Mean-field theory of spin glasses: Analysis of replicated TAP free energy

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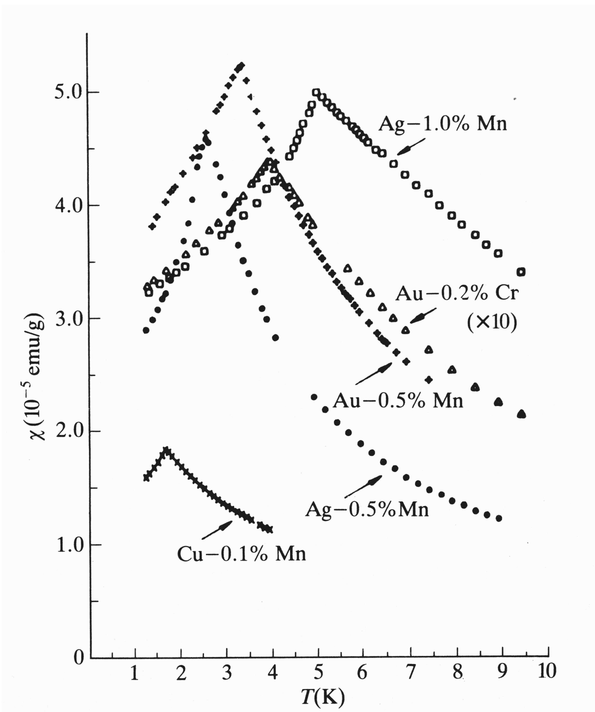
What is spin glass?



Magnetic disorder phase

- nonzero local magnetization
- zero global magnetization
- no magnetic periodic ordering

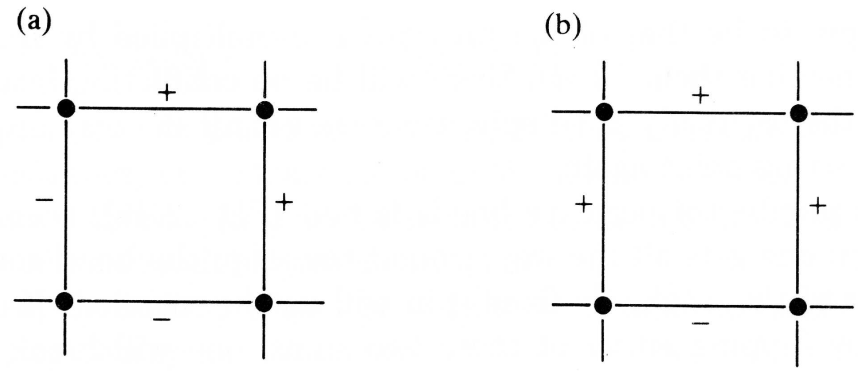
Fluctuation-dissipation theorem

$$\chi = \frac{1}{N}\sum_i \chi_{ii} = \frac{1 - N^{-1}\sum_i m_i^2}{kT}$$

Theoretical model

Two important ingredients

- frustration
- quenched disorder



Sherrington-Kirkpatrick model, Ising Hamiltonian, Gaussian interaction

$$H = -\frac{1}{2}\sum_{ij} J_{ij} S_i S_j - h \sum_i S_i$$

Self-averaging of the free energy: $F(J_{ij}) = \langle F(J_{ij}) \rangle_{av}$.

Replica trick $\langle \ln Z \rangle_{av} = \lim_{n\to 0} \frac{\langle Z^n \rangle_{av} - 1}{n}$

- replica symmetric solution $\rightarrow$ wrong
- Parisi replica symmetry breaking $\rightarrow$ believed to be correct

$$\begin{pmatrix} \begin{matrix}0 & q_2 & q_2\\ q_2 & 0 & q_2\\ q_2 & q_2 & 0\end{matrix} & q_1 & & \\ q_1 & \begin{matrix}0 & q_2 & q_2\\ q_2 & 0 & q_2\\ q_2 & q_2 & 0\end{matrix} & & q_0 \\ & & \begin{matrix}0 & q_2 & q_2\\ q_2 & 0 & q_2\\ q_2 & q_2 & 0\end{matrix} & q_1 \\ q_0 & & q_1 & \begin{matrix}0 & q_2 & q_2\\ q_2 & 0 & q_2\\ q_2 & q_2 & 0\end{matrix} \end{pmatrix}.$$

