Spin models on random graphs with controlled topologies beyond degree constraints

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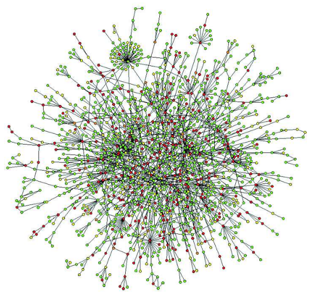
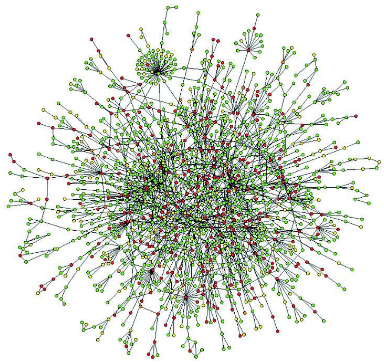
(work in progress)



Motivation - processes on random graphs
Deformed random graph ensembles
Replica analysis
Phase diagrams for specific deformations
Summary and outlook

1. MOTIVATION



Model processes on complex real graphs
by *solvable* processes on suitable *random* graphs

e.g. Ising systems,
graph $\mathbf{c}^\star = \{c^\star_{ij}\}$ $\qquad H = -J\sum_{i<j} c^\star_{ij}\sigma_i\sigma_j \qquad c^\star_{ij}\in\{0,1\}$

level 0 :

measure average connectivity $\langle k\rangle = N^{-1}\sum_{ij} c^\star_{ij}$
draw random $\mathbf{c}$ from Erdös-Rényi ensemble

$$\text{Prob}(\mathbf{c}) = \prod_{i<j}[\frac{\langle k\rangle}{N}\delta_{c_{ij},1} + (1-\frac{\langle k\rangle}{N})\delta_{c_{ij},0}]$$

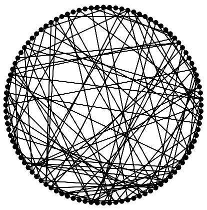
level 1 :

measure degrees $\{k^\star_1,\ldots,k^\star_N\}$, $\;k^\star_i = \sum_j c^\star_{ij}$
draw random $\mathbf{c}$ from degree-constrained ensemble

$$\text{Prob}(\mathbf{c}) = \frac{1}{\mathcal{Z}_N}\prod_{i<j}[\frac{\langle k\rangle}{N}\delta_{c_{ij},1} + (1-\frac{\langle k\rangle}{N})\delta_{c_{ij},0}].\prod_i \delta_{k^\star_i,\sum_j c_{ij}}$$

Examples:

	Erdös-Renyi (level 0)	*degree-constrained (level 1)*	*exact solution*
1D Ising model:	$\langle k \rangle = 2$	$p(k) = \delta_{k,2}$	
	$T_c/J \approx 1.820$	$T_c/J = 0$	$T_c/J = 0$
2D Ising model:	$\langle k \rangle = 4$	$p(k) = \delta_{k,4}$	
	$T_c/J \approx 3.915$	$T_c/J \approx 2.885$	$T_c/J \approx 2.269$
3D Ising model:	$\langle k \rangle = 6$	$p(k) = \delta_{k,6}$	
	$T_c/J \approx 5.944$	$T_c/J \approx 4.933$	$T_c/J \approx 4.51?$
small world model:	$\langle k \rangle = 2 + c$	$p(k \geq 2) = \frac{e^{-c}c^{k-2}}{(k-2)!}$	
$c = 0:$	$T_c/J \approx 1.820$	$T_c/J = 0$	$T_c/J = 0$
$c = 1:$	$T_c/J \approx 2.885$	$T_c/J \approx 2.183$	$T_c/J \approx 2.269$
$c = 2:$	$T_c/J \approx 3.915$	$T_c/J \approx 3.403$	$T_c/J \approx 3.466$



models with the same $p(k)$ can behave quite differently ...

Level 2 random graph ensembles?

