Replica Symmetry Breaking in Spin Glasses

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"Celebrating the Science of Giorgio Parisi"
ICTS, Bangalore
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Awarded the Nobel Prize in Physics, 2021 for
'the discovery of the interplay of disorder
and fluctuations in physical systems from
atomic to planetary scales'.

Replica Symmetry Breaking in Spin Glasses

Outline

I. Pedagogical account of replica symmetry breaking in the Parisi solution for the Sherrington-Kirkpatrick model of spin glass.

- ►Derivation
- ►Physical interpretation
- ►Applicability to experimental systems

II. Significance of this work: how it has influenced subsequent developments in many areas of science.

Interacting spin systems

$$\mathcal{H} = -\sum_{i>j} J_{ij}\vec{S}_i \cdot \vec{S}_j - \sum_i \vec{h} \cdot \vec{S}_i$$ Heisenberg Model

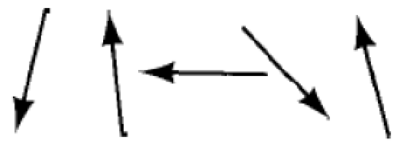
$$\mathcal{H} = -\sum_{i>j} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i$$ Ising Model

$J_{ij} = J > 0$ if i and j are nearest neighbors, and

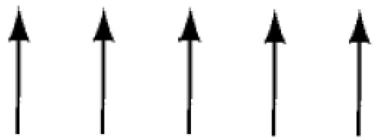
$J_{ij} = 0$ otherwise

Ferromagnetic model

Ferromagnetic ordering in which $m \equiv \langle \sigma_i \rangle \neq 0$ for $h = 0$.

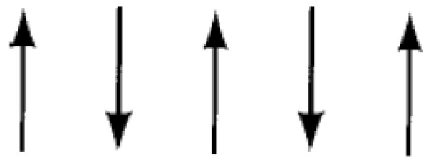


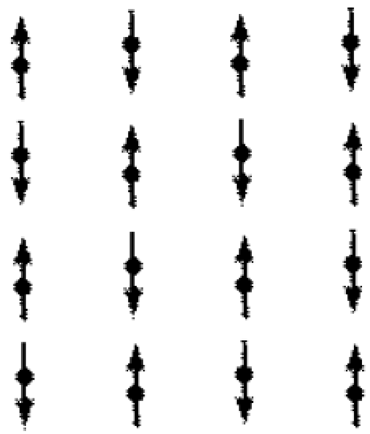
Paramagnetic state



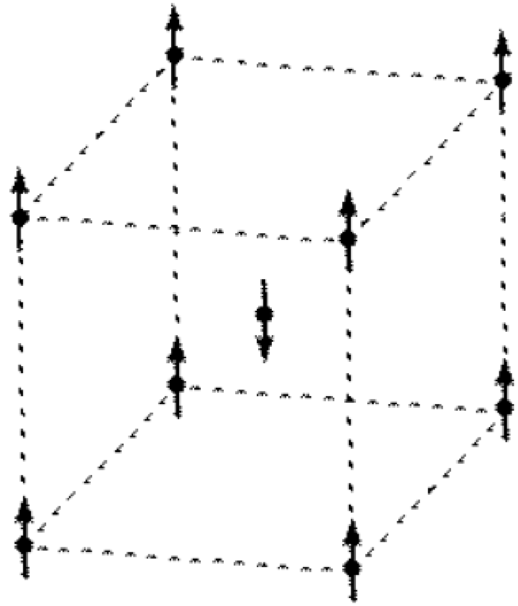
Ferromagnetic state

For J < 0, antiferromagnetic ordering may occur





2d square lattice



3d BCC lattice

What are Spin Glasses?

- Magnetic systems with **quenched disorder**.
- Competition between ferromagnetic and antiferromagnetic interactions.