TAP - first thermodynamical averaging

- Trivial configuration averaging $\Rightarrow$ RS solution
- Considering of many TAP solutions $\Rightarrow$ RSB solution

Derivation of the TAP-like free energy

The Euler condition for thermodynamic homogeneity leads to

$$F = -\frac{1}{\beta}\langle \ln \operatorname*{Tr}_{S_i} e^{-\beta H} \rangle_{av} = -\frac{1}{\beta\nu}\langle \ln \operatorname*{Tr}_{S_i^\alpha} e^{-\beta H_\nu} \rangle_{av}$$

H_ν is ν-times replicated SK Hamiltonian plus interactions between replicas

$$H_\nu = -\sum_{\alpha}^{\nu}\left(\frac{1}{2}\sum_{i\neq j} J_{ij} S_i^\alpha S_j^\alpha + \sum_i h_i^\alpha S_i^\alpha\right) - \frac{1}{2}\sum_{\alpha\neq\beta}\sum_i \mu^{\alpha\beta} S_i^\alpha S_i^\beta$$

- $\mu^{\alpha\beta}$ is the interaction between real replicas, i. e. replica independence breaking interaction
- J_{ij} random spin-spin interaction with Gaussian distribution
- h_i^α external magnetic field, S_i^α spin on the position i in the replica α

With some conventional technique the TAP-like free energy can be derived

$$
\begin{aligned}
-\beta F_\nu &= \sum_{\alpha=1}^{\nu}\left\{\frac{\beta}{2}\sum_{ij} J_{ij} m_i^\alpha m_j^\alpha + \frac{\beta^2}{4}\sum_{ij} J_{ij}^2[1-(m_i^\alpha)^2][1-(m_j^\alpha)^2] -\right.\\
&- \left.\beta\sum_i m_i^\alpha \eta_i^\alpha\right\} - \sum_{\alpha\neq\beta}\left\{\frac{\beta^2}{4}J^2 N(\chi_{\alpha\beta})^2 + \frac{\beta^2}{2}J^2\chi_{\alpha\beta}\sum_i m_i^\alpha m_i^\beta\right\} +\\
&+ \sum_i \ln \mathrm{Tr}\exp\left[\frac{\beta^2}{2}J^2\sum_{\alpha\neq\beta}\chi_{\alpha\beta}S_i^\alpha S_i^\beta + \beta\sum_\alpha S_i^\alpha(\eta_i^\alpha + h_i^\alpha)\right]
\end{aligned}
$$

- m_i^α thermodynamical mean value of S_i^α; $J^2 = \langle J_{ij}\rangle_{av}$,
- $\chi_{\alpha\beta}$ linear response to the interaction $\mu^{\alpha\beta} \to 0$
- $\eta_i^\alpha = \sum_j J_{ij} m_j^\alpha - \beta J^2 \sum_\beta \chi_{\alpha\beta} m_i^\beta$ local internal magnetic field, Gaussian

TAP like free energy can be averaged over nonlocal J_{ij}.

Averaged TAP-like free energy

$$f_\nu = -\frac{\beta J^2}{4\nu}\sum_{\alpha=1}^{\nu}(1-q_{\alpha\alpha})^2 + \frac{\beta J^2}{4\nu}\sum_{\alpha\neq\beta}\chi_{\alpha\beta}(2q_{\alpha\beta}+\chi_{\alpha\beta})$$

$$- \frac{1}{\beta\nu}\left\langle \ln\left\{ \operatorname*{Tr}_S \exp\left[\frac{\beta^2 J^2}{2}\sum_{\alpha\neq\beta}\chi_{\alpha\beta}S^\alpha S^\beta + \beta\sum_{\alpha=1}^{\nu}\eta_\alpha S^\alpha\right]\right\}\right\rangle_{av},$$

$$\langle X(\eta)\rangle_{av} = \frac{\int\prod_{\alpha=1}^{\nu}\frac{\mathrm{d}\eta_\alpha}{\sqrt{2\pi}}\exp\left(-\frac{1}{2J^2}\sum_{\alpha\beta}\eta_\alpha[Q^{-1}]_{\alpha\beta}\eta_\beta\right)X(\eta)}{\int\prod_{\alpha=1}^{\nu}\frac{\mathrm{d}\eta_\alpha}{\sqrt{2\pi}}\exp\left(-\frac{1}{2J^2}\sum_{\alpha\beta}\eta_\alpha[Q^{-1}]_{\alpha\beta}\eta_\beta\right)}.$$