- include topological information on $\mathbf{c}^\star$ beyond degrees
- keep model solvable
- additional information must be relevant (phase diagram)

Deformed degree-constrained ensembles

$$\text{level 0}: \qquad \text{Prob}(\mathbf{c}) = \prod_{i<j}[\frac{\langle k\rangle}{N}\delta_{c_{ij},1} + (1-\frac{\langle k\rangle}{N})\delta_{c_{ij},0}]$$

$$\text{level 1}: \qquad \text{Prob}(\mathbf{c}) = \frac{1}{\mathcal{Z}_N}\prod_{i<j}[\frac{\langle k\rangle}{N}\delta_{c_{ij},1} + (1-\frac{\langle k\rangle}{N})\delta_{c_{ij},0}].\prod_i \delta_{k_i^\star,\sum_j c_{ij}}$$

$$\text{level 2}: \qquad \text{Prob}(\mathbf{c}) = \frac{1}{\mathcal{Z}_N}\prod_{i<j}[\frac{\langle k\rangle}{N}Q(k_i,k_j)\delta_{c_{ij},1} + (1-\frac{\langle k\rangle}{N}Q(k_i,k_j))\delta_{c_{ij},0}].\prod_i \delta_{k_i^\star,\sum_j c_{ij}}$$

$$\text{with}: \qquad Q(k,k')\geq 0 \;\; \forall k,k' \qquad \sum_{k,k'\geq 0} p(k)p(k')Q(k,k') = 1$$

Ising models on random graphs
drawn from deformed degree-constrained ensembles

$$H(\boldsymbol{\sigma}) = -\sum_{i<j} c_{ij}\sigma_i J_{ij}\sigma_j$$

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

characteristics:

- $\{k_1,\ldots,k_N\}$ drawn randomly from $p(k)$
- $\{J_{ij}\}$ drawn randomly from $P(J)$
- ensemble parametrized by: $p(k)$ and $Q(k,k')$
- graphs locally tree-like, e.g. $\lim_{N\to\infty} p(k,r) = p(k)\delta_{r,0}$
  $p(k,r) = N^{-1}\sum_i \delta_{k,\sum_j c_{ij}}\delta_{r,\sum_{jk} c_{ij}c_{jk}c_{ki}}$

These models are *solvable*,
calculate average of free energy per spin over disorder (bonds, graphs)
how do phase diagrams depend on $p(k)$ and $Q(k,k')$?

question:
Before we start, should we expect that
introducing $Q(k,k')$ can make a serious difference?

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

answer:
choose arbitrary degree distribution $p(k)$,
with $\langle k\rangle > 0$ and $\langle k^2\rangle - \langle k\rangle^2 > 0$,
compare the following microscopic realizations:

$A:$	$Q(k,k') = 1$	standard degree constrained ensemble, phase diagram depends on $\langle k^2\rangle$ and $\langle k\rangle$ only
$B:$	$Q(k,k') = \gamma\delta_{kk'}$	collection of *disconnected* regular graphs, one for each degree k with $p(k) > 0$ transitions : those of regular graph with $k = k^\star$ $k^\star$: largest k with $p(k) > 0$

3. EQUILIBRIUM REPLICA ANALYSIS

In a nutshell ...

exploit $\overline{\log Z} = \lim_{n\to 0} n^{-1} \log \overline{Z^n}$,
and assume initially that n integer

$$\begin{aligned}\overline{f} &= -\lim_{N\to\infty} \frac{1}{\beta N} \overline{\log \sum_{\boldsymbol{\sigma}} e^{-\beta H(\boldsymbol{\sigma})}} = -\lim_{N\to\infty} \lim_{n\to 0} \frac{1}{\beta n N} \log \overline{[\sum_{\boldsymbol{\sigma}} e^{-\beta H(\boldsymbol{\sigma})}]^n} \\ &= -\lim_{N\to\infty} \lim_{n\to 0} \frac{1}{\beta n N} \log \sum_{\boldsymbol{\sigma}^1} \ldots \sum_{\boldsymbol{\sigma}^n} \overline{e^{-\beta \sum_{\alpha=1}^n H(\boldsymbol{\sigma}^\alpha)}}\end{aligned}$$

- carry out average $\overline{\cdots}$ over bonds and graphs *first*
- exchange limits $N \to \infty$ and $n \to 0$
- steepest descent integration as $N \to \infty$, for finite n
- ergodicity ansatz for order parameters of replicated spin system
- take the limit $n \to 0$
- order parameters: functions (effective & cavity field distributions)
- study bifurcations in order parameter eqns via moment expansions