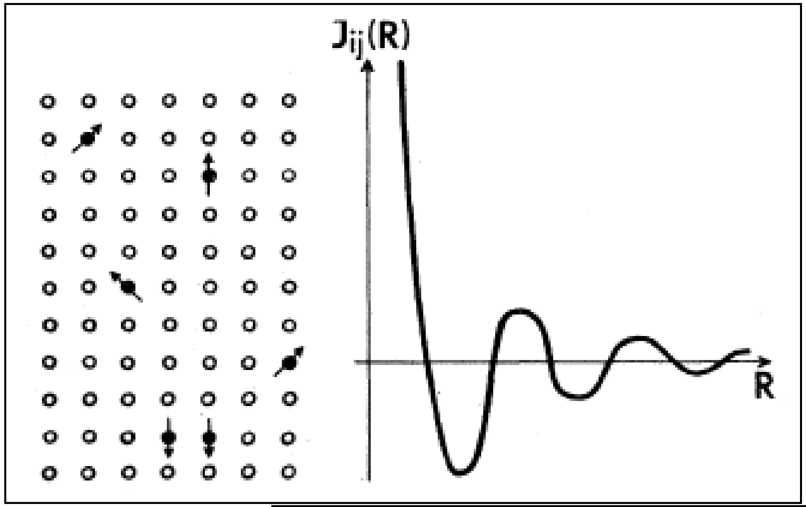
“Glass”: Disorder + Slow Dynamics

Example: CuMn, AuFe, …

$$J(r) = J_0 \frac{\cos(2k_F r + \phi_0)}{(k_F r)^3}$$

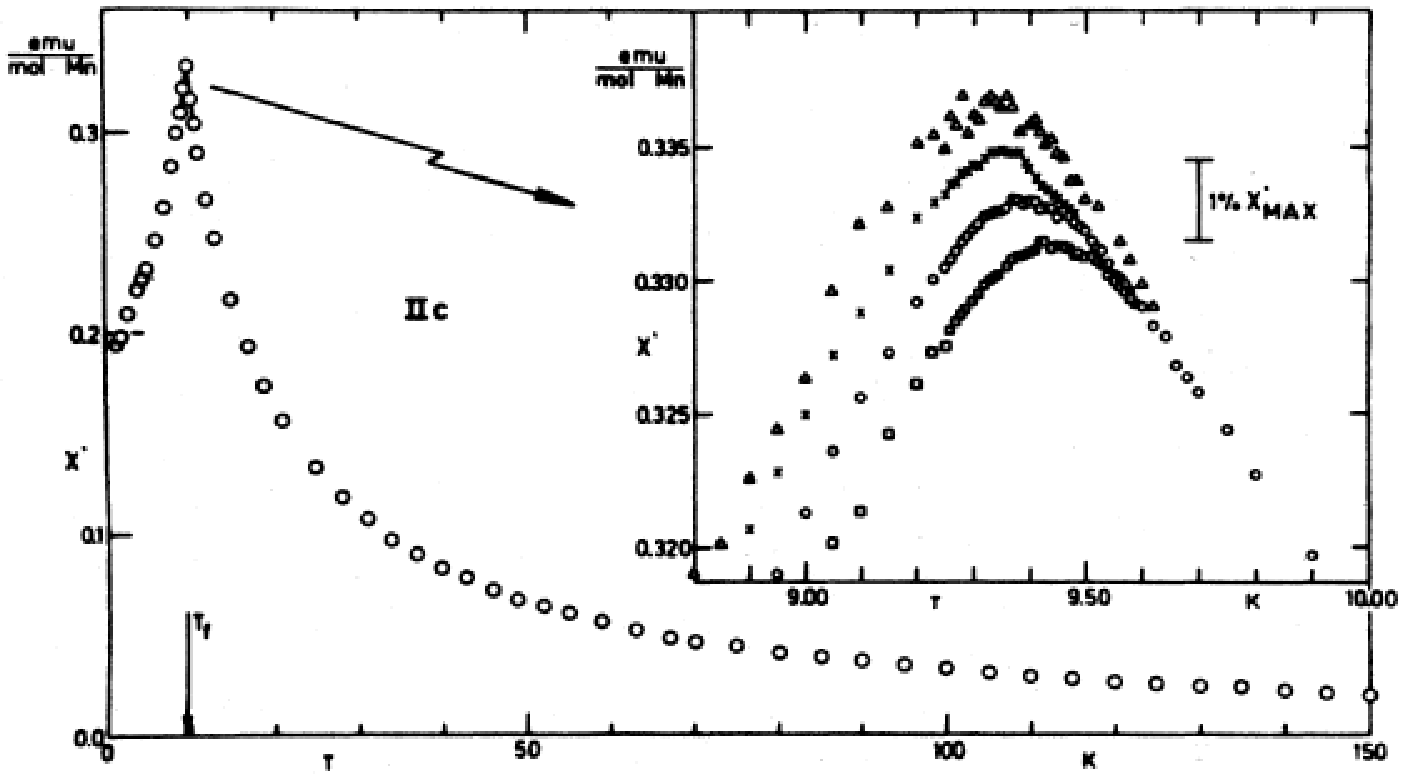
RKKY Interaction between localized spins

V. Cannella and J.A. Mydosh, Phys. Rev. B **6**, 4220 (1972): provided the first experimental evidence for the occurrence of a phase transition in these systems.



Figures from K. Binder and A.P. Young, Rev. Mod. Phys. **58**, 801 (1986).

Experimental results: (1) Cusp in the magnetic susceptibility



AC Susceptibility of CuMn as a function of temperature

Mulder *et al*, Phys. Rev. B **23**, 1384 (1981)