Stationarity equations for the order parameters are

susceptibilities $\chi_{\alpha\beta} = \langle\langle S^\alpha S^\beta\rangle\rangle_{av} - \langle\langle S^\alpha\rangle\langle S^\beta\rangle\rangle_{av} \qquad \alpha\neq\beta,$

overlaps $q_{\alpha\beta} \equiv \frac{1}{N}\sum_i m_i^\alpha m_i^\beta = \langle\langle S^\alpha\rangle\langle S^\beta\rangle\rangle_{av},$

Summary

- We have averaged TAP-like free energy
- Two sorts of order parameters
  - $q_{\alpha\beta}$ spin overlaps
  - $\chi_{\alpha\beta}$, $\alpha \neq \beta$ overlap susceptibilities, response to the replica independence breaking interaction
- Demand of homogeneity of free energy $\Rightarrow$ independence on the number of replicas.

What to do now?

Find the symmetry of the order parameters so that the free energy does not depend on the number of replicas!

Beginning of the technical part

Two replicas $\nu = 2$

- $q_{11} = q_{22} = q_0$
- $q_{12} = q_{21} = q_1$
- $\chi_{12} = \chi_{21} = \chi$

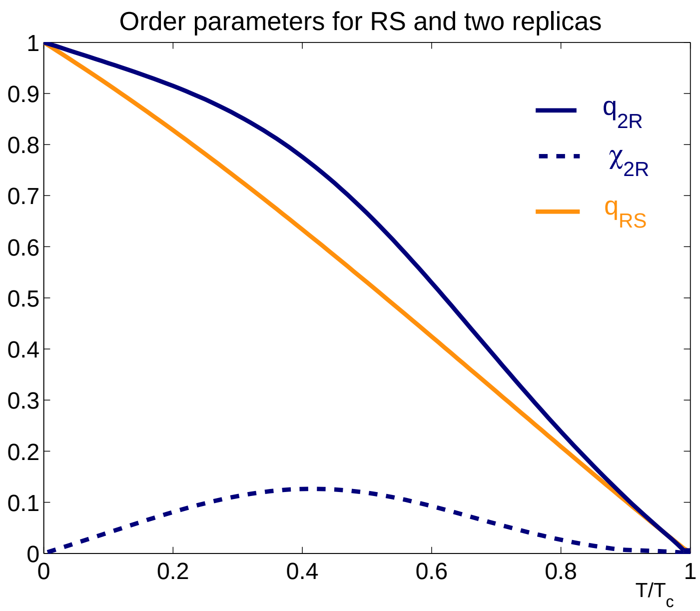
Rewrite the free energy. Numerical solution $\rightarrow$ three possibilities

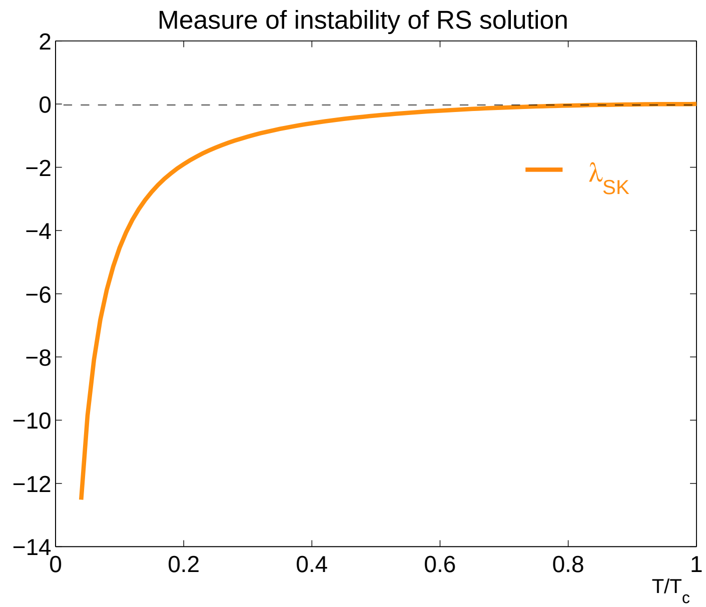
- $q_0 = q_1 = q_{RS}$, $\chi = 0 \Rightarrow$ RS solution
- $q_0 = q_{RS}$, $q_1 = 0$, $\chi = 0 \Rightarrow$ RS solution
- $\chi \neq 0$, $q_{RS} \neq q_1 = q_2 \neq 0$

What do we want?