Stage 1:
order parameter eqns after limit $N \to \infty$
(steepest descent)
$\boldsymbol{\sigma} = (\sigma_1, \ldots, \sigma_n)$

$$
\begin{aligned}
F(k, \boldsymbol{\sigma}) &= \sum_{k'} Q(k, k') \sum_{\boldsymbol{\sigma}'} D(k', \boldsymbol{\sigma}') \int dJ \; P(J) e^{\beta J \boldsymbol{\sigma} \cdot \boldsymbol{\sigma}'} \\
D(k, \boldsymbol{\sigma}) &= \frac{p(k) k}{\langle k \rangle} \frac{F^{k-1}(k, \boldsymbol{\sigma})}{\sum_{\boldsymbol{\sigma}'} F^k(k, \boldsymbol{\sigma}')} \\
\overline{f} &= -\lim_{n \to 0} \frac{1}{\beta n} \sum_k p(k) \log \left[\sum_{\boldsymbol{\sigma}} [F(k, \boldsymbol{\sigma}) / F(k)]^k \right]
\end{aligned}
$$

Stage 2:
make ergodic ansatz ('replica symmetry')

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

$$
D(k, h) = D(h|k) D(k), \;\; \int dh \; D(h|k) = 1 \qquad F(k, h) = F(h|k) F(k), \;\; \int dh \; F(h|k) = 1
$$

Stage 3:
take the limit $n \to 0$,
eliminate $D(k)$ and $D(h|k)$,
leaves closed eqns for $F(k)$ and $F(h|k)$:

$$
\begin{aligned}
F(k) &= \langle k\rangle^{-1} \sum_{k'} p(k')k'Q(k,k')F^{-1}(k') \\
F(h|k) &= \sum_{k'} \frac{Q(k,k')p(k')k'}{\langle k\rangle F(k)F(k')} \int dJ\ P(J) \int \prod_{\ell<k} [dh_\ell F(h_\ell|k')] \\
&\qquad \times \delta[h - \beta^{-1}\text{atanh}[\tanh(\beta J)\tanh(\beta \sum_{\ell<k} h_\ell)]]
\end{aligned}
$$

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

Stage 4:

Physical meaning of replica-symmetric (RS) order parameters

$$\boldsymbol{\sigma}=(\sigma_1,\ldots,\sigma_n): \qquad P(k,\boldsymbol{\sigma}) = \lim_{N\to\infty}\frac{1}{N}\sum_i \overline{\left[\frac{\sum_{\boldsymbol{\sigma}_1\ldots\boldsymbol{\sigma}_N}\delta_{k,k_i}\delta_{\boldsymbol{\sigma},\boldsymbol{\sigma}_i}e^{-\beta\sum_\alpha H(\boldsymbol{\sigma}^\alpha)}}{\sum_{\boldsymbol{\sigma}_1\ldots\boldsymbol{\sigma}_N}e^{-\beta\sum_\alpha H(\boldsymbol{\sigma}^\alpha)}}\right]}$$

$$= p(k)\int dh\; W(h|k)\frac{e^{\beta h\sum_{\alpha=1}^n\sigma_\alpha}}{[2\cosh(\beta h)]^n}$$

degree-conditioned effective field distr:

$$W(h|k)=\int\prod_{\ell\leq k}[dh_\ell F(h_\ell|k)]\;\delta[h-\sum_{\ell\leq k}h_\ell]$$

$W(h)=\sum_k p(k)W(h|k)$:

$$m = \lim_{N\to\infty}\frac{1}{N}\sum_i\overline{\langle\sigma_i\rangle} = \int dh\; W(h)\tanh(\beta h)$$

$$q = \lim_{N\to\infty}\frac{1}{N}\sum_i\overline{\langle\sigma_i\rangle^2} = \int dh\; W(h)\tanh^2(\beta h)$$

$$\overline{f}=-\frac{1}{\beta}\int dh\; W(h)\log[2\cosh(\beta h)]$$

4. PHASE DIAGRAMS FOR SPECIFIC DEFORMATION FUNCTIONS

choose bond distribution

$$P(J) = \frac{1}{2}(1+\eta)\delta(J-J_0) + \frac{1}{2}(1-\eta)\delta(J+J_0)$$

Procedure:

