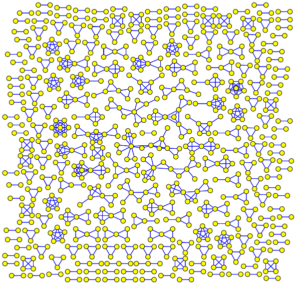
Tools for stochastic processes on loopy networks

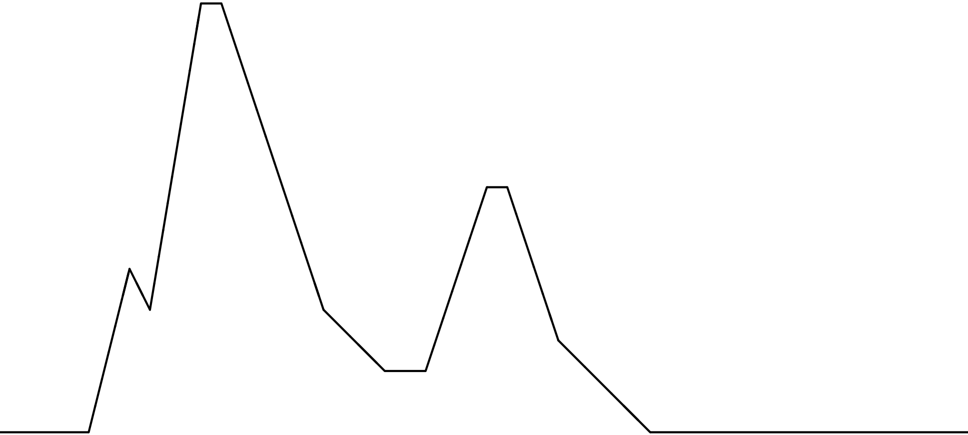
Bardonecchia, Feb 2nd 2015

ACC Coolen

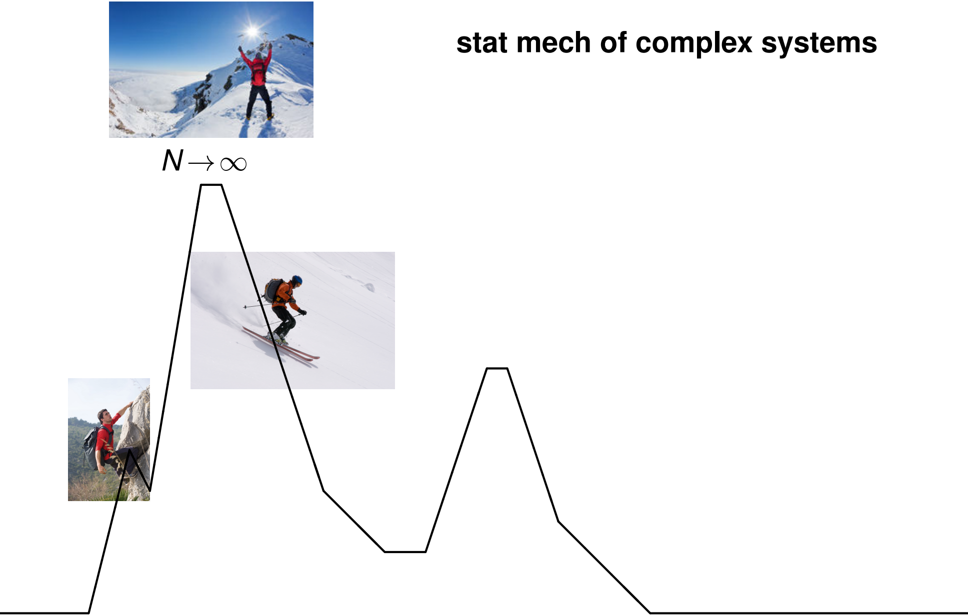
King's College London



stat mech of complex systems

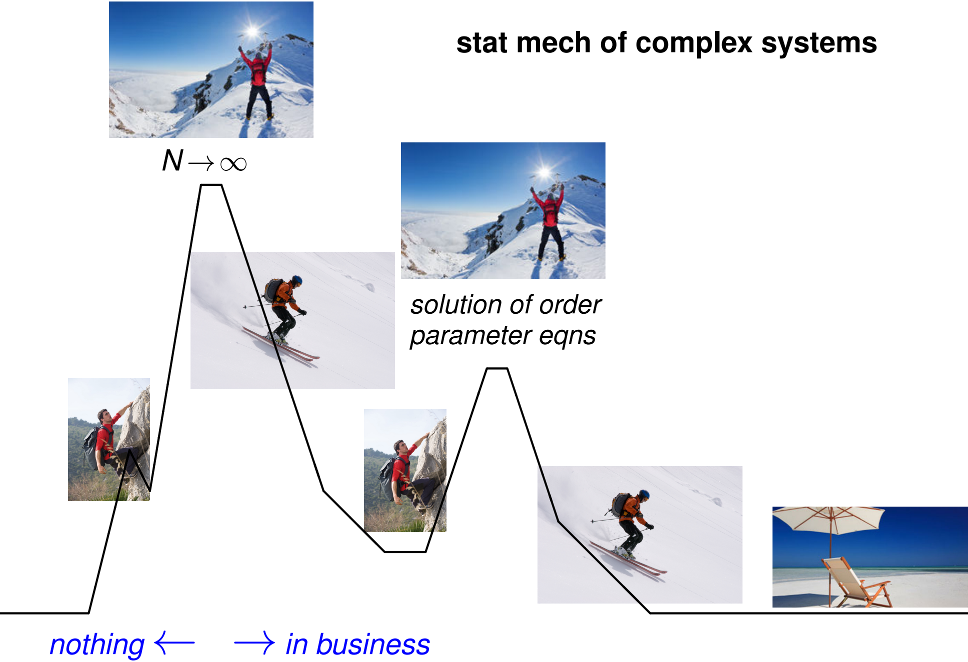


stat mech of complex systems

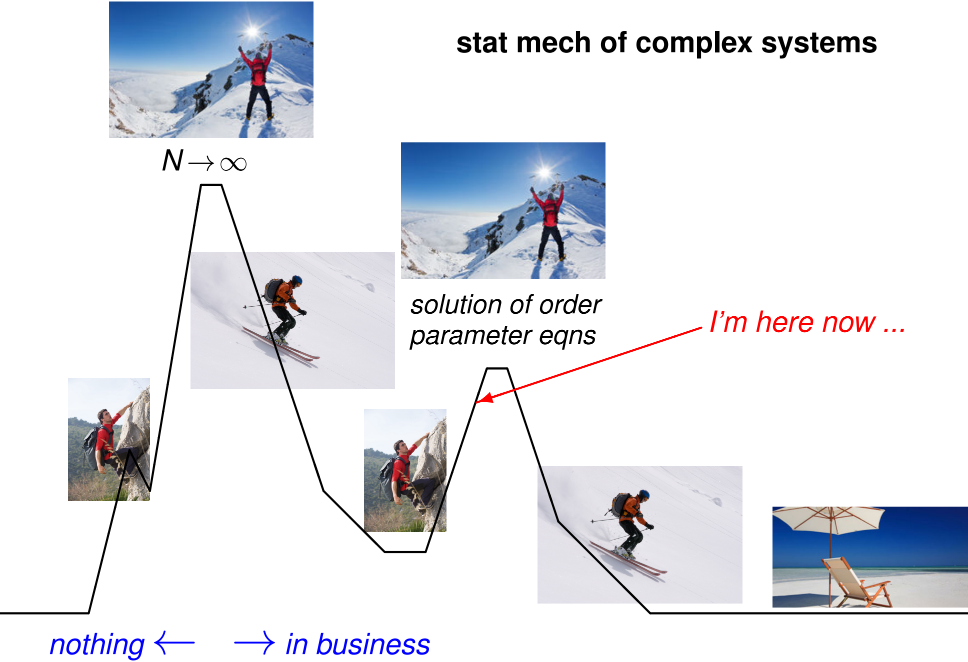


nothing $\leftarrow$ $\rightarrow$ *in business*

stat mech of complex systems



stat mech of complex systems



Outline

Biological processes on networks

- **protein interaction networks**

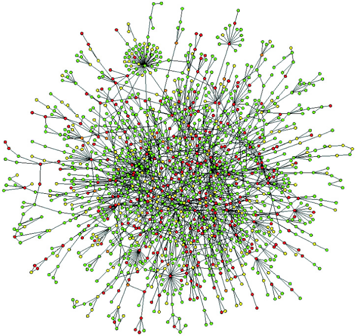
  process: chemical reactions

  nodes: proteins species

  links: $c_{ij} = 1$ if i can bind to j
  $c_{ij} = 0$ otherwise

  nondirected

  $N \sim 10^4$, links/node ~ 7



- **gene regulation networks**

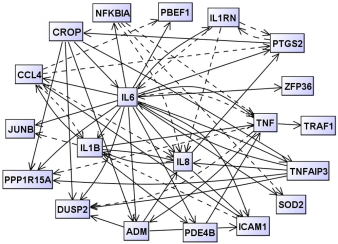
  process: transcription

  nodes: genes

  links: $c_{ij} = 1$ if j is transcription factor of i
  $c_{ij} = 0$ otherwise

  directed

  $N \sim 10^4$, links/node ~ 5



Problem I was interested in

- non-equilibrium statistical mechanics of biochemical reaction processes using generating functional analysis (proteome, transcriptome)

  [ACCC, Rabello 2009]

then got side-tracked ...

- need realistic graph ensembles in GFA:
  tailoring random graphs to resemble observed networks

  [ACCC, Perez-Vicente 2008; Bianconi, ACCC, Perez-Vicente 2008; Annibale et al 2009, Roberts, ACCC, Schlitt 2011; Roberts, ACCC 2014; Annibale, ACCC, Planell-Morell 2015]

- protein interaction data very unreliable:
  modelling/decontaminating experimental bias

  [Annibale, ACCC 2011]

- algorithms for generating random graphs from tailored ensembles

  [ACCC, De Martino, Annibale 2009; Roberts, ACCC 2012]

Random graphs as proxies

stat mech of process on network $\mathbf{c}^\star$,
use *random* graph $\mathbf{c}$ as proxy

- tailored random graph ensemble Ω_L:

  max entropy ensemble, constrained by values of $\omega_1(\mathbf{c})\ldots\omega_L(\mathbf{c})$

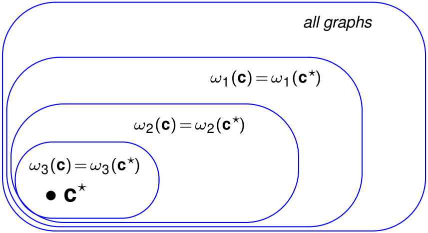
$$\Omega_L^{\rm hard}: \qquad p(\mathbf{c}) \propto \prod_{\ell\leq L} \delta_{\omega_\ell(\mathbf{c}),\omega_\ell(\mathbf{c}^\star)}$$

$$\Omega_L^{\rm soft}: \qquad p(\mathbf{c}) \propto {\rm e}^{\sum_{\ell=1}^L \hat{\omega}_\ell \omega_\ell(\mathbf{c})}, \quad \langle \omega_\ell(\mathbf{c})\rangle = \omega_\ell(\mathbf{c}^\star)\ \ \forall \ell$$