Experimental results: (2) Slow dynamics at low temperatures

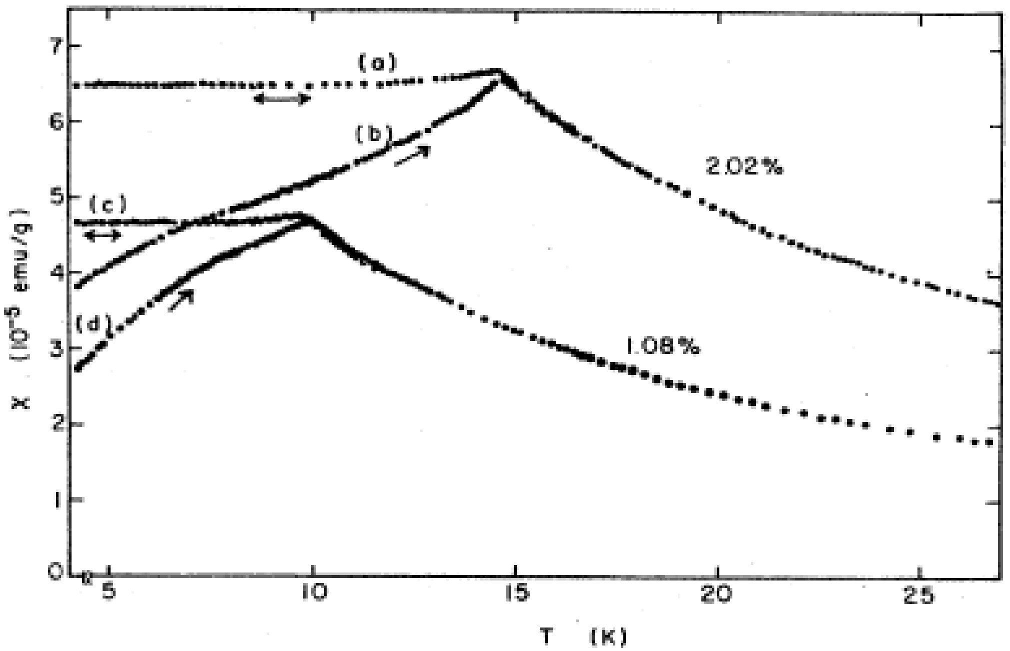


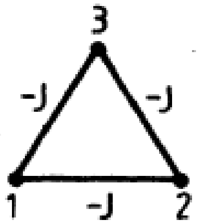
FIG. 7. Static susceptibilities of *Cu*Mn vs temperature for 1.08 and 2.02 at. % Mn. After zero-field cooling ($H < 0.05$ Oe), initial susceptibilities (b) and (d) were taken for increasing temperature in a field of $H = 5.9$ Oe. The susceptibilities (a) and (c) were obtained in the field $H = 5.9$ Oe, which was applied above T_f before cooling the samples. From Nagata *et al.* (1979).

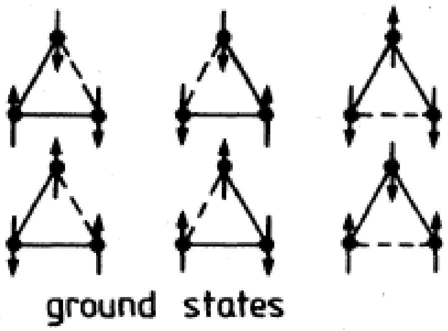
Difference between zero-field-cooled and field-cooled magnetization for T<T(cusp)

Nagata *et al*, Phys. Rev. B **19**, 1633 (1979)

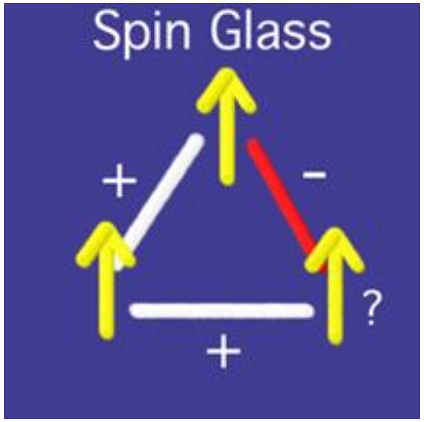
Frustration

All pair interactions can not be satisfied simultaneously





Frustration leads to a multiplicity of ground states of the spin system



Frustration is present if the product of the signs of the interactions is -1.

Conventional spin ordering is not possible in systems with strong frustration

Edwards-Anderson Model

S. F. Edwards and P. W. Anderson, J. Phys. F **5**, 965 (1975).

$$\mathcal{H} = -\sum_{<ij>} J_{ij}\sigma_i\sigma_j \quad \sigma_i = \pm 1$$

Ising spins on a regular lattice
Nearest-neighbour interactions
Quenched disorder

$$\tilde{P}(\{J_{ij}\}) = \Pi_{<ij>} P(J_{ij})$$

$$P(J_{ij}) = \frac{1}{\sqrt{2\pi J^2}} \exp[-J_{ij}^2/2J^2]$$

or

$$P(J_{ij}) = \frac{1}{2}[\delta(J_{ij} + J) + \delta(J_{ij} - J)]$$

$$[J_{ij}]_{av} = 0, \quad [J_{ij}^2]_{av} = J^2$$

No ferromagnetic or antiferromagnetic phase is possible

Spin Glass Phase

High-temperature $\langle\sigma_i\rangle = 0 \quad M \equiv \frac{1}{N}\sum_{i=1}^{N}\langle\sigma_i\rangle = 0$
paramagnetic phase

Low-temperature $\langle\sigma_i\rangle \neq 0 \quad M \equiv \frac{1}{N}\sum_{i=1}^{N}\langle\sigma_i\rangle = 0$
spin glass phase

Edwards-Anderson Order Parameter $q \equiv \frac{1}{N}\sum_{i=1}^{N}(\langle\sigma_i\rangle)^2 \neq 0$

Temporal autocorrelation function

$$C(t) \equiv \frac{1}{N}\sum_{i=1}^{N}\langle\sigma_i(t)\sigma_i(0)\rangle$$

$$C(t)|_{t\to\infty} = \frac{1}{N}\sum_{i=1}^{N}(\langle\sigma_i\rangle)^2 = q$$

Spin glass transition :
"Freezing" of the spins
in random orientations

The Replica Method Disorder-averaged Free Energy

$$F = Nf = -T[\ln Z(\{J_{ij}\})]_{av}$$
$$= -T \int \Pi_{<ij>} dJ_{ij} \tilde{P}(\{J_{ij}\}) \ln Z(\{J_{ij}\})$$

Mathematical identity: $\ln(x) = \lim_{n\to 0} \frac{x^n - 1}{n}$

$$[\ln Z(\{J_{ij}\})]_{av} = \lim_{n\to 0} \frac{[Z^n(\{J_{ij}\})]_{av} - 1}{n}$$

$$[Z^n(\{J_{ij}\})]_{av} = [\mathrm{Tr}_{\{\sigma_i^\alpha\}} \exp[-\sum_{\alpha=1}^{n} \mathcal{H}(\{\sigma_i^\alpha\}, \{J_{ij}\})/T]]_{av}$$
$$= \mathrm{Tr}_{\{\sigma_i^\alpha\}} \exp[-\mathcal{H}_{eff}(\{\sigma_i^\alpha\})/T]$$

$$\mathcal{H}_{eff}(\{\sigma_i^\alpha\}) = -T \ln[\int \Pi_{<ij>} dJ_{ij} \tilde{P}(\{J_{ij}\})$$
$$\times \exp[-\sum_{\alpha=1}^{n} \mathcal{H}(\{\sigma_i^\alpha\}, \{J_{ij}\})/T]]$$

$\mathcal{H}_{eff}(\{\sigma_i^\alpha\})$ **does not** have any quenched disorder

Use standard methods to treat the replicated (n-component) spin model described by $\mathcal{H}_{eff}(\{\sigma_i^\alpha\})$. Take n → 0 limit at the end of the calculation.