- always the paramagnetic (P) soln $F(h|k) = \delta(h)$, where $m = q = 0$
- it is the *only* solution for $T \to \infty$
- assume bifurcations away from $F(h|k) = \delta(h)$ are *continuous*,
  so expand in moments of $F(h|k)$:
  assume $\exists\epsilon$ with $0 < |\epsilon| \ll 1$ such that

$$\int dh\ h^\ell F(h|k) = \mathcal{O}(\epsilon^\ell)$$

- bifurcating order ϵ: state has $m \neq 0$, $q > 0$ $\rightarrow$ ferromagnet (F)
  bifurcating order ϵ^2: state has $m = 0$, $q > 0$ $\rightarrow$ spin-glass (SG)

result of bifurcation analysis:

$$\eta > \tanh(\beta J_0): \qquad \mathrm{P}\to\mathrm{F}, \qquad T_{\mathrm{F}}/J_0 = 2/\log\left[\frac{\eta\lambda_{\max}(Q,p)+1}{\eta\lambda_{\max}(Q,p)-1}\right]$$

$$\eta < \tanh(\beta J_0): \qquad \mathrm{P}\to\mathrm{SG}, \quad T_{\mathrm{SG}}/J_0 = 2/\log\left[\frac{\sqrt{\lambda_{\max}(Q,p)}+1}{\sqrt{\lambda_{\max}(Q,p)}-1}\right]$$

$$\lambda(Q,p): \qquad \text{eigenvalues of} \quad M_{kk'} = \frac{Q(k,k')p(k')k'(k'-1)}{\langle k\rangle F(k)F(k')}, \qquad k,k'=0,1,2,3,\ldots$$

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

notes:

- one expects RSB solutions (broken replica symmetry), but *at or below* the RS critical temperatures
- the F→SG transition is much harder to find analytically, but could be constructed via Parisi-Toulouse hypothesis

Choices considered

$$
\begin{aligned}
\text{Type I}: &\quad Q(k,k') = g(k)g(k')/\langle g\rangle^2, && g(k)\geq 0\ \forall k, \quad \langle g\rangle = \sum_k p(k)g(k) > 0 \\
\text{Type II}: &\quad Q(k,k') = [g(k)+g(k')]/2\langle g\rangle, && g(k)\geq 0\ \forall k, \quad \langle g\rangle > 0 \\
\text{Type III}: &\quad Q(k,k') = \gamma_0 + \gamma\delta_{kk'}, && \gamma_0 = 1-\gamma\sum_k p^2(k), \quad |\gamma| \leq [\sum_k p^2(k)]^{-1}
\end{aligned}
$$

no deformation: $Q(k,k')=1$

$$
\eta > \tanh(\beta J_0): \qquad \mathrm{P}\to\mathrm{F}, \qquad T_{\mathrm{F}}/J_0 = 2/\log\left[\frac{\eta[\langle k^2\rangle/\langle k\rangle - 1]+1}{\eta[\langle k^2\rangle/\langle k\rangle - 1]-1}\right]
$$

$$
\eta < \tanh(\beta J_0): \qquad \mathrm{P}\to\mathrm{SG}, \quad T_{\mathrm{SG}}/J_0 = 2/\log\left[\frac{\sqrt{\langle k^2\rangle/\langle k\rangle - 1}+1}{\sqrt{[\langle k^2\rangle/\langle k\rangle - 1]}-1}\right]
$$

Type I: $Q(k,k') = g(k)g(k')/\langle g\rangle^2$

trivial: $g(k)$ drops out of transition lines and order parameter eqns, for any $p(k)$, complete solution identical to that of $Q(k,k')=1$ ...