- approximate process on $\mathbf{c}^\star$:

  average generating function of process over graphs in Ω_L

  larger $L \to$ better approx



which observables
$\boldsymbol{\omega}(\mathbf{c}) = \{\omega_1(\mathbf{c}), \ldots, \omega_L(\mathbf{c})\}$
to carry over from real network?

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

- in statics:

$$\overline{\mathrm{e}^{-\beta \sum_{\alpha=1}^{n} H(\boldsymbol{\sigma}^{\alpha})}} = \frac{\sum_{\mathbf{c}} \delta_{\boldsymbol{\omega},\boldsymbol{\omega}(\mathbf{c})} \mathrm{e}^{\sum_{i<j} c_{ij} L_{ij}}}{\sum_{\mathbf{c}} \delta_{\boldsymbol{\omega},\boldsymbol{\omega}(\mathbf{c})}}, \qquad L_{ij} = \beta J_{ij} \sum_{\alpha=1}^{n} \sigma_i^{\alpha} \sigma_j^{\alpha}$$

- in dynamics:

$$\overline{\mathrm{e}^{-\mathrm{i} \sum_{it} \hat{h}_i(t) \sum_j c_{ij} J_{ij} \sigma_j(t)}} = \frac{\sum_{\mathbf{c}} \delta_{\boldsymbol{\omega},\boldsymbol{\omega}(\mathbf{c})} \mathrm{e}^{\sum_{i<j} c_{ij} L_{ij}}}{\sum_{\mathbf{c}} \delta_{\boldsymbol{\omega},\boldsymbol{\omega}(\mathbf{c})}}, \qquad L_{ij} = -\mathrm{i} J_{ij} \sum_{t} [\hat{h}_i(t)\sigma_j(t) + \hat{h}_j(t)\sigma_i(t)]$$

in both cases
to do *analytically*:

$$\sum_{\mathbf{c}} \underbrace{\delta_{\boldsymbol{\omega},\boldsymbol{\omega}(\mathbf{c})}}_{\textit{hard}} \underbrace{\mathrm{e}^{\sum_{i<j} c_{ij} L_{ij}}}_{\textit{easy}}$$

seems to boil down to:
can we calculate ensemble entropy?

Shannon entropy per node
of tailored graph ensembles

- constraint: $\langle k\rangle$
  (ER ensemble)

$$S = \frac{1}{2}[1+\log(\frac{N}{\langle k\rangle})] + \ \ldots$$

- constraints:
  $p(k) = \frac{1}{N}\sum_i \delta_{k,k_i(\mathbf{c})}$

$$S = \frac{1}{2}[1+\log(\frac{N}{\langle k\rangle})] - \frac{1}{\langle k\rangle}\sum_k p(k)\log[\frac{p(k)}{\pi(k)}] + \ \ldots$$

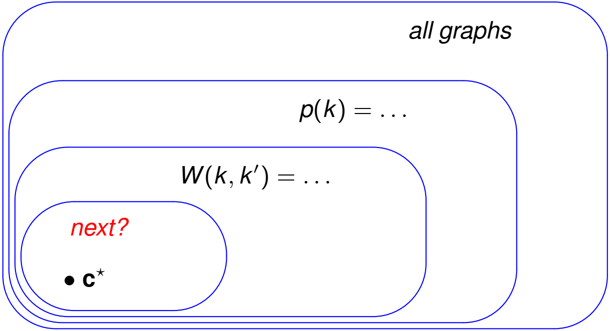
$$\pi(k) = \mathrm{e}^{-\langle k\rangle}\langle k\rangle^k/k!$$

- constraints:
  $p(k) = \frac{1}{N}\sum_i \delta_{k,k_i(\mathbf{c})}$
  $W(k,k') = \frac{1}{\langle k\rangle N}\sum_{ij} c_{ij}\delta_{k,k_i(\mathbf{c})}\delta_{k',k_j(\mathbf{c})}$

$$S = \frac{1}{2}[1+\log(\frac{N}{\langle k\rangle})] - \frac{1}{\langle k\rangle}\sum_k p(k)\log[\frac{p(k)}{\pi(k)}]$$
$$-\frac{1}{2}\sum_{k,k'} W(k,k')\log\left[\frac{W(k,k')}{W(k)W(k')}\right] + \ \ldots$$

