathrm{d}\phi' \chi_{k'}(\phi') \, \mathrm{e}^{-\mathrm{i}\phi'}}}{\int_{-\pi}^{\pi} \mathrm{d}\phi' \, \mathrm{e}^{\mathrm{i}\phi' k + \langle k \rangle \sum_{k'} p_{k'} \mathcal{Q}(k,k') \, \mathrm{e}^{-\mathrm{i}\phi'} \int \mathrm{d}\phi'' \chi_{k'}(\phi'') \, \mathrm{e}^{-\mathrm{i}\phi''}}}.$$
(A.20)

One defines $a_k = \int d\phi' \chi_k(\phi') e^{-i\phi'}$ and $b_k = \langle k \rangle \sum_{k'} p_{k'} Q(k, k') a_{k'}$, and finds after some simple manipulations that $a_0 = 0$ and $a_{k>0} = k/b_k$. This leaves a closed equation for b_k , which shows that $\lim_{N\to\infty} b_k = \langle k \rangle F(k)$, see (32), and a corresponding formula for $\chi_k(\phi)$

$$b_{k} = \langle k \rangle \sum_{k'>0} p_{k'} Q(k, k') k' / b_{k'}$$
(A.21)

$$\chi_k(\phi) = \frac{k!}{2\pi} (b_k \,\mathrm{e}^{-\mathrm{i}\phi})^{-k} \exp[b_k \,\mathrm{e}^{-\mathrm{i}\phi}]. \tag{A.22}$$

At the relevant saddle point, we find as a direct consequence of the form $W_{sk}(\phi) = \delta_{s0} p_k \chi_k(\phi)$ that the functions $\Psi(W, \hat{W}, \psi)$ and $\Phi(W, \hat{W}, \psi)$ are both independent of the variable ψ . This ensures that expression (A.17) is well defined, but it also gives us $L_k(\psi) = 1$, and hence

$$P(r|k) = \delta_{r0}.\tag{A.23}$$

We conclude that in our ensemble (2) the fraction of nodes in a loop of length three vanishes in the limit $N \to \infty$, independent of the degree distribution p(k) and independent of the choice made for the deformation function Q(k, k').

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