

Modelling of Complex Real-World Systems

Part B. Tools for Heterogeneous Systems

B2. The replica method

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- 1 Self-averaging
- 2 The basic replica identity
- 3 Replicas and minimisation
- 4 Alternative forms
- 5 More complicated objects

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Self-averaging

Site-heterogeneity

heterogeneity in *single-site properties*, e.g. $J_{ij} \rightarrow \xi_i \xi_j / N$, $\theta_i \rightarrow \theta_i$ (Mattis model)

- repeat analysis with $N \rightarrow \infty$

parallel dynamics :
$$m(t+1) = \int d\xi d\theta \rho(\xi, \theta) \xi \tanh[\beta(\xi m(t) + \theta)]$$

sequential dynamics :
$$\frac{d}{dt} m = \int d\xi d\theta \rho(\xi, \theta) \xi \tanh[\beta(\xi m + \theta)] - m$$

$$m(t) = \frac{1}{N} \sum_i \xi_i \sigma_i, \quad \rho(\xi, \eta) = \lim_{N \rightarrow \infty} \frac{1}{N} \sum_i \delta(\xi - \xi_i) \delta(\eta - \theta_i)$$

(see exercises)

- observations

- again deterministic macroscopic laws
- again spontaneous order, but not in terms of $N^{-1} \sum_i \sigma_i$
- details of $\{\xi_i, \theta_i\}$ not important, only $\rho(\xi, \theta)$: 'self-averaging'
- interactions mediated via single observable: $h_i(\sigma) = \xi_i m(\sigma) + \theta_i$

Interaction heterogeneity

site-heterogeneity: $\mathcal{O}(N)$ parameters, harmless

interaction heterogeneity: $\mathcal{O}(N^2)$ parameters ... ?

- simulation examples, $\sigma \in \{-1, 1\}^N$

$$J_{ij} = \frac{Jz_{ij}}{\sqrt{N}}(1 - \delta_{ij}), \quad z_{ij} = z_{ji} : \text{ drawn indep from } p(z) = (2\pi)^{-\frac{1}{2}} e^{-\frac{1}{2}z^2}$$

$$\text{measure: } m(\sigma) = \frac{1}{N} \sum_i \sigma_i, \quad E(\sigma) = -\frac{1}{2N} \sum_{i \neq j} \sigma_i J_{ij} \sigma_j$$

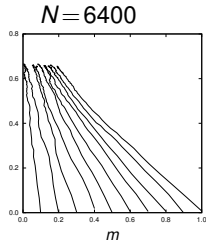
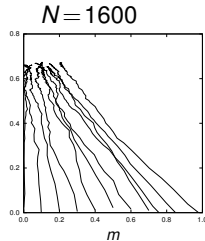
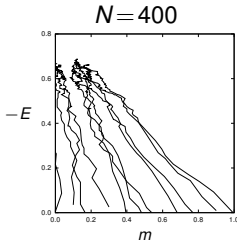
sequential
dynamics,

$$\beta J = 10$$

$$\beta \theta = 0$$

$$E_0 = 0,$$

$$m_0 = \ell/10$$



plotted versus time ...

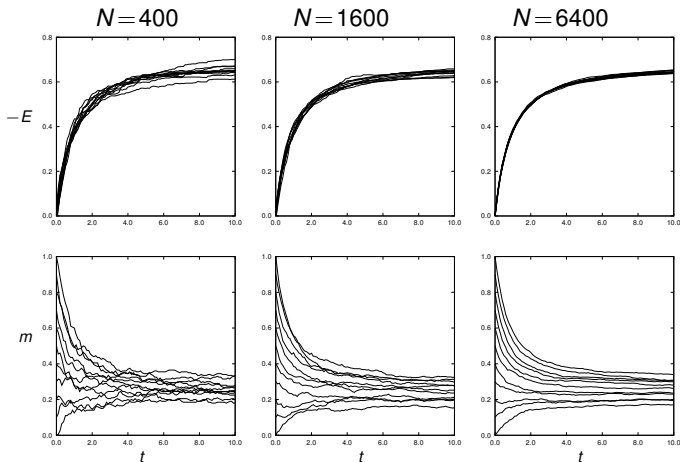
sequential
dynamics,

$$\beta J = 10$$

$$\beta \theta = 2$$

$$E_0 = 0,$$

$$m_0 = \ell/10$$



previous analysis routes no longer work,
but macroscopic dynamics again self-averaging!