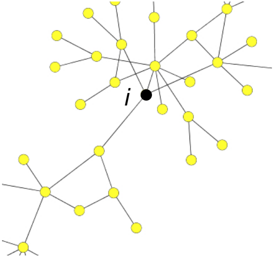
[Annibale, ACCC, Roberts, ... 2009-2011]

Tailoring graphs further ...



candidates:

generalised degrees, node neighbourhoods,
...



$$k_i = \sum_j c_{ij} = 4$$
$$m_i = \sum_{jk} c_{ij} c_{jk} = 20$$

$$n_i = (k_i;\ \{\xi_i^s\}) = (4;\ 3, 4, 6, 7)$$

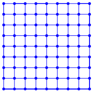
[Roberts & ACCC 2014]

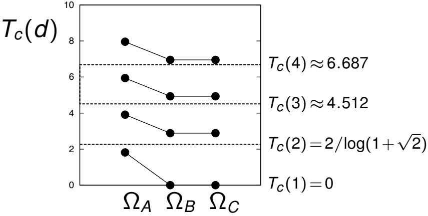
Graphs with many short loops

Ising spin models on tailored random graphs

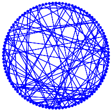
Ω_A: correct $\langle k \rangle$
Ω_B: correct $p(k)$
Ω_C: correct $p(k)$ and $W(k,k')$

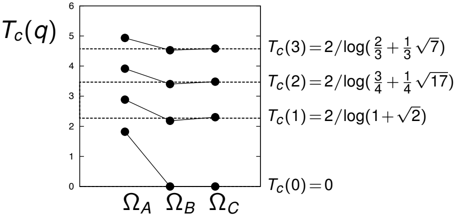
- $\mathbf{c}^\star$ = d-dim cubic lattice
  $p(k) = \delta_{k,2^d}$





- $\mathbf{c}^\star$ = ‘small world’ lattice
  $p(k \geq 2) = \mathrm{e}^{-q} q^{k-2}/(k-2)!$



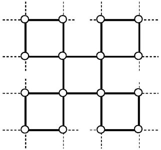


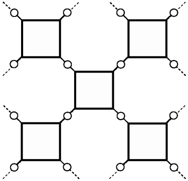
It is all about short loops ...

			critical temperatures $T_c(d)$			
	degrees	4-loops	$d=1$	$d=2$	$d=3$	$d=4$
random, $\langle k\rangle=2d$			1.820	3.915	5.944	7.958
random, $p(k)=\delta_{k,2d}$	✓		0	2.885	4.933	6.952
hypercubic Bethe	✓	✓	0	2.771	4.839	6.879
true cubic lattice	✓	✓	0	2.269	4.511	6.680

hypercubic Bethe lattice:
'tree of hypercubes'

– *correct local degrees*
– *geometric (non-random)*
– *finite nr of short loops per site*





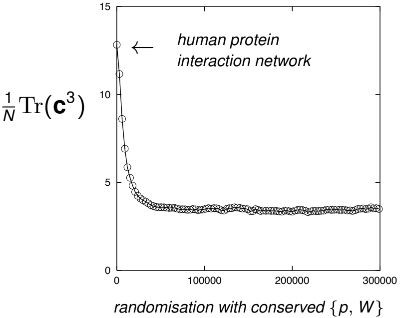
[Roberts & ACCC 2014, Mozeika & ACCC 2015]

most informative
next observable $\omega(\mathbf{c})$
to add?

- random graphs with prescribed $p(k)$, $W(k,k')$:
  locally tree-like ...

  protein interaction networks:
  many short loops ...

  realistic physical lattices:
  many short loops ...



- realistic graphs:
  $\omega(\mathbf{c})$ *must count short loops*

  most analysis methods,
  e.g. replicas, GFA, cavity, belief prop, ...
  require locally tree-like graphs

  (modulo loop corrections)

exceptions:

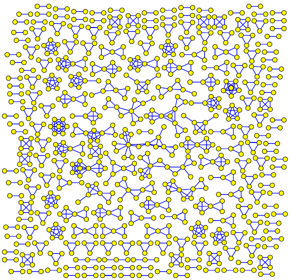
cubic lattices $d < 3$
spherical models
recent immune models

Immune model
of Agliari and Barra

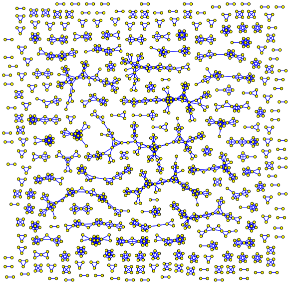
B-clones $\{b_\mu\}$, T-clones $\{\sigma_i\}$ and cytokines $\{\xi_i^\mu\}$
map to model with effective T-T interactions

$$H = -\sum_{i<j} J_{ij}\sigma_i\sigma_j, \qquad J_{ij} = \sum_{\mu=1}^{\alpha N} \xi_i^\mu \xi_j^\mu, \qquad p(\xi_i^\mu) = \frac{c}{2N}\left[\delta_{\xi_i^\mu,1} + \delta_{\xi_i^\mu,-1}\right] + (1-\frac{c}{N})\delta_{\xi_i^\mu,0}$$

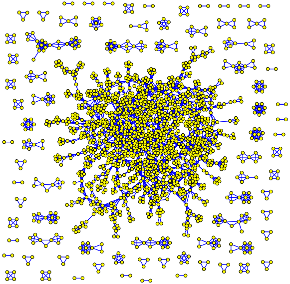
$\alpha c^2 < 1$



$\alpha c^2 = 1$

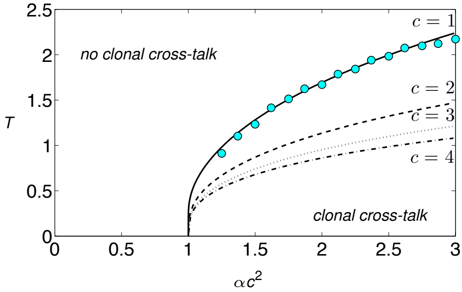


$\alpha c^2 > 1$



Exactly solvable
in spite of short loops ...

[Agliari, Annibale, Barra, ACCC, Tantari, 2013]



here: $\mathbf{J} = \boldsymbol{\xi}^\dagger \boldsymbol{\xi}$
$\boldsymbol{\xi}$: sparse $p \times N$ matrix with iid entries

map to model with spins + Gaussian fields,
on tree-like bipartite graph $\boldsymbol{\xi}$

$$\sum_{\boldsymbol{\sigma}} \mathrm{e}^{\beta \sum_{i<j} J_{ij} \sigma_i \sigma_j} = \int \frac{\mathrm{d}\mathbf{z}}{(2\pi)^{p/2}} \sum_{\boldsymbol{\sigma}} \mathrm{e}^{\sqrt{\beta} \sum_{\mu i} z_\mu \xi_{\mu i} \sigma_i - \frac{1}{2} \sum_\mu z_\mu^2}$$

is a special case!