Type II: $Q(k,k') = [g(k)+g(k')]/2\langle g\rangle$

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

y to be solved from $$\langle\frac{k}{yg(k)+1}\rangle = \frac{1}{2}\langle k\rangle$$

Type III: $Q(k,k') = \gamma_0 + \gamma\delta_{kk'}$

$\lambda_{\max}(Q,p)$: largest soln of

$$\begin{aligned} 1 &= [1-\gamma\langle p(k)\rangle]\langle\frac{4k(k-1)}{\lambda\langle k\rangle[y+\sqrt{y^2+4\gamma p(k)k/\langle k\rangle}]^2 - 4\gamma p(k)k(k-1)}\rangle \\ y &= \frac{1-\gamma\langle p(k)\rangle}{\langle k\rangle}\langle\frac{2k}{y+\sqrt{y^2+4\gamma p(k)k/\langle k\rangle}}\rangle \end{aligned}$$

$\lim_{\gamma_0\to 0}\lambda_{\max}(Q,p) = k^\star - 1$,
$k^\star$: largest degree with $p(k) > 0$

Results for ensembles with type II and type III deformations

Example degree distributions:

$$\text{Poissonnian :} \qquad p(k) = c^k e^{-c}/k!$$
$$\text{power law :} \qquad p(k) = (1-\frac{c\,\zeta(3+\alpha)}{\zeta(2+\alpha)})\delta_{k0} + (1-\delta_{k0})\frac{ck^{-3-\alpha}}{\zeta(2+\alpha)}$$

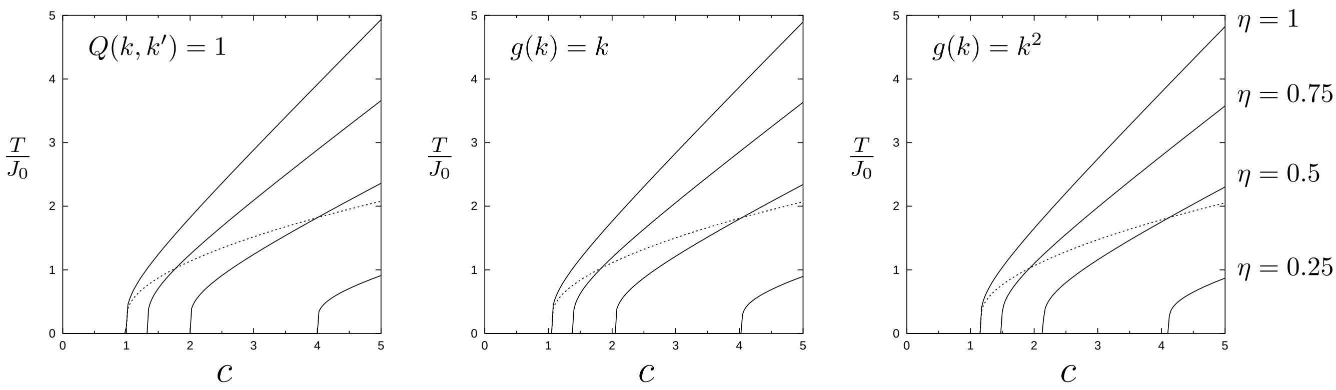
$\zeta(x) = \sum_{k>0} k^{-x}$,
$\alpha \in [0,1]$, so $\langle k \rangle < \infty$ but $\langle k^2 \rangle \to \infty$ for $\alpha \downarrow 0$

notes:

- always $\langle k \rangle = c$
- power-law: bifurcation lines type II deformations indep of c
- In practice: $k \leq k_{\max} = 10^8$