Edwards-Anderson (Spin Glass) Order Parameter

$$q = [\langle \sigma_i \rangle^2]_{av} = \langle \sigma_i^\alpha \sigma_i^\beta \rangle_{\mathcal{H}_{eff}}, \ \alpha \neq \beta$$

The spin glass transition is from the paramagnetic state with q=0 to a spin glass state with nonzero q as the temperature is decreased.

Magnetic susceptibility

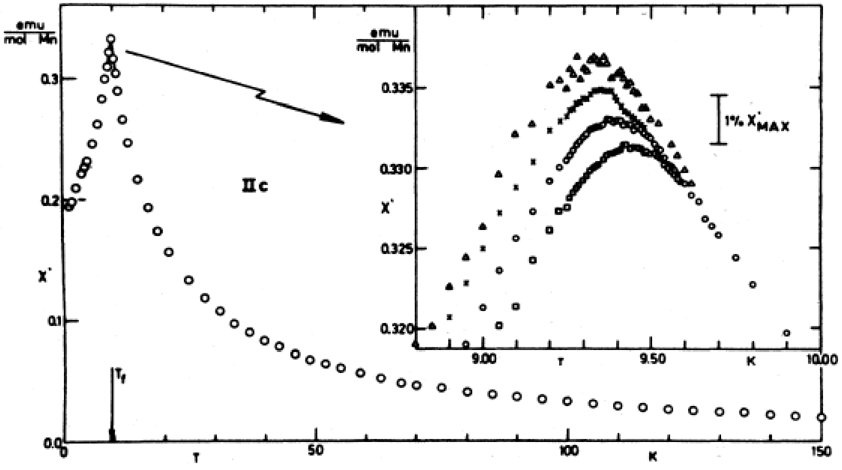
$$\chi(T) = \frac{1}{NT}[\sum_{i,j}(\langle\sigma_i\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle)]_{av}$$

For spin glasses,

$$[\langle\sigma_i\sigma_j\rangle]_{av} = 0 \text{ for } i \neq j, \; = 1 \text{ for } i = j.$$

Also, $[\langle\sigma_i\rangle]_{av} = 0$ and $[\langle\sigma_i\rangle^2]_{av} \neq 0$ in the SG phase

$$\chi(T) = \frac{1}{T}(1-q)$$



The Sherrington-Kirkpatrick Model

D. Sherrington and S. Kirkpatrick, Phys. Rev. Lett. **35**, 1972 (1975).

Infinite-range (mean field) model of Ising spin glass

$$\mathcal{H} = -\frac{1}{2}\sum_{i\neq j} J_{ij}\sigma_i\sigma_j = -\sum_{<ij>} J_{ij}\sigma_i\sigma_j.$$

$$P(J_{ij}) = \sqrt{\frac{N}{2\pi J^2}}\exp\left[-\frac{NJ_{ij}^2}{2J^2}\right] \qquad [J_{ij}]_{av} = 0,\ [J_{ij}^2]_{av} = J^2/N.$$

$$[Z^n]_{av} = \mathrm{Tr}_{\{\sigma_i^\alpha\}}\exp\left[\frac{\beta^2 J^2}{2N}\sum_{<ij>}\sum_{\alpha,\beta}\sigma_i^\alpha\sigma_i^\beta\sigma_j^\alpha\sigma_j^\beta\right]$$

Hubbard-Stratonovich Identity:

$$\exp[\lambda a^2/2] = \sqrt{\frac{\lambda}{2\pi}}\int_{-\infty}^{\infty} dx\,\exp[-\lambda x^2/2 + \lambda a x].$$

S-K Model (contd.)

→ $$[Z^n]_{av} = \exp\left[\frac{\beta^2 J^2 n N}{4}\right] \int_{-\infty}^{\infty} \Pi_{\alpha<\beta} \sqrt{\frac{N}{2\pi}} \beta J dq_{\alpha\beta}$$

$$\times \exp\left[-\frac{N\beta^2 J^2}{2} \sum_{\alpha<\beta} q_{\alpha\beta}^2 + N \ln \mathrm{Tr}_{\{\sigma^\alpha\}} e^{L(\{q_{\alpha\beta}\},\{\sigma^\alpha\})}\right]$$

where $L(\{q_{\alpha\beta}\}, \{\sigma^\alpha\}) \equiv \beta^2 J^2 \sum_{\alpha<\beta} q_{\alpha\beta} \sigma^\alpha \sigma^\beta$

→ $$-\beta f = \lim_{n\to 0}\left[\frac{\beta^2 J^2}{4}(1 - \frac{1}{n} \sum_{\alpha\neq\beta} q_{\alpha\beta}^2) + \frac{1}{n} \ln \mathrm{Tr} e^L\right]$$

$q_{\alpha\beta}$ are to be determined from $\dfrac{\partial f}{\partial q_{\alpha\beta}} = 0$

S-K Model (contd.)