Strauss ensemble (aka random triangle model)

Simplest loopy graph ensemble

control $\langle k \rangle$
and nr of triangles

$$p(\mathbf{c}) \propto \mathrm{e}^{u\sum_{ij} c_{ij} + v\sum_{ijk} c_{ij}c_{jk}c_{ki}}$$

[Strauss 1986; Jonasson 1999]

- to calculate:

$$\langle k \rangle = \langle \frac{1}{N}\sum_{ij} c_{ij} \rangle, \qquad \langle m \rangle = \langle \frac{1}{N}\sum_{ijk} c_{ij}c_{jk}c_{ki} \rangle, \qquad S = -\frac{1}{N}\sum_{\mathbf{c}} p(\mathbf{c}) \log p(\mathbf{c})$$

- generating function:

$$\phi = \frac{1}{N}\log\sum_{\mathbf{c}} \mathrm{e}^{u\sum_{ij} c_{ij} + v\sum_{ijk} c_{ij}c_{jk}c_{ki}}$$

$$\langle k \rangle = \partial\phi/\partial u$$
$$\langle m \rangle = \partial\phi/\partial v$$
$$S = \phi - u\langle k \rangle - v\langle m \rangle$$

challenge:
sum over graphs

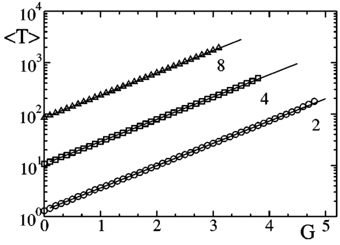
Early results

- Strauss 1986
  - — no theory
  - — triangles 'clump together'
- Jonasson 1999
  - — $u = -\frac{1}{2}\alpha \log N + \ldots$
  - — phase transition, $v_c = \frac{\alpha}{2N} \log N + \ldots$
- Burda et al 2004
  - — $u = -\frac{1}{2} \log N + \ldots$
  - — perturbation theory in v: formula for nr of triangles $\langle T \rangle$, $v_c = \mathcal{O}(\log N) \ldots$
- Park & Newman 2005
  - — $u = \mathcal{O}(1)$ so $\langle k \rangle = \mathcal{O}(N)$
  - — mean-field approx:

$$p(\mathbf{c}) \rightarrow e^{u \sum_{ij} c_{ij} + v \sum_{ijk} c_{ij} \langle c_{jk} c_{ki} \rangle}, \quad \textit{eqns for} \;\; m = \langle c_{ij} \rangle, \; q = \langle c_{ik} c_{kj} \rangle$$

ensemble:

$$p(\mathbf{c}) \propto e^{u \sum_{ij} c_{ij} + v \sum_{ijk} c_{ij} c_{jk} c_{ki}}$$



$G = 6v$

Generalisation to spectrally constrained ensembles

- control **closed paths of all lengths**

$$p(\mathbf{c}) \propto \mathrm{e}^{u\sum_{ij} c_{ij} + \sum_{\ell\geq 3} v_\ell \sum_{i_1\ldots i_\ell} c_{i_1 i_2} c_{i_2 i_3} \ldots c_{i_\ell i_1}}$$

  generating function:
  use $c_{ij} = c_{ij}c_{ji}$

$$\phi = \frac{1}{N}\log\sum_{\mathbf{c}} \mathrm{e}^{u\,\mathrm{Tr}(\mathbf{c}^2) + \sum_{\ell\geq 3} v_\ell \mathrm{Tr}(\mathbf{c}^\ell)}$$

$$\langle k\rangle = \partial\phi/\partial u$$

$$\langle m_\ell\rangle = \tfrac{1}{N}\langle \mathrm{Tr}(\mathbf{c}^\ell)\rangle = \partial\phi/\partial v_\ell$$

$$S = \phi - u\langle k\rangle - \sum_{\ell\geq 3} v_\ell\langle m_\ell\rangle$$

- since $\mathrm{Tr}(\mathbf{c}^\ell) = N\int\mathrm{d}\mu\ \mu^\ell \varrho(\mu|\mathbf{c})$:
  control **spectrum** $\varrho(\mu)$

$$p(\mathbf{c}) \propto \mathrm{e}^{N\int\mathrm{d}\mu\ \hat{\varrho}(\mu)\varrho(\mu|\mathbf{c})}$$

  generating function:

$$\phi = \frac{1}{N}\log\sum_{\mathbf{c}} \mathrm{e}^{N\int\mathrm{d}\mu\ \hat{\varrho}(\mu)\varrho(\mu|\mathbf{c})}$$

$$\varrho(\mu) = \delta\phi/\delta\hat{\varrho}(\mu)$$

$$S = \phi - \int\mathrm{d}\mu\ \hat{\varrho}(\mu)\varrho(\mu)$$

A possible analytical route

$$\phi = \frac{1}{N}\log\sum_{\mathbf{c}} \mathrm{e}^{u\sum_{ij} c_{ij} + N\int \mathrm{d}\mu\;\hat{\varrho}(\mu)\varrho(\mu|\mathbf{c})}$$

$$\mathit{ER/Burda\ regime}:\;\; u = -\frac{1}{2}\log N + \mathcal{O}(1)$$

- derive

$$\phi = \lim_{\varepsilon,\Delta\downarrow 0}\frac{1}{N}\log\sum_{\mathbf{c}} \mathrm{e}^{u\sum_{ij} c_{ij}} \prod_{\mu}\Big[Z(\mu+\mathrm{i}\varepsilon|\mathbf{c})^{\mathrm{i}\Delta\lambda(\mu)}\;\overline{Z(\mu+\mathrm{i}\varepsilon|\mathbf{c})}^{\,-\mathrm{i}\Delta\lambda(\mu)}\Big]$$

$$Z(\mu|\mathbf{c}) = \int \mathrm{d}\boldsymbol{\phi}\;\mathrm{e}^{-\frac{1}{2}\mathrm{i}\boldsymbol{\phi}\cdot[\mathbf{c}-\mu\mathbf{1}]\boldsymbol{\phi}}, \qquad \lambda(\mu) = \frac{1}{\pi}\frac{\mathrm{d}}{\mathrm{d}\mu}\hat{\varrho}(\mu)$$

- replicas, steepest descent for $N\!\to\!\infty$, continuation to *imaginary* dimensions, limits $\epsilon\!\downarrow\!0$ and $\Delta\!\downarrow\!0$
- replica symmetry, bifurcation analysis, phase transitions and entropy, RSB

feasible?

Key identity

spectral ensemble constraints,
use Edwards-Jones (1976):

$$\varrho(\mu|\mathbf{c}) = \frac{2}{N\pi}\lim_{\varepsilon\downarrow 0}\mathrm{Im}\frac{\partial}{\partial\mu}\log Z(\mu+\mathrm{i}\varepsilon|\mathbf{c}), \qquad Z(\mu|\mathbf{c}) = \int \mathrm{d}\boldsymbol{\phi}\ \mathrm{e}^{-\frac{1}{2}\mathrm{i}\boldsymbol{\phi}\cdot[\mathbf{c}-\mu\mathbb{1}]\boldsymbol{\phi}}$$

insert into ϕ,
integrate by parts,

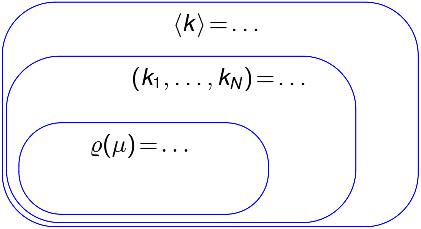
discretise
μ-integral:

$$\begin{aligned}\phi &= \frac{1}{N}\log\sum_{\mathbf{c}}\mathrm{e}^{u\sum_{ij}c_{ij}+N\int\mathrm{d}\mu\ \hat{\varrho}(\mu)\frac{2}{N\pi}\lim_{\varepsilon\downarrow 0}\mathrm{Im}\frac{\partial}{\partial\mu}\log Z(\mu+\mathrm{i}\varepsilon|\mathbf{c})} \\ &= \ldots\ldots \\ &= \lim_{\varepsilon,\Delta\downarrow 0}\frac{1}{N}\log\sum_{\mathbf{c}}\mathrm{e}^{u\sum_{ij}c_{ij}}\prod_{\mu}\mathrm{e}^{-2\mathrm{Im}\log Z(\mu+\mathrm{i}\varepsilon|\mathbf{c}).\ \frac{\Delta}{\pi}\frac{\mathrm{d}}{\mathrm{d}\mu}\hat{\varrho}(\mu)}\end{aligned}$$

$$\mathrm{e}^{-2\ \mathrm{Im}\log z} = z^{\mathrm{i}}.\overline{z}^{\ -\mathrm{i}}$$

$$\phi = \lim_{\varepsilon,\Delta\downarrow 0}\frac{1}{N}\log\sum_{\mathbf{c}}\mathrm{e}^{u\sum_{ij}c_{ij}}\prod_{\mu}\Big[Z(\mu+\mathrm{i}\varepsilon|\mathbf{c})^{\mathrm{i}}\ \overline{Z(\mu+\mathrm{i}\varepsilon|\mathbf{c})}^{-\mathrm{i}}\Big]^{\frac{\Delta}{\pi}\frac{\mathrm{d}}{\mathrm{d}\mu}\hat{\varrho}(\mu)}$$