Poissonian $p(k)$ with type II deformations

$Q(k,k') = [k^\ell + (k')^\ell]/2\langle k^\ell \rangle$



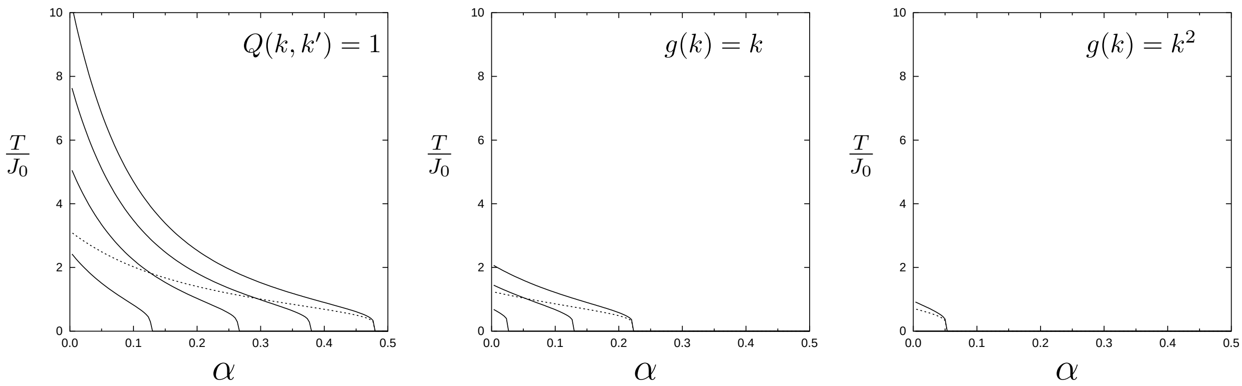
P→SG (dotted) and P→F (solid)

$$P(J)=\tfrac{1}{2}(1+\eta)\delta(J-J_0)+\tfrac{1}{2}(1-\eta)\delta(J+J_0)$$

impact of deformation:
small reduction of all critical temperatures

Power law $p(k) \sim k^{-3-\alpha}$ with type II deformations

$Q(k,k') = [k^\ell + (k')^\ell]/2\langle k^\ell \rangle$



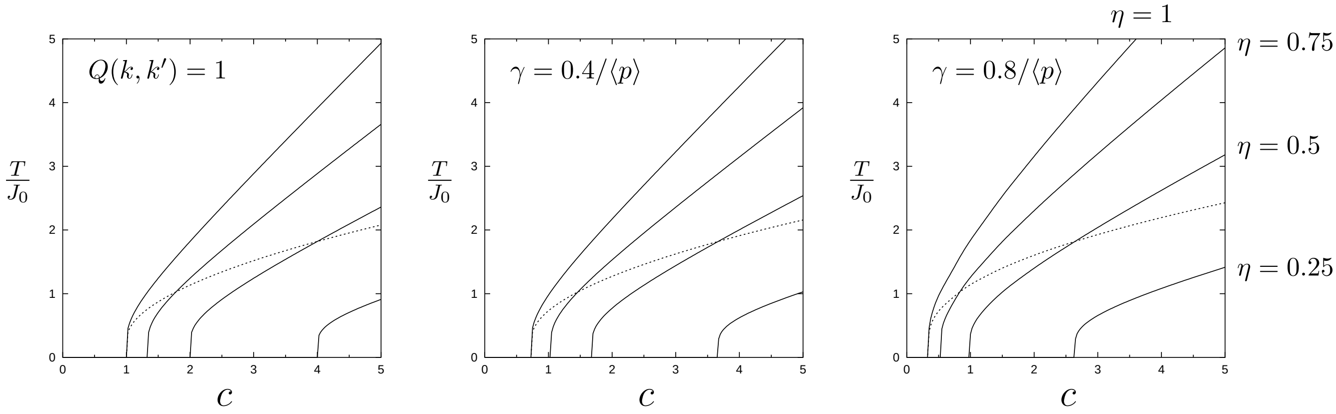
P→SG (dotted) and P→F (solid)