Implications of self-averaging

let ξ be (static) system parameters

drawn from $p(\xi)$

notation:
$$\overline{g(\xi)} = \int d\xi p(\xi)g(\xi)$$

- $\omega(\sigma)$ self-averaging:

for all $t \geq 0$:

$$\lim_{N \rightarrow \infty} \langle \omega(\sigma(t)) \rangle = \lim_{N \rightarrow \infty} \overline{\langle \omega(\sigma(t)) \rangle}$$

- generating functions:

if $\lim_{N \rightarrow \infty} f(\lambda)$ exists and is self-averaging

$$\lim_{N \rightarrow \infty} \langle \omega_k(\sigma) \rangle = \lim_{N \rightarrow \infty} \frac{\partial f}{\partial \lambda_k} = \lim_{N \rightarrow \infty} \frac{\partial \bar{f}}{\partial \lambda_k}$$

- can **work with \bar{f}** instead of f , for $N \rightarrow \infty$
- fruitful new route to solving complex models
- generating functions exist for *statics and dynamics*

Previous example

$$h_i(\boldsymbol{\sigma}) = \sum_j J_{ij} \sigma_j + \theta, \quad J_{ij} = \frac{J z_{ij}}{\sqrt{N}} (1 - \delta_{ij}), \quad z_{ij} = z_{ji} : \text{static random pars}$$

$$\text{observables: } m(\boldsymbol{\sigma}) = \frac{1}{N} \sum_i \sigma_i, \quad E(\boldsymbol{\sigma}) = -\frac{1}{2N} \sum_{i \neq j} \sigma_i J_{ij} \sigma_j$$

Sherrington-Kirkpatrick spin-glass model

- equilibrium

$$\rho(\boldsymbol{\sigma}) = \frac{1}{Z} e^{-\beta H(\boldsymbol{\sigma})}, \quad H(\boldsymbol{\sigma}) = -\frac{1}{2} \sum_{i \neq j} J_{ij} \sigma_i \sigma_j - \theta \sum_i \sigma_i$$

$$f = -\frac{1}{\beta N} \log Z = -\frac{1}{\beta N} \log \left[\sum_{\boldsymbol{\sigma}} e^{\frac{\beta J}{2\sqrt{N}} \sum_{i \neq j} z_{ij} \sigma_i \sigma_j + \beta \theta \sum_i \sigma_i} \right]$$

large N

$$\overline{\langle E(\boldsymbol{\sigma}) \rangle} = J \frac{\partial \bar{f}}{\partial J}, \quad \overline{\langle m(\boldsymbol{\sigma}) \rangle} = -\frac{\partial \bar{f}}{\partial \theta} : \quad \bar{f} = -\frac{1}{\beta N} \overline{\log \left[\sum_{\boldsymbol{\sigma}} e^{\frac{\beta J}{2\sqrt{N}} \sum_{i \neq j} z_{ij} \sigma_i \sigma_j + \beta \theta \sum_i \sigma_i} \right]}$$

see also: <https://scitechdaily.com/new-whirling-state-of-matter-discovered-self-induced-spin-glass/>

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The basic replica identity

the replica method

A clever trick that enables the analytical calculation of averages that are normally impossible to do, except numerically

is particularly useful for

Complex heterogeneous systems composed of *many* interacting variables, and with *many* parameters on which we have only statistical information (too large for numerical averages to be computationally feasible)

gives us

Analytical predictions for the behaviour of *macroscopic* quantities in *typical* realisations of the systems under study.

first appearance: Marc Kac 1968

first in physics: Sherrington & Kirkpatrick 1975

first in biology: Amit, Gutfreund & Sompolinsky 1985

since then: computer science, economics, statistics, ...