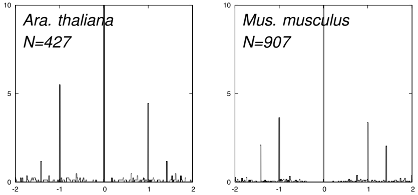
Some relevant questions

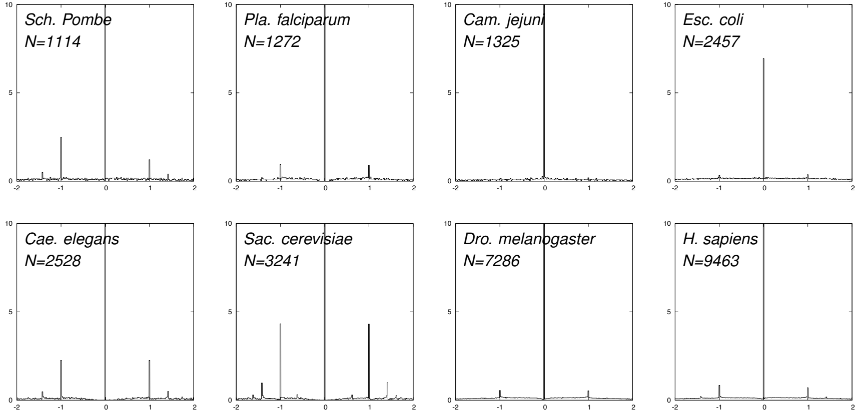


- Q1: How informative are spectra of finitely connected graphs?
- Q2: How many non-isomorphic graphs are there with
  given degrees $(k_1, \ldots, k_N)$ and a given spectrum $\varrho(\mu)$?
- Q3: How similar are processes running on non-isomorphic graphs with
  the same degrees $(k_1, \ldots, k_N)$ and the same spectrum $\varrho(\mu)$?

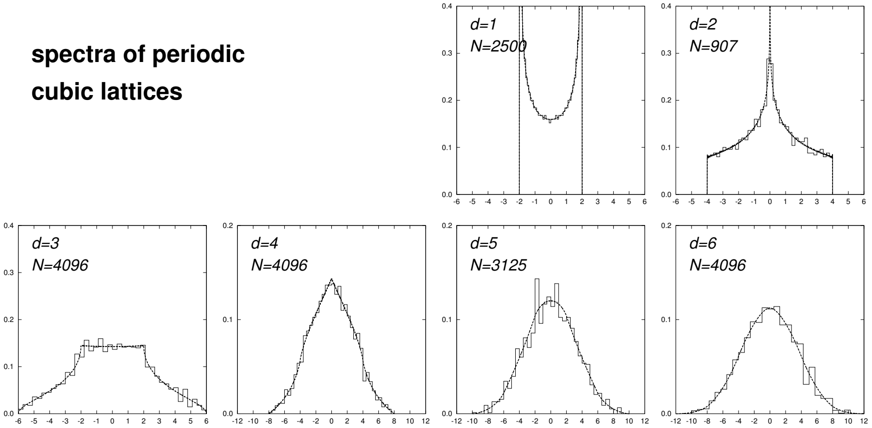
  (spherical spins: free energies identical!)

spectra of protein interaction networks





spectra of periodic cubic lattices



$$N \to \infty: \qquad \varrho_{d+1}(\mu) = \int_0^1 \mathrm{d}x \; \varrho_d(\mu - 2\cos(\pi x)), \qquad \varrho_1(\mu) = \frac{\theta(2-|\mu|)}{\pi\sqrt{4-\mu^2}}$$

[Berlin, Kac 1952]

Co-spectral and DS graphs

co-spectral graphs

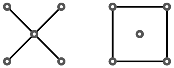
identical nr of edges and closed paths of any length

DS graphs

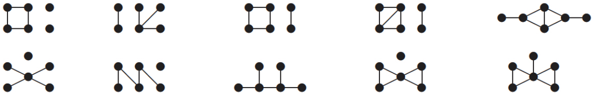
determined fully by their spectrum (modulo isomorphisms)

examples of **non-DS** pairs

$N = 5$: one pair



$N = 6$: five pairs



$N = 10$: regular example pair

$N = 13$: example of co-spectral trees

- $N < 5$: all graphs are DS
- $N = 5, 6$: some non-DS, but different degrees
- almost all trees are non-DS
- $N \to \infty$ expectation: nearly all graphs are DS

[Schwenk 1973,
Van Dam & Haemers 2002]

n	# graphs	A
2	2	0
3	4	0
4	11	0
5	34	0.059
6	156	0.064
7	1044	0.105
8	12346	0.139
9	274668	0.186
10	12005168	0.213
11	1018997864	0.211
12	165091172592	0.188

↑ *size* ↑ *non-DS fraction*

DSDS graphs

determined fully by
spectrum and degree sequence

nothing known ...

Order parameter eqns

does the entropy calculation work
for the generalised Strauss model?

$$\phi = \lim_{\epsilon,\Delta\downarrow 0} \frac{1}{N} \log \sum_{\mathbf{c}} e^{u\sum_{ij} c_{ij}} \prod_{\mu} \Big[Z(\mu + i\varepsilon|\mathbf{c})^{n_\mu}\, \overline{Z(\mu+i\varepsilon|\mathbf{c})}^{m_\mu} \Big]$$

$$n_\mu = -m_\mu = \frac{i\Delta}{\pi} \frac{d}{d\mu} \hat{\varrho}(\mu)$$

- preparation:
  $u = -\frac{1}{2}\log(N/\bar{k})$:

$$\phi = \frac{1}{2}\bar{k} + \lim_{\epsilon,\Delta\downarrow 0} \frac{1}{N} \log \Big\langle \prod_{\mu} \Big[Z(\mu + i\varepsilon|\mathbf{c})^{n_\mu}\, \overline{Z(\mu+i\varepsilon|\mathbf{c})}^{m_\mu} \Big\rangle_{\rm ER} + \mathcal{O}(\frac{1}{N})$$

$$Z(\mu|\mathbf{c}) = \int_{{\rm I\!R}^N} d\boldsymbol{\phi}\; e^{-\frac{1}{2} i \boldsymbol{\phi}\cdot[\mathbf{c}-\mu \mathbb{I}]\boldsymbol{\phi}}$$

$$p_{\rm ER}(\mathbf{c}|\bar{k}) = \prod_{i<j} \Big[\frac{\bar{k}}{N} \delta_{c_{ij},1} + (1 - \frac{\bar{k}}{N}) \delta_{c_{ij},0} \Big]$$