To improve upon RS solution. $\Rightarrow$ We have to take the third possibility.

More about two-replica solution



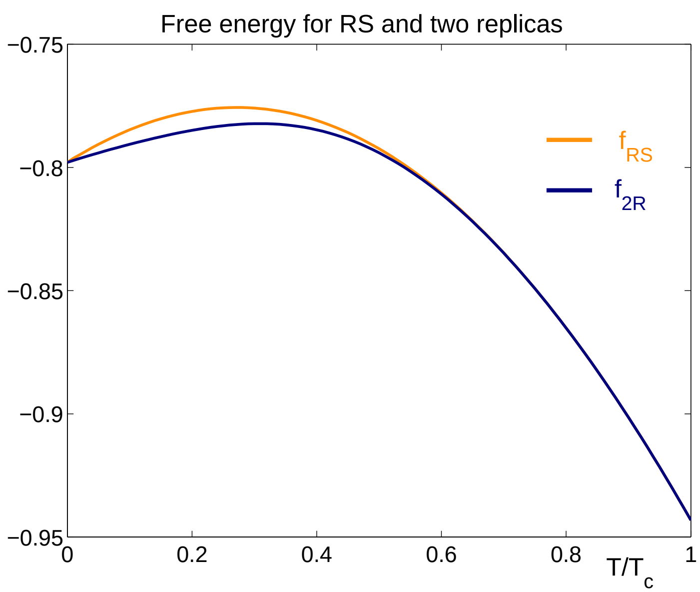


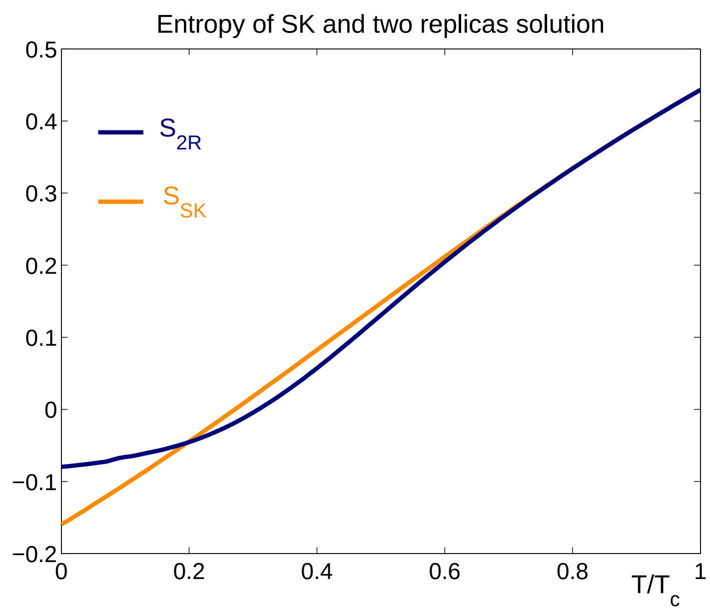
Instability of the RS solution with respect to the 2R solution, $\chi = f_\chi(\chi, q)$.

$$\lambda_{RS} = 1 - \frac{\partial f_\chi}{\partial \chi}\bigg|_{0,q_{RS}} \quad \Rightarrow \quad \lambda_{RS} = 1 - \beta^2 \int \mathrm{D}z \left(1 - \tanh^2\left(\beta z \sqrt{q_{RS}}\right)\right)^2$$

This is well known equation for AT-line. RS solution is unstable $\Leftrightarrow \lambda_{RS} < 0$.