Disorder-averaged generating functions

- Consider processes with many fixed (pseudo-)random parameters ξ ('disorder'), distributed according to $\mathcal{P}(\xi)$

$$p(\sigma|\xi) = \frac{e^{\sum_{\ell=1}^L \lambda_{\ell} \omega_{\ell}(\sigma, \xi)}}{Z(\lambda, \xi)}, \quad Z(\lambda, \xi) = \sum_{\sigma} e^{\sum_{\ell=1}^L \lambda_{\ell} \omega_{\ell}(\sigma, \xi)}$$

- calculating $\langle g(\sigma, \xi) \rangle$ for *each* realisation of ξ usually impossible
- we are mostly interested in *typical* values of state averages
- for $N \rightarrow \infty$ macroscopic averages will not depend on ξ , only on $\mathcal{P}(\xi)$, 'self-averaging': $\lim_{N \rightarrow \infty} \langle g(\sigma, \xi) \rangle$ indep of ξ

so focus on

$$\overline{\langle g(\sigma, \xi) \rangle} = \sum_{\xi} \mathcal{P}(\xi) \langle g(\sigma, \xi) \rangle = \sum_{\xi} \mathcal{P}(\xi) \sum_{\sigma} p(\sigma|\xi) g(\sigma, \xi)$$

- new generating function

$$\bar{F}(\lambda, \mu) = \sum_{\xi} \mathcal{P}(\xi) \log Z(\lambda, \mu, \xi), \quad Z(\lambda, \mu, \xi) = \sum_{\sigma} e^{\mu\psi(\sigma, \xi) + \sum_{\ell} \lambda_{\ell} \omega_{\ell}(\sigma, \xi)}$$

$$\begin{aligned} \lim_{\mu \rightarrow 0} \frac{\partial}{\partial \mu} \bar{F}(\lambda, \mu) &= \lim_{\mu \rightarrow 0} \sum_{\xi} \mathcal{P}(\xi) \left\{ \frac{\sum_{\sigma} \psi(\sigma, \xi) e^{\mu\psi(\sigma, \xi) + \sum_{\ell} \lambda_{\ell} \omega_{\ell}(\sigma, \xi)}}{\sum_{\sigma} e^{\mu\psi(\sigma, \xi) + \sum_{\ell} \lambda_{\ell} \omega_{\ell}(\sigma, \xi)}} \right\} \\ &= \sum_{\xi} \mathcal{P}(\xi) \left\{ \frac{\sum_{\sigma} \psi(\sigma, \xi) e^{\sum_{\ell} \lambda_{\ell} \omega_{\ell}(\sigma, \xi)}}{\sum_{\sigma} e^{\sum_{\ell} \lambda_{\ell} \omega_{\ell}(\sigma, \xi)}} \right\} = \overline{\langle \psi \rangle} \end{aligned}$$

- main obstacle in calculating \bar{F} :
the logarithm ...

$$\text{replica identity : } \overline{\log Z} = \lim_{n \rightarrow 0} \frac{1}{n} \log \overline{Z^n}$$

proof:

$$\begin{aligned} \lim_{n \rightarrow 0} \frac{1}{n} \log \overline{Z^n} &= \lim_{n \rightarrow 0} \frac{1}{n} \log \overline{[e^{n \log Z}]} = \lim_{n \rightarrow 0} \frac{1}{n} \log \overline{[1 + n \log Z + \mathcal{O}(n^2)]} \\ &= \lim_{n \rightarrow 0} \frac{1}{n} \log [1 + n \overline{\log Z} + \mathcal{O}(n^2)] = \overline{\log Z} \end{aligned}$$