- evaluate $Z(\mu+i\epsilon|\mathbf{c})^{n_\mu}$ and $\overline{Z(\mu+i\epsilon|\mathbf{c})}^{m_\mu}$ for *integer* n_μ and m_μ,

  average over graphs

$$\Big\langle \prod_\mu \Big\{ \Big[\prod_{\alpha_\mu=1}^{n_\mu} \int_{\mathbb{R}^N} d\boldsymbol{\phi}\; e^{-\frac{1}{2}\varepsilon\boldsymbol{\phi}^2-\frac{1}{2}i\boldsymbol{\phi}\cdot(\mathbf{c}-\mu\mathbf{1})\boldsymbol{\phi}} \Big] \Big[\prod_{\beta_\mu=1}^{m_\mu} \int_{\mathbb{R}^N} d\boldsymbol{\psi}\; e^{-\frac{1}{2}\varepsilon\boldsymbol{\psi}^2+\frac{1}{2}i\boldsymbol{\psi}\cdot(\mathbf{c}-\mu\mathbf{1})\boldsymbol{\psi}} \Big] \Big\} \Big\rangle_{\rm ER}$$

$$= \int \prod_i \Big[d\boldsymbol{\phi}^i d\boldsymbol{\psi}^i\; e^{-\frac{1}{2}(\varepsilon-i\mu)(\boldsymbol{\phi}^i)^2-\frac{1}{2}(\varepsilon+i\mu)(\boldsymbol{\psi}^i)^2} \Big] e^{\frac{1}{2}\sum_{i\neq j}\log\left\{1+\frac{\bar{k}}{N}\left[\exp[i(\boldsymbol{\psi}^i\cdot\boldsymbol{\psi}^j-\boldsymbol{\phi}^i\cdot\boldsymbol{\phi}^j)]-1\right]\right\}}$$

$$\boldsymbol{\phi}^i = \{\phi^i_{\mu,\alpha_\mu\leq n_\mu}\}, \quad \boldsymbol{\psi}^i = \{\psi^i_{\mu,\beta_\mu\leq m_\mu}\}$$

- functional order parameter

$$\begin{array}{l} \forall\boldsymbol{\phi} = \{\phi_{\mu,\alpha_\mu\leq n_\mu}\} \\ \forall\boldsymbol{\psi} = \{\psi_{\mu,\beta_\mu\leq m_\mu}\} \end{array} : \qquad 1 = \int d\mathcal{P}(\boldsymbol{\phi},\boldsymbol{\psi})\; \delta\Big[\mathcal{P}(\boldsymbol{\phi},\boldsymbol{\psi}) - \frac{1}{N}\sum_i \delta(\boldsymbol{\phi}-\boldsymbol{\phi}^i)\delta(\boldsymbol{\psi}-\boldsymbol{\psi}^i)\Big]$$

theory in terms of
$\mathcal{P}(\boldsymbol{\phi},\boldsymbol{\psi})$ *and* $\hat{\mathcal{P}}(\boldsymbol{\phi},\boldsymbol{\psi})$

- path integral form,
  steepest descent for $N \to \infty$:

$$\phi = \lim_{\epsilon,\Delta\downarrow 0} \text{extr}_{\{\mathcal{P},\hat{\mathcal{P}}\}} \Psi[\{\mathcal{P},\hat{\mathcal{P}}\}]$$

$$\begin{aligned}\Psi[\{\mathcal{P},\hat{\mathcal{P}}\}] &= \mathrm{i}\int \mathrm{d}\boldsymbol{\phi}\mathrm{d}\boldsymbol{\psi}\; \hat{\mathcal{P}}(\boldsymbol{\phi},\boldsymbol{\psi})\mathcal{P}(\boldsymbol{\phi},\boldsymbol{\psi}) \\ &\quad + \frac{1}{2}\bar{k}\int \mathrm{d}\boldsymbol{\phi}\mathrm{d}\boldsymbol{\psi}\mathrm{d}\boldsymbol{\phi}'\mathrm{d}\boldsymbol{\psi}'\mathcal{P}(\boldsymbol{\phi},\boldsymbol{\psi})\mathcal{P}(\boldsymbol{\phi}',\boldsymbol{\psi}')\mathrm{e}^{\mathrm{i}(\boldsymbol{\psi}\cdot\boldsymbol{\psi}'-\boldsymbol{\phi}\cdot\boldsymbol{\phi}')} \\ &\quad + \log\int \mathrm{d}\boldsymbol{\phi}\mathrm{d}\boldsymbol{\psi}\; \mathrm{e}^{-\frac{1}{2}\boldsymbol{\phi}\cdot(\varepsilon\mathbf{1}-\mathrm{i}\mathbf{M})\boldsymbol{\phi}-\frac{1}{2}\boldsymbol{\psi}\cdot(\varepsilon\mathbf{1}+\mathrm{i}\mathbf{M})\boldsymbol{\psi}-\mathrm{i}\hat{\mathcal{P}}(\boldsymbol{\phi},\boldsymbol{\psi})}\end{aligned}$$

$$M_{\mu,\alpha;\mu',\alpha'} = \mu\delta_{\mu\mu'}\delta_{\alpha\alpha'}$$

$$\boldsymbol{\phi} = \{\phi_{\mu,\alpha_\mu\leq n_\mu}\}, \qquad n_\mu = \frac{\mathrm{i}\Delta}{\pi}\frac{\mathrm{d}}{\mathrm{d}\mu}\hat{\varrho}(\mu)$$

$$\boldsymbol{\psi} = \{\psi_{\mu,\beta_\mu\leq m_\mu}\}, \qquad m_\mu = -\frac{\mathrm{i}\Delta}{\pi}\frac{\mathrm{d}}{\mathrm{d}\mu}\hat{\varrho}(\mu)$$

- saddle-point eqns,
  $\mathcal{Q} = \exp[-\mathrm{i}\hat{\mathcal{P}}]$:

$$\mathcal{Q}(\boldsymbol{\phi},\boldsymbol{\psi}) = \exp\left[\bar{k}\int \mathrm{d}\boldsymbol{\phi}'\mathrm{d}\boldsymbol{\psi}'\; \mathcal{P}(\boldsymbol{\phi}',\boldsymbol{\psi}')\mathrm{e}^{\mathrm{i}(\boldsymbol{\psi}\cdot\boldsymbol{\psi}'-\boldsymbol{\phi}\cdot\boldsymbol{\phi}')}\right]$$

$$\mathcal{P}(\boldsymbol{\phi},\boldsymbol{\psi}) = \frac{\mathcal{Q}(\boldsymbol{\phi},\boldsymbol{\psi})\mathrm{e}^{-\frac{1}{2}\boldsymbol{\phi}\cdot(\varepsilon\mathbf{1}-\mathrm{i}\mathbf{M})\boldsymbol{\phi}-\frac{1}{2}\boldsymbol{\psi}\cdot(\varepsilon\mathbf{1}+\mathrm{i}\mathbf{M})\boldsymbol{\psi}}}{\int \mathrm{d}\boldsymbol{\phi}'\mathrm{d}\boldsymbol{\psi}'\; \mathcal{Q}(\boldsymbol{\phi}',\boldsymbol{\psi}')\mathrm{e}^{-\frac{1}{2}\boldsymbol{\phi}'\cdot(\varepsilon\mathbf{1}-\mathrm{i}\mathbf{M})\boldsymbol{\phi}'-\frac{1}{2}\boldsymbol{\psi}'\cdot(\varepsilon\mathbf{1}+\mathrm{i}\mathbf{M})\boldsymbol{\psi}'}}$$

RS ansatz

- De Finetti, $\mathcal{P}(\boldsymbol{\psi},\boldsymbol{\phi})=\overline{\mathcal{P}(\boldsymbol{\phi},\boldsymbol{\psi})}$:

$$\mathcal{P}(\boldsymbol{\phi},\boldsymbol{\psi})=\int\{\mathrm{d}\pi\}\mathcal{W}[\{\pi\}]\Big[\prod_\mu\prod_{\alpha_\mu=1}^{n_\mu}\pi(\phi_{\mu,\alpha_\mu}|\mu)\Big]\Big[\prod_\mu\prod_{\beta_\mu=1}^{m_\mu}\overline{\pi(\psi_{\mu,\beta_\mu}|\mu)}\Big]$$

$$\int\{\mathrm{d}\pi\}\mathcal{W}[\{\pi\}]=1,\qquad\int\mathrm{d}\phi\;\pi(\phi|\mu)=1\;\;\textit{for all }\mu$$