Replica Symmetry: $q_{\alpha\beta} = q \text{ for all } \alpha \neq \beta$

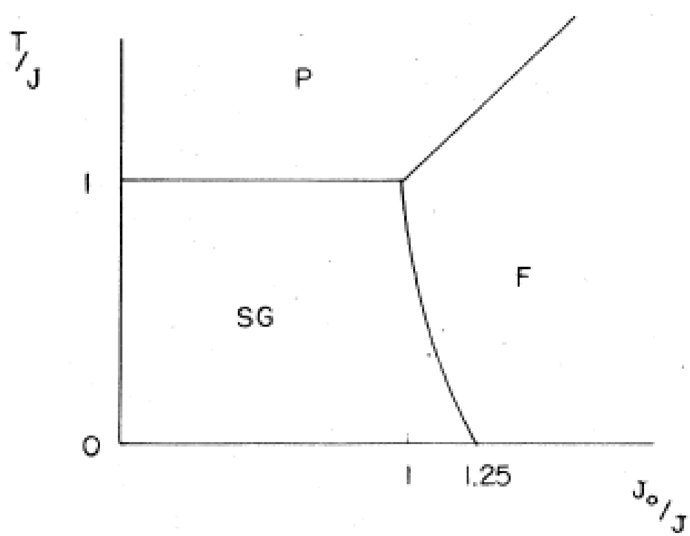
Self-consistency equation:

$$q = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} dz \exp(-z^2/2) \tanh^2(\beta J \sqrt{q} z)$$

$$q \neq 0 \text{ for } T < T_c = J$$

Continuous spin glass transition at T=J

Phase diagram



Replica Symmetry Breaking

The replica symmetric solution has unphysical properties for T < J.

Instability of the replica symmetric solution

$$-\beta f = \lim_{n\to 0}\left[\frac{\beta^2 J^2}{4}\left(1 - \frac{1}{n}\sum_{\alpha\neq\beta} q_{\alpha\beta}^2\right) + \frac{1}{n}\ln \mathrm{Tr} e^{L}\right]$$

Fluctuations: $q_{\alpha\beta} = q_0 + \delta q_{\alpha\beta}$

$$\beta f = \beta f(q_0) + \lim_{n\to 0}\frac{1}{2n}\sum_{\alpha<\beta,\gamma<\delta}\mathcal{R}^{\alpha\beta,\gamma\delta}\delta q_{\alpha\beta}\delta q_{\gamma\delta} + \cdots$$

All eigenvalues of $\mathcal{R}$ must be ≥ 0 for stability and physically meaningful behavior.

This condition is not satisfied for T < J.

Replica Symmetry Breaking (contd.)

H: magnetic field

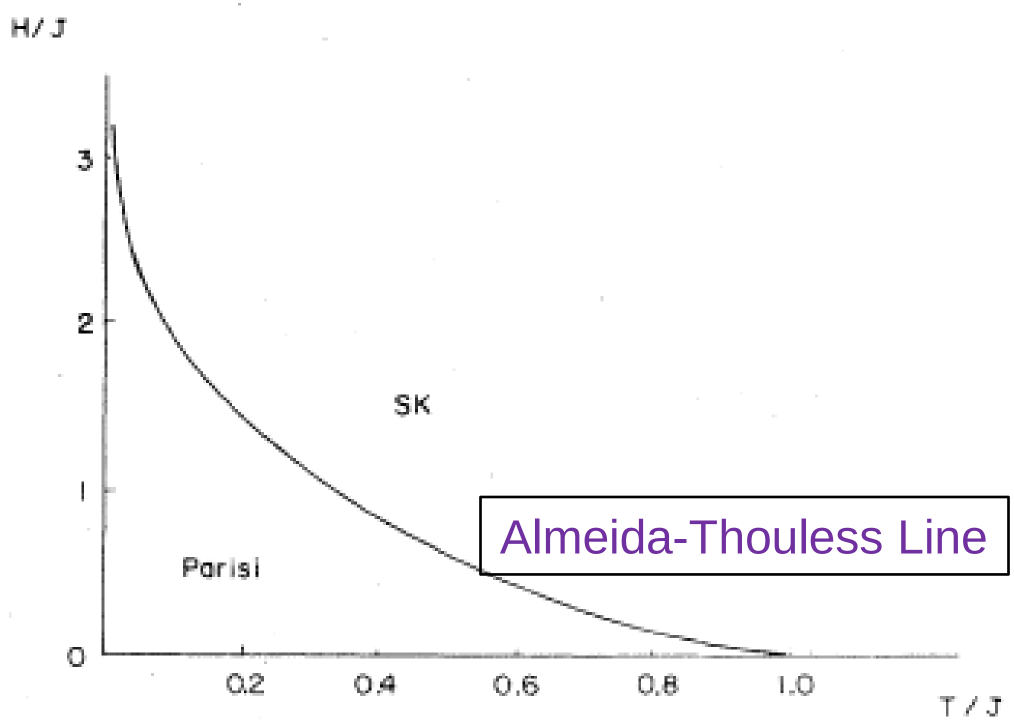
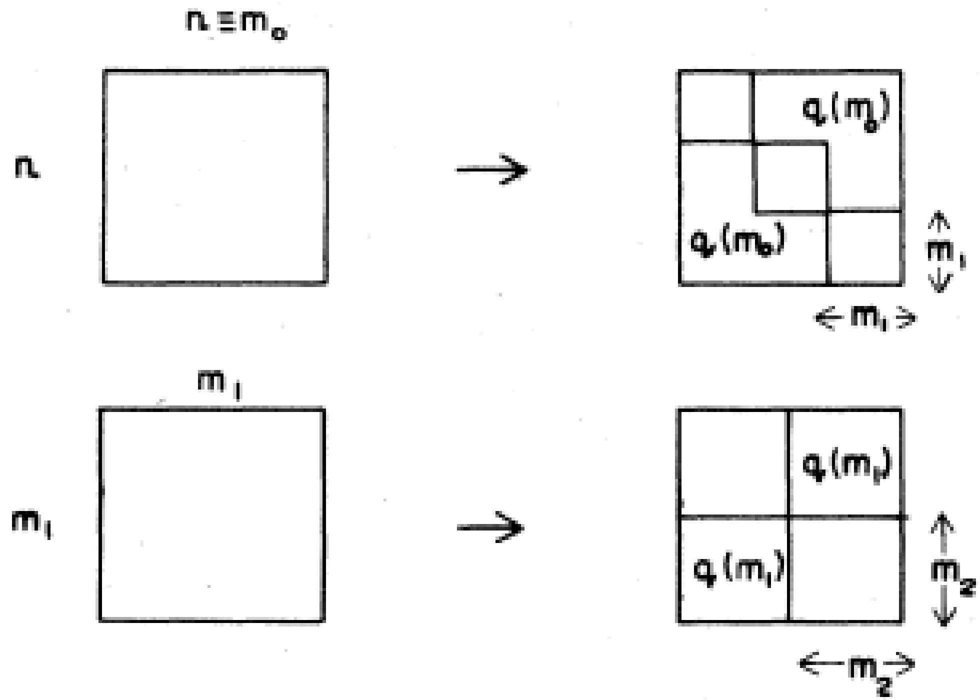