Free energy and entropy





Zero temperature limit

$$f_{RS}(0) = f_{2R}(0), \qquad \frac{1}{2}s_{RS}(0) = s_{2R}(0)$$

According to MC simulations $f(0)$ should be higher!

Free energy for $q_{\alpha\beta} = q$

$$f_\nu = -\frac{\beta}{4}(1-q)^2 + \frac{\beta}{4\nu}\sum_{\alpha\neq\beta}\chi_{\alpha\beta}(2q+\chi_{\alpha\beta}) - \frac{1}{\beta\nu}\cdot$$

$$\cdot \int D\xi \ln\left\{\operatorname*{Tr}_S \exp\left[\frac{\beta^2}{2}\sum_{\alpha\neq\beta}\chi_{\alpha\beta}S^\alpha S^\beta + \beta\xi\sqrt{q}\sum_{\alpha=1}^{\nu}S^\alpha\right]\right\}.$$

Numeric analysis of the stationarity equation for $\nu = 3, 4, 6, \ldots$.

- $\chi_{\alpha\beta} = \chi$, all χ are the same
- Some $\chi = 0 \to$ combination of solutions with a smaller ν

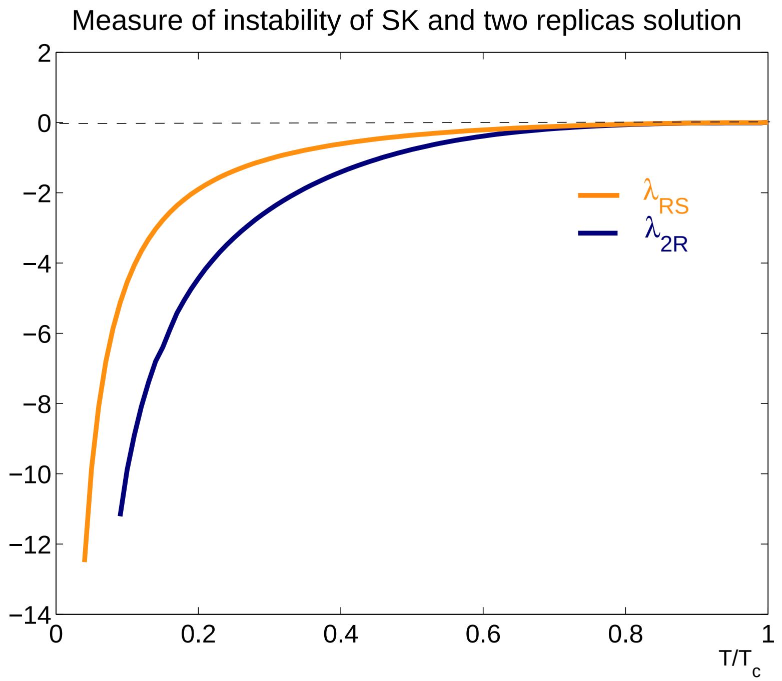
Example: four-replica solution, combination of two two-replica solution.

$$\begin{pmatrix} 0 & \chi & \chi & \chi \\ \chi & 0 & \chi & \chi \\ \chi & \chi & 0 & \chi \\ \chi & \chi & \chi & 0 \end{pmatrix}, \qquad \begin{pmatrix} 0 & \chi & 0 & 0 \\ \chi & 0 & 0 & 0 \\ 0 & 0 & 0 & \chi \\ 0 & 0 & \chi & 0 \end{pmatrix}.$$

Stability

How much the χ_2 wants to be nonzero?

Two-replica solution is unstable $\Leftrightarrow \lambda_{2R} < 0$.



$$\begin{pmatrix} 0 & \chi_1 & \chi_2 & \chi_2 \\ \chi_1 & 0 & \chi_2 & \chi_2 \\ \chi_2 & \chi_2 & 0 & \chi_1 \\ \chi_2 & \chi_2 & \chi_1 & 0 \end{pmatrix}.$$

Two-replica solution is more unstable than RS solution!!!

Is 2R solution better than RS?

- **Yes**
  - The entropy in zero temperature is less negative.
  - RS is unstable with respect to the 2R.
- **No**
  - The zero temperature free energy is still the same.
  - 2R is more unstable with respect to the 4R than RS to 2R.

Which ν is the best?

Remember: Free energy should not depend on ν !