- insert into saddle-point eqns,
  $\Delta\!\downarrow\!0$: $\Delta\sum_\mu\to\int\mathrm{d}\mu$

$$\mathcal{W}[\{\pi\}]=\frac{\sum_{\ell\geq 0}\mathrm{e}^{-\bar{k}}\frac{\bar{k}^\ell}{\ell!}\int\Big(\prod_{r\leq\ell}\{\mathrm{d}\pi_r\}\mathcal{W}[\{\pi_r\}]\Big)\mathcal{D}[\{\pi_1,\ldots,\pi_\ell\}]\delta\Big[\pi-\mathcal{F}[\{\pi_1,\ldots,\pi_\ell\}]\Big]}{\sum_{\ell\geq 0}\mathrm{e}^{-\bar{k}}\frac{\bar{k}^\ell}{\ell!}\int\Big(\prod_{r\leq\ell}\{\mathrm{d}\pi_r\}\mathcal{W}[\{\pi_r\}]\Big)\mathcal{D}[\{\pi_1,\ldots,\pi_\ell\}]}$$

$$\mathcal{F}(\phi|\mu;\pi_1,\ldots,\pi_\ell)=\ldots,\qquad\mathcal{D}[\{\pi_1,\ldots,\pi_\ell\}]=\ldots$$

if no loops: $\mathcal{D}[..]=1$

- further simplification:

$$\pi(\phi|\mu)=\frac{e^{-\frac{1}{2}\epsilon\phi^2-\frac{1}{2}ix(\mu)\phi^2+y(\mu)\phi}}{\int d\phi'\ e^{-\frac{1}{2}\epsilon\phi'^2-\frac{1}{2}ix(\mu)\phi'^2+y(\mu)\phi'}}:\qquad \mathcal{W}[\{\pi\}]\ \to\ W[\{x,y\}]$$

- insert into RS eqns,
  take $\epsilon\downarrow 0$

$$W[\{x,y\}]=\frac{\sum_{\ell\geq 0}p_\ell\int\left(\prod_{r\leq\ell}\{dx_r dy_r\}W[\{x_r,y_r\}]\right)\tilde{\mathcal{D}}[\ldots]\ \delta\left[x-F_x[\ldots]\right]\delta\left[y-F_y[\ldots]\right]}{\sum_{\ell\geq 0}p_\ell\int\left(\prod_{r\leq\ell}\{dx_r dy_r\}W[\{x_r,y_r\}]\right)\tilde{\mathcal{D}}[\ldots]}$$

$$F_x[\mu|\{x_1,\ldots,x_\ell\}]=-\mu-\sum_{r\leq\ell}\frac{1}{x_r(\mu)}$$

$$F_y[\mu|\{x_1,y_1,\ldots,x_\ell,y_\ell\}]=-\sum_{r\leq\ell}\frac{y_r(\mu)}{x_r(\mu)}\qquad\qquad p_\ell=e^{-\bar{k}}\bar{k}^\ell/\ell!$$

$$\tilde{\mathcal{D}}[\{x_1,y_1,\ldots,x_\ell,y_\ell\}]=e^{\int d\mu\ \frac{d}{d\mu}\hat{\varrho}(\mu)\ \left[\frac{1}{2}\mathrm{sgn}\left(F_x[\mu|x_1,\ldots,x_\ell]\right)+\frac{1}{\pi}\frac{F_y^2[\mu|x_1,y_1,\ldots,x_\ell,y_\ell]}{F_x[\mu|x_1,\ldots,x_\ell]}\right]}$$

everything real-valued!

Phase transitions

- symmetry:
  $\mathcal{P}(\phi,\psi) \to \mathcal{P}(-\phi,-\psi)$
  i.e. $\{y\} \to \{-y\}$

$$\begin{aligned} \textit{weakly symmetric}: &\quad W[\{x,-y\}] = W[\{x,y\}] \\ \textit{strongly symmetric}: &\quad W[\{x,y\}] = W[\{x\}]\,\delta[\{y\}] \end{aligned}$$

- symmetry-breaking:

$$\begin{aligned} \textit{SG type}: &\quad W[\{x,y\}] = W[\{x\}]\delta[\{y\}] \;\to\; W[\{x,-y\}] = W[\{x,y\}] \\ \textit{F type}: &\quad W[\{x,y\}] = W[\{x\}]\delta[\{y\}] \;\to\; W[\{x,-y\}] \neq W[\{x,y\}] \end{aligned}$$

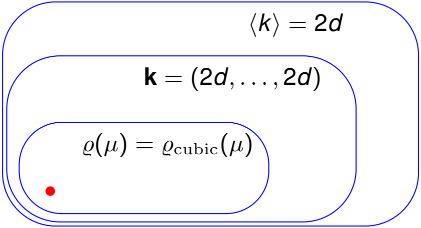
functional moment expansion

$$\psi(\mu_1,\ldots,\mu_n|\{x\}) = \int\{\mathrm{d}y\}W[\{y|x\}]\,y(\mu_1)\ldots y(\mu_n)$$
$$= \mathcal{O}(\varepsilon^n) \quad \textit{close to transition}$$

Loopy proxies for loopy lattices

method seems to work
for ensemble entropies ...

how about processes?



transition temp $T_c(d)$

	$d=1$	$d=2$	$d=3$	$d=4$
random, $\langle k \rangle = 2d$	1.820	3.915	5.944	7.958
random, $\mathbf{k} = (2d, \ldots, 2d)$	0	2.885	4.933	6.952
random, $\mathbf{k} = (2d, \ldots, 2d)$, $\varrho(\mu) = \varrho_{\text{cubic}}(\mu)$	?	?	?	?
d-dim cubic lattice	0	2.269	4.511	6.680

Free energy density

Ising model on random graph
from tailored loopy ensemble:

$$p(\boldsymbol{\sigma}|\mathbf{c}) \propto \exp[-\beta H(\boldsymbol{\sigma}|\mathbf{c})], \qquad H(\boldsymbol{\sigma}|\mathbf{c}) = -J\sum_{i<j} c_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i$$

replica approach:

$\overline{g(\mathbf{c})} = \sum_{\mathbf{c}} p(\mathbf{c})g(\mathbf{c})$

$$\overline{f} = -\lim_{N\to\infty}\lim_{n\to 0}\frac{1}{\beta N n}\log\sum_{\boldsymbol{\sigma}_1\ldots\boldsymbol{\sigma}_N} \mathrm{e}^{\beta h\sum_i\sum_{\alpha=1}^n \sigma_i^\alpha - \beta N E_{\rm eff}(\boldsymbol{\sigma}_1,\ldots,\boldsymbol{\sigma}_N)}$$

$$E_{\rm eff}(\boldsymbol{\sigma}_1,\ldots,\boldsymbol{\sigma}_N) = -\frac{1}{\beta N}\log\overline{\mathrm{e}^{\frac{1}{2}\beta J\sum_{ij} c_{ij}\boldsymbol{\sigma}_i\cdot\boldsymbol{\sigma}_j}}, \qquad \boldsymbol{\sigma}_i = (\sigma_i^1,\ldots,\sigma_i^n)$$

MaxEnt ensembles:
(soft/hard spectral
constraint)

$$p_A(\mathbf{c}) \propto \mathrm{e}^{N\int \mathrm{d}\mu\ \hat{\varrho}(\mu)\varrho(\mu|\mathbf{c})}\prod_{i=1}^N \delta_{k_i,\sum_j c_{ij}} \qquad \varrho(\mu) = \overline{\varrho(\mu|\mathbf{c})}$$

$$p_B(\mathbf{c}) \propto \delta_F\left[\varrho(\mu) - \varrho(\mu|\mathbf{c})\right]\prod_{i=1}^N \delta_{k_i,\sum_j c_{ij}}$$