FIG. 48. Plot of the Almeida-Thouless (AT) line for the SK model with $J_0=0$. To the right of the line the SK solution with a single order parameter is correct, while to the left of the line the Parisi solution is believed exact. The Parisi solution represents the many-valley structure of phase space and nonergodic behavior. The AT line, therefore, signals the onset of irreversibility.

J.R.L de Almeida and D.J Thouless, J. Phys A **11**, 983 (1978)

The Parisi Solution

G. Parisi, Phys. Rev. Lett. **43**, 1754 (1979)



Iterative scheme

Repeat this procedure K times:
K-step replica symmetry breaking

$$m_1, m_2, \ldots, m_K; \;\; m_0 \geq m_i \geq 1.$$

$$q(m_0), q(m_1), \ldots, q(m_K)$$

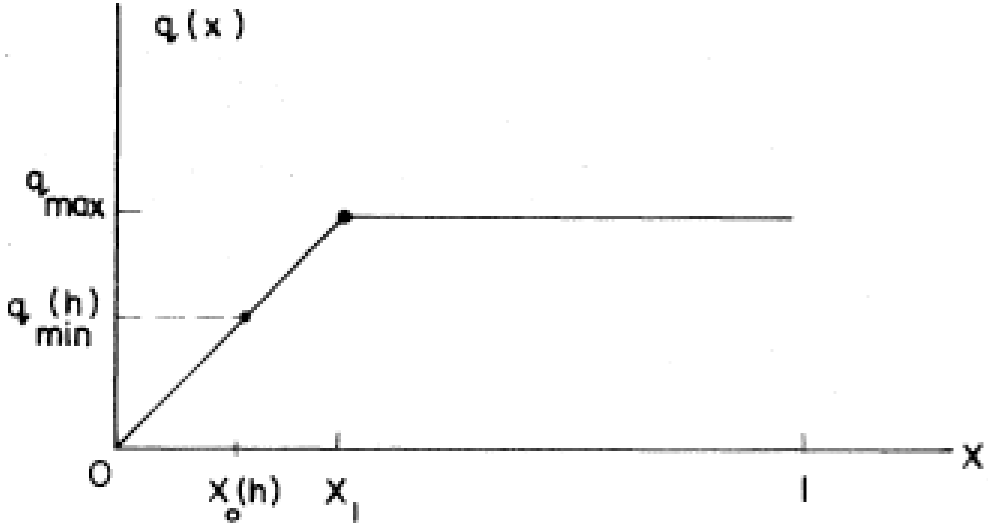
The Parisi Solution (contd.)

$$K \to \infty : \; m_i \to x, \; 0 \le x \le 1, \; q(m_i) \to q(x)$$

q(x): Order parameter function

Spin glass order parameter:

$$q_{eq} = [\langle \sigma_i \rangle^2]_{av} = \int_0^1 q(x) dx$$



q(x) at a temperature slightly below the critical temperature

Physical Interpretation of the Parisi Solution

Thouless-Anderson-Palmer Equations

D.J. Thouless, P.W. Anderson, R.G. Palmer, Phil. Mag. **35**, 593 (1977)

Free energy of the S-K model for a given set of interaction parameters

$$F = -\frac{1}{2}\sum_{i\neq j} J_{ij} m_i m_j + \frac{T}{2}\sum_i [(1+m_i)\ln\{(1+m_i)/2\} + (1-m_i)\ln\{(1-m_i)/2\}] - \frac{1}{4T}\sum_{i\neq j} J_{ij}^2 (1-m_i^2)(1-m_j^2).$$

Onsager Reaction term

$$\frac{\partial F}{\partial m_i} = 0 \rightarrow m_i = \tanh[\beta \sum_j J_{ij} m_j - \beta^2 \sum_j J_{ij}^2 (1-m_j^2) m_i]$$

Local field at site i:

Cavity Method

$$\sum_j J_{ij}(m_j - \chi_{jj} J_{ij} m_i) = \sum_j J_{ij} m_j - \sum_j J_{ij}^2 \beta (1-m_j^2) m_i$$

TAP Equations (contd.)