Let us fulfill it at least locally

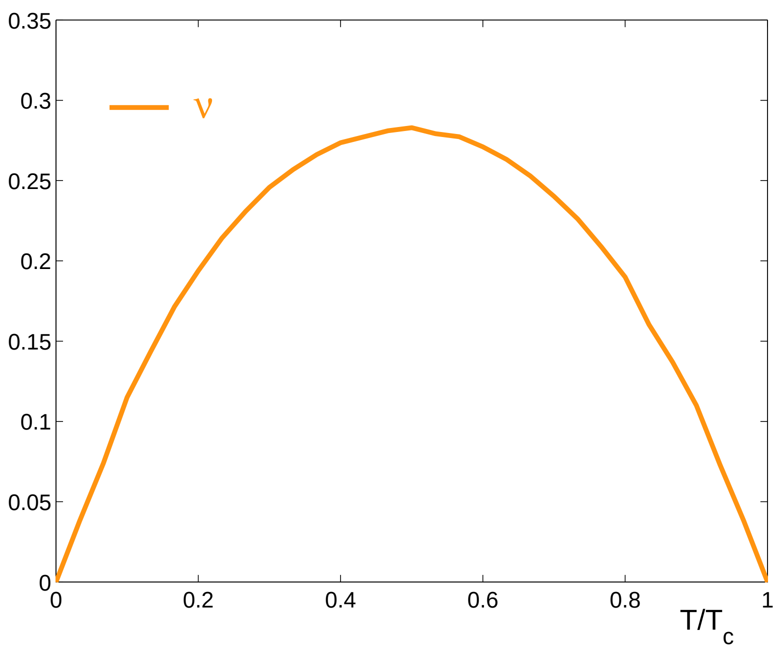
$$\frac{\partial f_\nu}{\partial \nu} = 0.$$

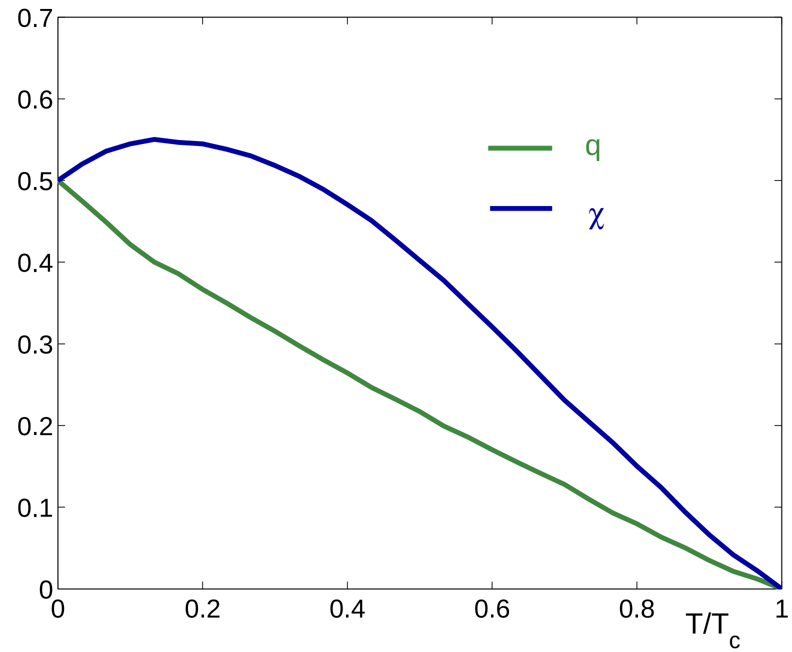
Take $\chi_{\alpha\beta} = \chi$. Free energy

$$f_\nu = -\frac{\beta}{4}(1-q)^2 + \frac{\beta}{4}(\nu-1)\chi(2q+\chi) + \frac{\beta}{2}\chi - \frac{1}{\beta\nu}\int \mathrm{D}\xi \ln \int \mathrm{D}z \left[2\cosh\beta(\xi\sqrt{q} + z\sqrt{\chi})\right]^\nu .$$

- Equivalent to the Parisi 1RSB free energy
- $f_0 = f_1 = f_{RS} \Rightarrow 0 \le \nu \le 1$