$$P(J) = \frac{1}{2}(1+\eta)\delta(J-J_0) + \frac{1}{2}(1-\eta)\delta(J+J_0)$$

impact of deformation:
dramatic reduction of all critical temperatures

Poissonian $p(k)$ with type III deformations

$Q(k,k') = \gamma_0 + \gamma\delta_{kk'}$



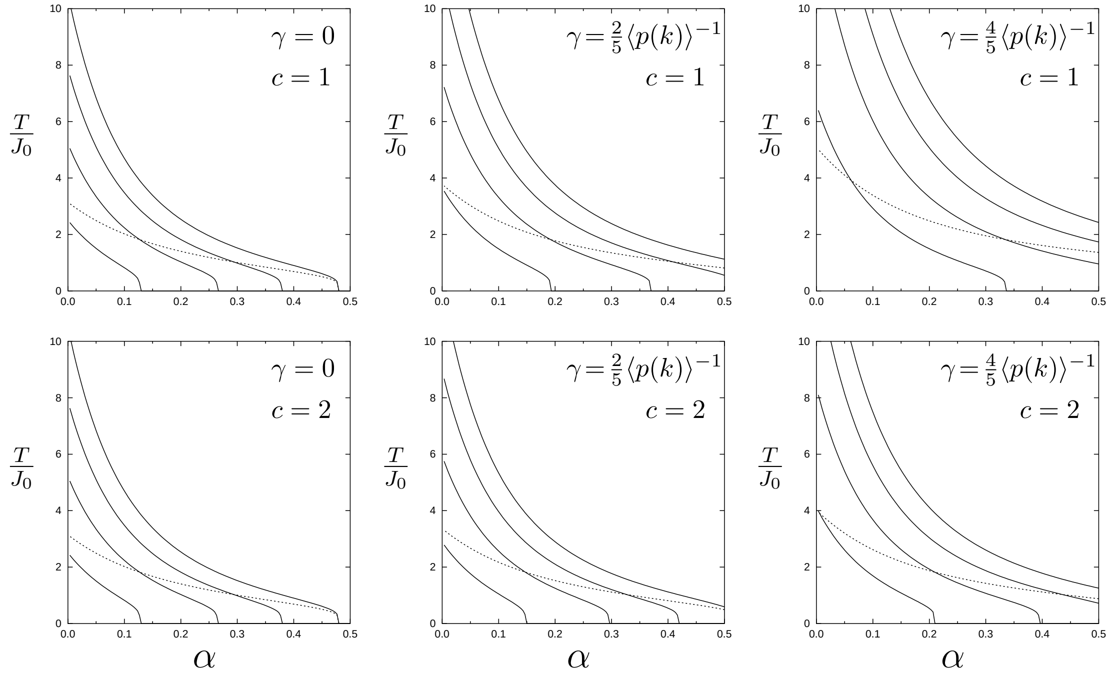
P→SG (dotted) and P→F (solid)

$P(J) = \frac{1}{2}(1+\eta)\delta(J-J_0) + \frac{1}{2}(1-\eta)\delta(J+J_0)$

impact of deformation:
significant increase in critical temperatures
$T_F \to \infty$ and $T_F \to \infty$ for $\gamma \to \langle p\rangle^{-1}$

Poissonian $p(k)$ with type III deformations

$$Q(k,k') = \gamma_0 + \gamma\delta_{kk'}$$



5. SUMMARY AND OUTLOOK

- Specifying just the degree distribution $p(k)$ of a connectivity graph for an interacting spin system does not permit reliable predictions on the phase diagram
- Proposed random graph ensembles, characterized by degree distribution $p(k)$ and additional deformation $Q(k,k')$

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

  - allow us to differentiate between models with same $p(k)$, but different microscopic realizations of these degree statistics
  - spin models with connectivity graphs from these ensembles still solvable
  - impact of deformation via $Q(k,k')$ on phase diagram can be non-negligible

- To be done:
  - physical meaning of the $F(k)$, RSB transition lines
  - application: what is optimal $Q(k,k')$ for a given real graph $\mathbf{c}^\star$?

Optimal random graph ensemble $\{p(k), Q(k,k')\}$
to serve as 'solvable proxy' for a given graph $\mathbf{c}^\star$:

- measure $k_i^\star = \sum_j c_{ij}^\star$, define $p(k) = N^{-1}\sum_i \delta_{k,k_i^\star}$
- maximizing log-likelihood of $\mathbf{c}^\star$ for deformed ensemble:
  minimize over Q, subject to $\sum_{kk'} p(k)p(k')Q(k,k') = 1$,
  the quantity

$$\begin{aligned}\Omega[Q] &= -\frac{1}{N}\log \text{Prob}(\mathbf{c}^\star)\\ &= \text{const} \;+\frac{1}{N}\sum_i k_i^\star \log F(k_i^\star|Q) - \frac{1}{N}\sum_{i<j} c_{ij}^\star \log Q(k_i^\star, k_j^\star) + \mathcal{O}(N^{-1})\end{aligned}$$

where $F(k|Q)$ is soln of

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