Only one solution of the TAP equations, $m_i = 0$ for all i, for $T > J$.

Many solutions with nonzero $\{m_i\}$ for $T < J$.

Number of minima with the lowest free energy per spin is not exponential in N.

Free energy barriers between different minima diverge in the thermodynamic limit.

Complex Free Energy Landscape

Physical interpretation of RSB

G. Parisi, Phys Rev Lett **50**, 1946 (1983)

Large number of "valleys" ["pure states", "ergodic components"] at temperatures lower than the critical temperature.

$P^{(\alpha)}$: Probability of the system being in valley α

$$\langle \sigma_i \rangle = \sum_\alpha P^{(\alpha)} m_i^{(\alpha)}$$

[Average over all valleys]

Take $t \to \infty$ limit before $N \to \infty$

$$\frac{1}{N}\sum_i \langle \sigma_i \rangle^2 = \frac{1}{N}\sum_{i=1}^{N}\sum_{\alpha\beta} P^{(\alpha)} P^{(\beta)} m_i^{(\alpha)} m_i^{(\beta)}$$

Define overlap between valleys α and β,

$$q_{\alpha\beta} = \frac{1}{N}\sum_{i=1}^{N} m_i^{(\alpha)} m_i^{(\beta)}$$

Distribution of the overlap: $P(q) = \sum_{\alpha\beta} P^{(\alpha)} P^{(\beta)} \delta(q - q_{\alpha\beta})$

Then $\frac{1}{N}\sum_i \langle \sigma_i \rangle^2 = \int_0^1 q P(q) dq$

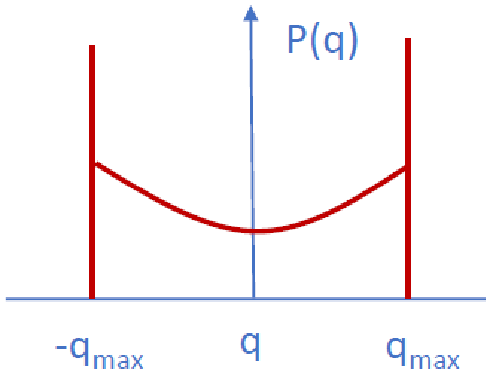
Physical interpretation of RSB (contd.)

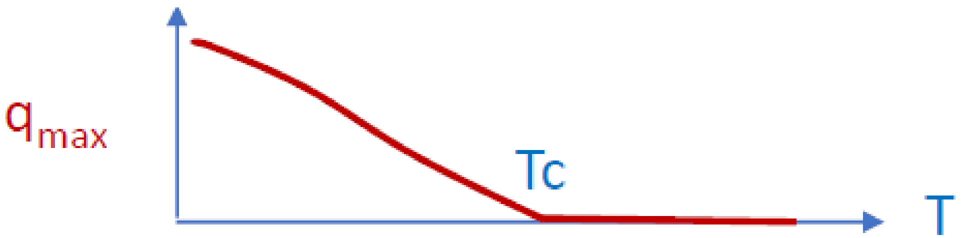
$$q_{eq} = [\langle \sigma_i \rangle^2]_{av} = \int_0^1 q(x)dx = \int q \frac{dx}{dq} dq$$

$$\boxed{P(q) = \frac{dx}{dq}}$$

Parisi function q(x) describes the distribution of overlaps between different free-energy minima.

$$q_{EA} = \frac{1}{N} \sum_i \sum_\alpha P^{(\alpha)} [m_i^{(\alpha)}]^2 = q(x=1)$$