Solution of saddle point equations, 1RSB

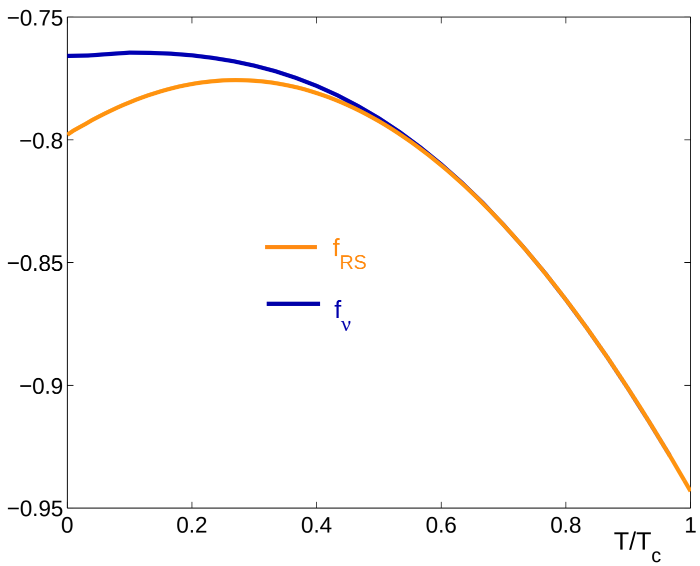


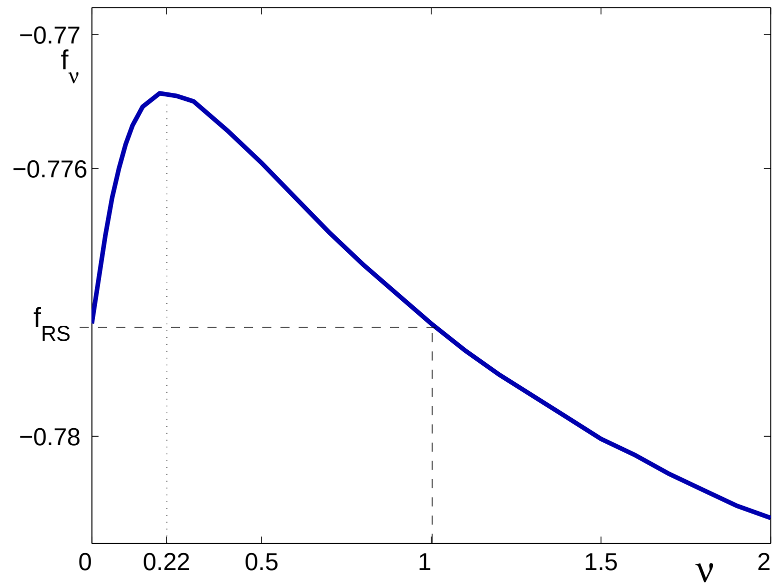


Zero temperature:

- ν temperature independent $\Rightarrow q(0) = 1, \quad \chi(0) = 0$
- ν temperature dependent $\Rightarrow q(0) = 0{,}5, \quad \chi(0) = 0{,}5$

Free energy of 1RSB





Zero temperature

- The free energy is higher $f_\nu(0) = -0{,}765$, MC result $-0{,}76 \pm 0{,}01$
- Entropy is about 16-times less negative

We are going the right way, but we have to continue!