Powers by replication

- apply $\overline{\log Z} = \lim_{n \rightarrow 0} \frac{1}{n} \log \overline{Z^n}$ (for simplest case $L=1$)

$$\begin{aligned} \overline{F}(\lambda) &= \sum_{\xi} \mathcal{P}(\xi) \log \left[\sum_{\sigma} e^{\lambda \omega(\sigma, \xi)} \right] = \lim_{n \rightarrow 0} \frac{1}{n} \log \sum_{\xi} \mathcal{P}(\xi) \left[\sum_{\sigma} e^{\lambda \omega(\sigma, \xi)} \right]^n \\ &= \lim_{n \rightarrow 0} \frac{1}{n} \log \sum_{\xi} \mathcal{P}(\xi) \left[\sum_{\sigma^1} \dots \sum_{\sigma^n} e^{\lambda \sum_{\alpha=1}^n \omega(\sigma^\alpha, \xi)} \right] \\ &= \lim_{n \rightarrow 0} \frac{1}{n} \log \left[\sum_{\sigma^1} \dots \sum_{\sigma^n} \sum_{\xi} \mathcal{P}(\xi) e^{\lambda \sum_{\alpha=1}^n \omega(\sigma^\alpha, \xi)} \right] \end{aligned}$$

notes

- ξ -average converted into doable one ...
- involves n 'replicas' σ^α of original system,
- but with $n \rightarrow 0$ at the end ...
- penultimate step true only for *integer* n ,
so limit requires *analytical continuation* ...



- imagine a physical system, with free energy density as generating function

$$f_N = -\frac{1}{\beta N} \log Z, \quad Z = \sum_{\sigma} e^{-\beta H(\sigma, \xi)}$$

replica method

$$\begin{aligned} \bar{f}_N &= -\frac{1}{\beta N} \overline{\log Z} = -\lim_{n \rightarrow 0} \frac{1}{n\beta N} \log \overline{Z^n} \\ &= -\lim_{n \rightarrow 0} \frac{1}{\beta n N} \log \left[\sum_{\sigma^1 \dots \sigma^n} \overline{e^{-\beta \sum_{\alpha=1}^n H(\sigma^\alpha, \xi)}} \right] \\ &= -\lim_{n \rightarrow 0} \frac{1}{\beta n N} \log Z', \quad Z' = \sum_{\sigma^1 \dots \sigma^n} e^{-\beta H_{\text{eff}}(\sigma^1, \dots, \sigma^n)} \\ & \quad H_{\text{eff}}(\sigma^1, \dots, \sigma^n) = -\frac{1}{\beta} \log \left(\overline{e^{-\beta \sum_{\alpha=1}^n H(\sigma^\alpha, \xi)}} \right) \end{aligned}$$

If f self-averaging:

disordered N -variable system with $H(\sigma, \xi)$ for $N \rightarrow \infty$

equivalent to homogeneous nN -variable system with $H_{\text{eff}}(\sigma^1, \dots, \sigma^n)$

But does the replica identity actually help?

- return to previous example ...