$\delta_{k_i,\sum_j c_{ij}}$ in integral form,
formula for spectral constraint,
spin order parameter $\mathcal{D}$,
steepest descent:

$$-\beta\overline{f} = \lim_{n\to 0} \mathrm{extr}_{\{\mathcal{D},\chi\}} \Psi[\mathcal{D},\chi]$$

$$\Psi[\mathcal{D},\chi] = \frac{1}{n}\Big\{ \log \sum_{\boldsymbol{\sigma}} \chi(\boldsymbol{\sigma}) \mathrm{e}^{\beta h \sum_\alpha \sigma^\alpha} - \sum_{\boldsymbol{\sigma}} \mathcal{D}(\boldsymbol{\sigma}) \log \chi(\boldsymbol{\sigma}) - \beta E_{\rm eff}(\mathcal{D}) \Big\}$$

$$\boldsymbol{\sigma} = (\sigma^1,\ldots,\sigma^n), \qquad \mathcal{D}(\boldsymbol{\sigma}) = \lim_{N\to\infty} \frac{1}{N} \sum_i \overline{\langle \prod_{\alpha\leq n} \delta_{\sigma^\alpha,\sigma_i^\alpha} \rangle}$$

Effective interaction energies:

$$-\beta E^A_{\rm eff}(\mathcal{D}) = \mathcal{E}_{\beta J}[\hat{\varrho}_0,\mathcal{D}] - \mathcal{E}_0[\hat{\varrho}_0,\mathcal{D}]$$

$$-\beta E^B_{\rm eff}(\mathcal{D}) = \mathcal{E}_{\beta J}[\hat{\varrho}_{\beta J},\mathcal{D}] - \mathcal{E}_0[\hat{\varrho}_0,\mathcal{D}]$$

$\hat{\varrho}_K(\mu)$
solved from

$$\varrho(\mu) = \frac{\delta}{\delta \hat{\varrho}_K(\mu)} \mathcal{E}_K[\hat{\varrho}_K,\mathcal{D}]$$

$$\mathcal{E}_K[\hat{\varrho},\mathcal{D}] = \lim_{\Delta\downarrow 0} \lim_{\varepsilon\downarrow 0} \lim_{n_\mu \to \frac{\mathrm{i}\Delta}{\pi}\frac{\mathrm{d}}{\mathrm{d}\mu}\hat{\varrho}(\mu)} \lim_{m_\mu\to -n_\mu} \mathrm{extr}_{\{\mathcal{P},\mathcal{Q}\}} \overbrace{\Psi_K[\mathcal{P},\mathcal{Q}|\mathcal{D}]}^{\textit{as in generalised Strauss!}}$$

spins on $\bar{k}$-regular lattice:

$$\Psi_K[\mathcal{P},\mathcal{Q}|\mathcal{D}] = -\sum_{\boldsymbol{\sigma}}\int_{-\pi}^{\pi}\mathrm{d}\omega\int\mathrm{d}\boldsymbol{\phi}\mathrm{d}\boldsymbol{\psi}\;\mathcal{P}(\boldsymbol{\sigma},\boldsymbol{\phi},\boldsymbol{\psi},\omega)\log\mathcal{Q}(\boldsymbol{\sigma},\boldsymbol{\phi},\boldsymbol{\psi},\omega)$$

$$+\frac{1}{2}\bar{k}\sum_{\boldsymbol{\sigma},\boldsymbol{\sigma}'}\int_{-\pi}^{\pi}\mathrm{d}\omega\mathrm{d}\omega'\mathrm{e}^{K\boldsymbol{\sigma}\cdot\boldsymbol{\sigma}'-\mathrm{i}(\omega+\omega')}\int\mathrm{d}\boldsymbol{\phi}\mathrm{d}\boldsymbol{\psi}\mathrm{d}\boldsymbol{\phi}'\mathrm{d}\boldsymbol{\psi}'\;\mathcal{P}(\boldsymbol{\sigma},\boldsymbol{\phi},\boldsymbol{\psi},\omega)\mathcal{P}(\boldsymbol{\sigma}',\boldsymbol{\phi}',\boldsymbol{\psi}',\omega')$$

$$\times\mathrm{e}^{\mathrm{i}(\boldsymbol{\psi}\cdot\boldsymbol{\psi}'-\boldsymbol{\phi}\cdot\boldsymbol{\phi}')}$$

$$+\sum_{\boldsymbol{\sigma}}\mathcal{D}(\boldsymbol{\sigma})\log\int_{-\pi}^{\pi}\frac{\mathrm{d}\omega}{2\pi}\mathrm{e}^{\mathrm{i}\bar{k}\omega}\int\mathrm{d}\boldsymbol{\phi}\mathrm{d}\boldsymbol{\psi}\;\mathcal{Q}(\boldsymbol{\sigma},\boldsymbol{\phi},\boldsymbol{\psi},\omega)\mathrm{e}^{-\frac{1}{2}\boldsymbol{\phi}\cdot(\varepsilon\mathbf{1}-\mathrm{i}\mathbf{M})\boldsymbol{\phi}-\frac{1}{2}\boldsymbol{\psi}\cdot(\varepsilon\mathbf{1}+\mathrm{i}\mathbf{M})\boldsymbol{\psi}}$$

$$\boldsymbol{\phi}=\{\phi_{\mu,\alpha_\mu\leq n_\mu}\},\quad \boldsymbol{\psi}=\{\psi_{\mu,\beta_\mu\leq m_\mu}\},\quad M_{\mu,\alpha;\mu',\alpha'}=\mu\delta_{\mu\mu'}\delta_{\alpha\alpha'}$$

comparison: generalised Strauss entropy

$$\Psi[\mathcal{P},\mathcal{Q}] = -\int\mathrm{d}\boldsymbol{\phi}\mathrm{d}\boldsymbol{\psi}\;\mathcal{P}(\boldsymbol{\phi},\boldsymbol{\psi})\log\mathcal{Q}(\boldsymbol{\phi},\boldsymbol{\psi})$$

$$+\frac{1}{2}\bar{k}\int\mathrm{d}\boldsymbol{\phi}\mathrm{d}\boldsymbol{\psi}\mathrm{d}\boldsymbol{\phi}'\mathrm{d}\boldsymbol{\psi}'\;\mathcal{P}(\boldsymbol{\phi},\boldsymbol{\psi})\mathcal{P}(\boldsymbol{\phi}',\boldsymbol{\psi}')\mathrm{e}^{\mathrm{i}(\boldsymbol{\psi}\cdot\boldsymbol{\psi}'-\boldsymbol{\phi}\cdot\boldsymbol{\phi}')}$$

$$+\log\int\mathrm{d}\boldsymbol{\phi}\mathrm{d}\boldsymbol{\psi}\;\mathcal{Q}(\boldsymbol{\phi},\boldsymbol{\psi})\mathrm{e}^{-\frac{1}{2}\boldsymbol{\phi}\cdot(\varepsilon\mathbf{1}-\mathrm{i}\mathbf{M})\boldsymbol{\phi}-\frac{1}{2}\boldsymbol{\psi}\cdot(\varepsilon\mathbf{1}+\mathrm{i}\mathbf{M})\boldsymbol{\psi}}$$

Summary

- new analytical approach to (processes on) loopy networks, based on graph ensembles characterised by *degrees and spectrum*
- replica formula for tricky constraint in which sum over graphs can be done (via Edwards-Jones)

$$e^{N\int d\mu\ \hat{\varrho}(\mu)\varrho(\mu|\mathbf{c})} = \lim_{\varepsilon,\Delta\downarrow 0} \prod_{\mu} \Big[Z(\mu+i\varepsilon|\mathbf{c})^{in(\mu)}\ \overline{Z(\mu+i\varepsilon|\mathbf{c})}^{\,-in(\mu)} \Big]$$

$$Z(\mu|\mathbf{c}) = \int d\boldsymbol{\phi}\ e^{-\frac{1}{2}i\boldsymbol{\phi}\cdot[\mathbf{c}-\mu\mathbb{1}]\boldsymbol{\phi}}, \qquad n(\mu) = \frac{\Delta}{\pi}\frac{d}{d\mu}\hat{\varrho}(\mu)$$

- exact order parameter eqns in replica language
- imaginary replica dimensions become real at saddle-point
- RS order parameter equations for *loopy* graphs similar to RSB order parameter equations for *tree-like* ones