Two-step replica symmetry breaking

Consider

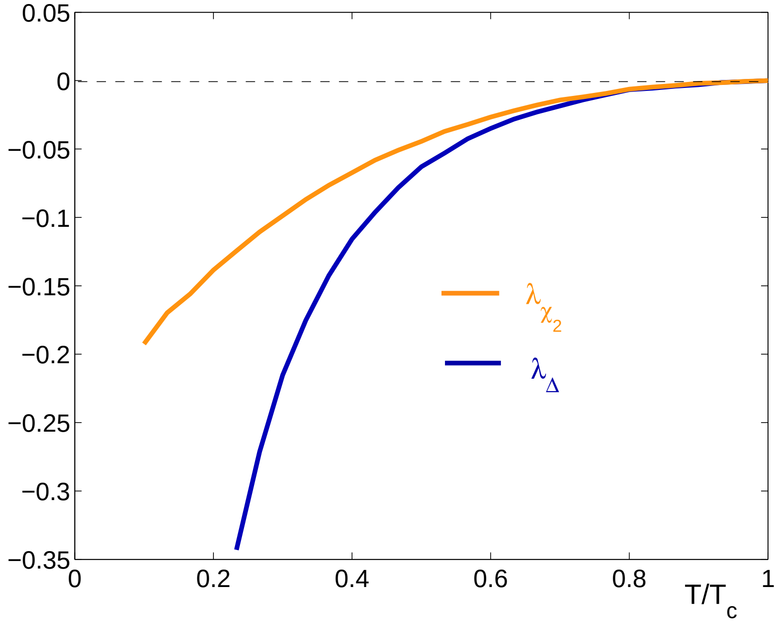
- ν_1 replicas is one super-replica
- take ν_2 super-replicas, $\nu = \nu_1 \nu_2$
- response to interaction between replicas is χ_1
- response to interaction between super-replicas is χ_2

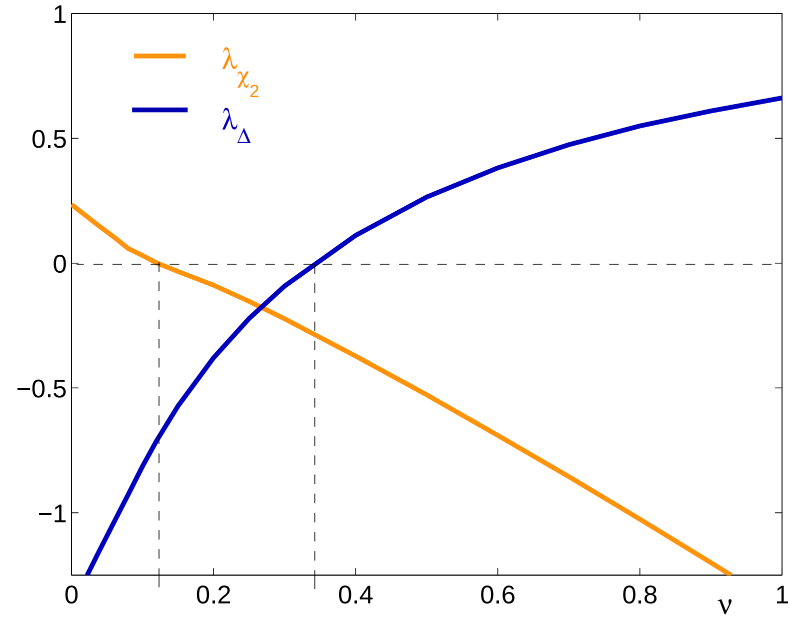
With this the free energy is

$$\begin{aligned} f_\nu &= -\frac{\beta}{4}(1-q)^2 + \frac{\beta}{4}(\nu_1 - 1)(2q+\chi_1)\chi_1 + \frac{\beta}{4}(\nu - \nu_1)(2q+\chi_2)\chi_2 + \frac{\beta}{2}\chi_1 - \\ &- \frac{1}{\beta\nu}\int \mathrm{D}\xi \ln \int \mathrm{D}z \left(\int \mathrm{D}u \; 2\cosh^{\nu_1} \beta(z\sqrt{\chi_2} + u\sqrt{\chi_1 - \chi_2} + \xi\sqrt{q})\right)^{\frac{\nu}{\nu_1}} . \end{aligned}$$

This is Parisi's 2RSB. We can continue and get the FRBS.

Stability of 1RSB





1RSB is unstable, but less than RS. Look at the scale of y-axes!

Now we have the answer why with 4 replicas we had nothing new.

Is 1RSB solution better than RS?

- **Yes**
  - The entropy at zero temperature is less negative.
  - RS is unstable with respect to the 1RSB.
- **Yes**
  - The zero temperature free energy is higher.
  - 1RSB is less unstable with respect to the 2RBS than RS to 1RSB.

Conclusions

- FRSB derived without replica trick and without any ansatz
- FRSB can be derived with replica trick without any ansatz
  - Do we have something Parisi didn't? The homogeneity demand!
- Final FRBS equations are too complicated.
  - At least zero and critical temperature limit?
- What about the real replicas and other random spin systems?