$$\begin{aligned}
 \bar{f}_N &= -\frac{1}{\beta N} \log \left[\overline{\sum_{\sigma} e^{\frac{\beta J}{\sqrt{N}} \sum_{i<j} z_{ij} \sigma_i \sigma_j + \beta \theta \sum_i \sigma_i}} \right] \\
 &= -\lim_{n \rightarrow 0} \frac{1}{n\beta N} \log \left[\overline{\sum_{\sigma} e^{\frac{\beta J}{\sqrt{N}} \sum_{i<j} z_{ij} \sigma_i \sigma_j + \beta \theta \sum_i \sigma_i}}^n \right] \\
 &= -\lim_{n \rightarrow 0} \frac{1}{n\beta N} \log \left[\sum_{\sigma^1 \dots \sigma^n} \overline{e^{\frac{\beta J}{\sqrt{N}} \sum_{i<j} z_{ij} \sum_{\alpha=1}^n \sigma_i^\alpha \sigma_j^\alpha + \beta \theta \sum_i \sum_{\alpha=1}^n \sigma_i^\alpha}} \right] \\
 &= -\lim_{n \rightarrow 0} \frac{1}{n\beta N} \log \left[\sum_{\sigma^1 \dots \sigma^n} e^{\beta \theta \sum_i \sum_{\alpha=1}^n \sigma_i^\alpha} \prod_{i<j} \int \frac{dz}{\sqrt{2\pi}} e^{-\frac{1}{2} z^2 + \frac{\beta J z}{\sqrt{N}} \sum_{\alpha=1}^n \sigma_i^\alpha \sigma_j^\alpha} \right] \\
 &= -\lim_{n \rightarrow 0} \frac{1}{n\beta N} \log \left[\sum_{\sigma^1 \dots \sigma^n} e^{\beta \theta \sum_i \sum_{\alpha=1}^n \sigma_i^\alpha} \prod_{i<j} e^{\frac{(\beta J)^2}{2N} \left(\sum_{\alpha=1}^n \sigma_i^\alpha \sigma_j^\alpha \right)^2} \right]
 \end{aligned}$$

$$\begin{aligned} \bar{f}_N &= -\lim_{n \rightarrow 0} \frac{1}{n\beta N} \log \left[\sum_{\sigma^1 \dots \sigma^n} e^{\beta\theta \sum_i \sum_{\alpha=1}^n \sigma_i^\alpha + \frac{(\beta J)^2}{4N} \sum_{i \neq j} \left(\sum_{\alpha=1}^n \sigma_i^\alpha \sigma_j^\alpha \right)^2} \right] \\ &= -\lim_{n \rightarrow 0} \frac{1}{n\beta N} \log \left[\sum_{\sigma^1 \dots \sigma^n} e^{N\beta\theta \sum_{\alpha=1}^n \left(\frac{1}{N} \sum_i \sigma_i^\alpha \right) + \frac{N(\beta J)^2}{4} \sum_{\alpha, \beta=1}^n \left(\frac{1}{N} \sum_i \sigma_i^\alpha \sigma_i^\beta \right)^2 + \mathcal{O}(1)} \right] \end{aligned}$$

new key macroscopic observables:

$$m_\alpha = \frac{1}{N} \sum_{i=1}^N \sigma_i^\alpha, \quad q_{\alpha\beta} = \frac{1}{N} \sum_{i=1}^N \sigma_i^\alpha \sigma_i^\beta, \quad \alpha, \beta = 1 \dots n$$

- unusual mathematics,
 n -vectors and $n \times n$ matrices with $n \rightarrow 0$...
- new types of statistical theories
- but results turn out to be *correct*, confirmed by computer simulations and alternative (much more tedious) routes

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Replicas and minimization

Suppose we have data D , with prob distr $\mathcal{P}(D)$
and an algorithm which minimises an error function $E(D, \theta)$

(maximum likelihood, logistic,
Cox & Bayesian regression, machine
learning, discriminant analysis, ...)

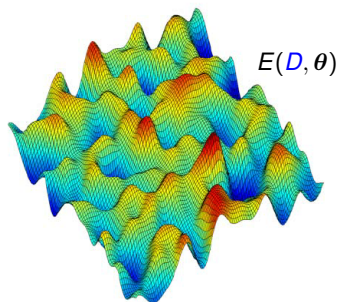
- algorithm outcome

$$\theta^*(D) = \arg \min_{\theta} E(D, \theta)$$

$$E_{\min}(D) = \min_{\theta} E(D, \theta)$$

most computer science analyses
focus on *worst case* performance
(i.e. on most difficult data)

not always useful in practice ...



Typical performance of algorithms

- typical performance

$$\theta^* = \sum_D \mathcal{P}(D) \theta^*(D) = \overline{\theta^*(D)}$$

$$E_{\min} = \sum_D \mathcal{P}(D) E_{\min}(D) = \overline{E_{\min}(D)}$$

- steepest descent identity
combined with replica trick

$$E_{\min}(D) = \min_{\theta} E(D, \theta) = - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log \int d\theta e^{-\beta E(D, \theta)}$$

$$E_{\min} = \overline{E_{\min}(D)} = - \lim_{\beta \rightarrow \infty} \frac{1}{\beta} \log \overline{\int d\theta e^{-\beta E(D, \theta)}}$$

$$= - \lim_{\beta \rightarrow \infty} \lim_{n \rightarrow 0} \frac{1}{\beta n} \log \left[\overline{\int d\theta e^{-\beta E(D, \theta)}}^n \right]$$

$$= - \lim_{\beta \rightarrow \infty} \lim_{n \rightarrow 0} \frac{1}{\beta n} \log \int d\theta^1 \dots \theta^n e^{-\beta \sum_{\alpha=1}^n E(D, \theta^\alpha)}$$

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Alternative forms of the replica identity

suppose we need disorder averages, but for a $p(\sigma|\xi)$ that is not of an exponential form?

$$p(\sigma|\xi) = \frac{W(\sigma, \xi)}{\sum_{\sigma'} W(\sigma', \xi)}, \quad \overline{\langle g \rangle} = \overline{\sum_{\sigma} p(\sigma|\xi) g(\sigma, \xi)}$$

- main obstacle: the fraction ...

$$\begin{aligned} \overline{\langle g \rangle} &= \overline{\left[\frac{\sum_{\sigma} W(\sigma, \xi) g(\sigma, \xi)}{\sum_{\sigma} W(\sigma, \xi)} \right]} = \overline{\left[\sum_{\sigma} W(\sigma, \xi) g(\sigma, \xi) \right] \left[\sum_{\sigma} W(\sigma, \xi) \right]^{-1}} \\ &= \lim_{n \rightarrow 0} \overline{\left[\sum_{\sigma} W(\sigma, \xi) g(\sigma, \xi) \right] \left[\sum_{\sigma} W(\sigma, \xi) \right]^{n-1}} \\ &= \lim_{n \rightarrow 0} \sum_{\sigma^1} \dots \sum_{\sigma^n} \overline{g(\sigma^1, \xi) W(\sigma^1, \xi) \dots W(\sigma^n, \xi)} \end{aligned}$$

(again: used integer n , but $n \rightarrow 0$...)

- equivalence of the two forms of replica identity, if

$$W(\sigma, \xi) = e^{\sum_{\ell} \lambda_{\ell} \phi_{\ell}(\sigma, \xi)}$$

$$\begin{aligned} \overline{\langle g \rangle} &= \lim_{n \rightarrow 0} \sum_{\sigma^1} \dots \sum_{\sigma^n} \overline{g(\sigma^1, \xi) W(\sigma^1, \xi) \dots W(\sigma^n, \xi)} \\ &= \lim_{n \rightarrow 0} \sum_{\sigma^1} \dots \sum_{\sigma^n} \overline{g(\sigma^1, \xi) e^{\sum_{\alpha=1}^n \sum_{\ell} \lambda_{\ell} \phi_{\ell}(\sigma^{\alpha}, \xi)}} \\ &= \lim_{n \rightarrow 0} \frac{1}{n} \sum_{\sigma^1} \dots \sum_{\sigma^n} \overline{\left[\sum_{\alpha=1}^n g(\sigma^{\alpha}, \xi) \right] e^{\sum_{\alpha=1}^n \sum_{\ell} \lambda_{\ell} \phi_{\ell}(\sigma^{\alpha}, \xi)}} \\ &= \lim_{n \rightarrow 0} \frac{1}{n} \lim_{\mu \rightarrow 0} \frac{\partial}{\partial \mu} \sum_{\sigma^1} \dots \sum_{\sigma^n} \overline{e^{\sum_{\alpha=1}^n \sum_{\ell} \lambda_{\ell} \phi_{\ell}(\sigma^{\alpha}, \xi) + \mu \sum_{\alpha=1}^n g(\sigma^{\alpha}, \xi)}} \\ &= \lim_{n \rightarrow 0} \lim_{\mu \rightarrow 0} \frac{\partial}{\partial \mu} \frac{1}{n} \sum_{\sigma^1} \dots \sum_{\sigma^n} \overline{e^{\sum_{\alpha=1}^n \left[\sum_{\ell} \lambda_{\ell} \phi_{\ell}(\sigma^{\alpha}, \xi) + \mu g(\sigma^{\alpha}, \xi) \right]}} \\ &= \lim_{n \rightarrow 0} \lim_{\mu \rightarrow 0} \frac{\partial}{\partial \mu} \frac{1}{n} \overline{Z^n(\lambda, \mu, \xi)}, \quad Z(\lambda, \mu, \xi) = \sum_{\sigma} e^{\sum_{\ell} \lambda_{\ell} \phi_{\ell}(\sigma, \xi) + \mu g(\sigma, \xi)} \\ &= \lim_{\mu \rightarrow 0} \frac{\partial}{\partial \mu} \overline{\log Z(\lambda, \mu, \xi)} \end{aligned}$$

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More complicated objects

- let $p(\sigma|\xi) = Z^{-1}(\xi)e^{-\beta H(\sigma,\xi)}$

$$\begin{aligned} \overline{\langle \sigma_i \rangle \langle \sigma_j \rangle} &= \overline{\left[\frac{\sum_{\sigma} e^{-\beta H(\sigma,\xi)} \sigma_i}{\sum_{\sigma} e^{-\beta H(\sigma,\xi)}} \right] \left[\frac{\sum_{\sigma} e^{-\beta H(\sigma,\xi)} \sigma_j}{\sum_{\sigma} e^{-\beta H(\sigma,\xi)}} \right]} \\ &= \lim_{n \rightarrow 0} \overline{\left[\sum_{\sigma} e^{-\beta H(\sigma,\xi)} \sigma_i \right] \left[\sum_{\sigma} e^{-\beta H(\sigma,\xi)} \sigma_j \right] \left[\sum_{\sigma} e^{-\beta H(\sigma,\xi)} \right]^{n-2}} \\ &= \lim_{n \rightarrow 0} \sum_{\sigma^1} \dots \sum_{\sigma^n} \sigma_i^1 \sigma_j^2 e^{-\beta \sum_{\alpha=1}^n H(\sigma^\alpha, \xi)} \\ \overline{\langle \sigma_i \rangle \langle \sigma_j \rangle \langle \sigma_k \rangle} &= \lim_{n \rightarrow 0} \sum_{\sigma^1} \dots \sum_{\sigma^n} \sigma_i^1 \sigma_j^2 \sigma_k^3 e^{-\beta \sum_{\alpha=1}^n H(\sigma^\alpha, \xi)} \end{aligned}$$

- detect macroscopic order,
not visible in $m = N^{-1} \sum_i \langle \sigma_i \rangle$

$$q_{\text{EA}} = \frac{1}{N} \sum_i \overline{\langle \sigma_i \rangle^2} = \lim_{n \rightarrow 0} \sum_{\sigma^1} \dots \sum_{\sigma^n} \left(\frac{1}{N} \sum_i \sigma_i^1 \sigma_i^2 \right) e^{-\beta \sum_{\alpha=1}^n H(\sigma^\alpha, \xi)}$$

(Edwards-Anderson parameter)