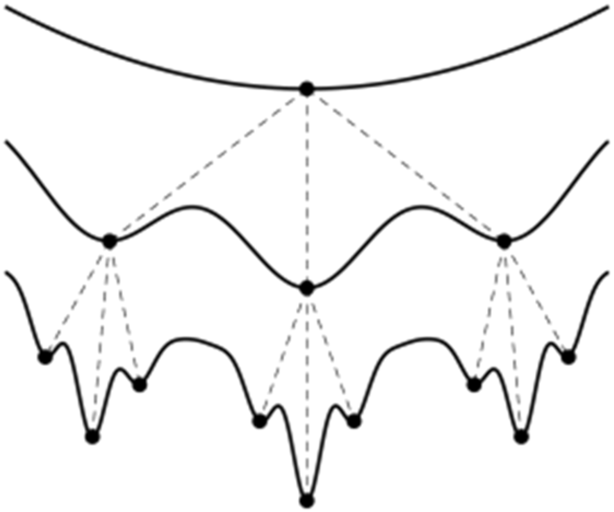




Sketches from Srikanth Sastry

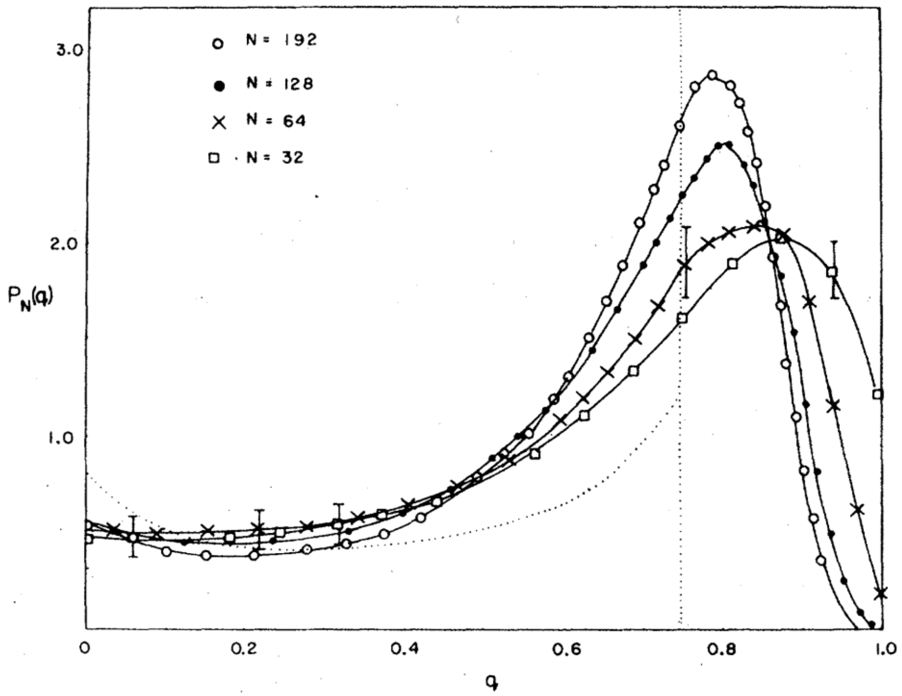
Ultrametricity: The valleys are arranged in a hierarchical tree-like ('ultrametric') structure

Consider three valleys, 1, 2 and 3 and their overlaps $q_{12},\ q_{23},\ q_{31}$
Only two possibilities: all three overlaps are equal, or two of them are equal and the third one is larger.
Valleys are arranged in a tree-like structure and the overlap between two valleys is determined by how far up the tree one must go to find a common ancestor.



Picture from Srikanth Sastry

Predictions of the Parisi solution have been confirmed from simulations.



A. P. Young, Phys Rev Lett **51**, 1206 (1983)

Correctness of the Parisi solution has been established from rigorous analysis.

M Talagrand, *Mean Field Models for Spin Glasses*, Springer-Verlag, 2010
http://michel.talagrand.net/challenge/volume1.pdf

Does the Parisi solution explain experimentally observed behaviour in real spin glasses?

Spin glasses do exhibit a thermodynamic phase transition in three dimensions.

The question of whether 3D spin glasses with short-range interactions exhibit RSB is still controversial.

Alternative theories:

"Droplet" picture [D.S. Fisher and D.A. Huse: Phys. Rev. B **38**, 386 (1988)]: Only a pair of pure states related to each other by global spin flip, excitations arising from reversals of clusters of spins.

"Chaotic pair" picture [C.M. Newman and D.L. Stein: Phys. Rev. E **57**, 1356 (1998)]: Infinitely many pure states in the thermodynamic limit, but the overlap distribution function is a δ-function at zero.

Talk of Enzo Marinari

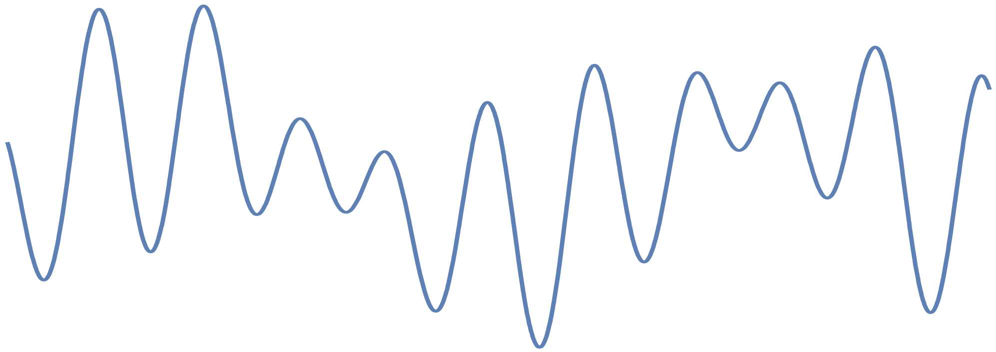
Dynamics: Slow relaxation, hysteresis, memory effects, aging, ….

Talk of Jorge Kurchan

Significance of the Parisi Solution

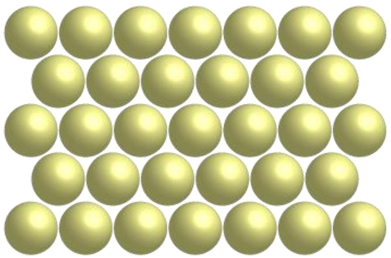
- Exact solution of the equilibrium properties of a system with (quenched) disorder and (thermal) fluctuations.
  - Order parameter function q(x) with x between 0 and 1
  - Novel symmetry breaking at the transition
  - Ordered (ultrametric) organization of pure states

- New paradigm of theoretical treatment of systems with a complex (free) energy landscape.

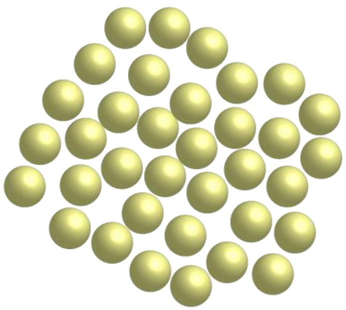


Landscape paradigm

Structural Glass: Disordered solid-like state obtained by rapidly cooling a liquid to a temperature lower than the equilibrium crystallization temperature



Crystal



Glass

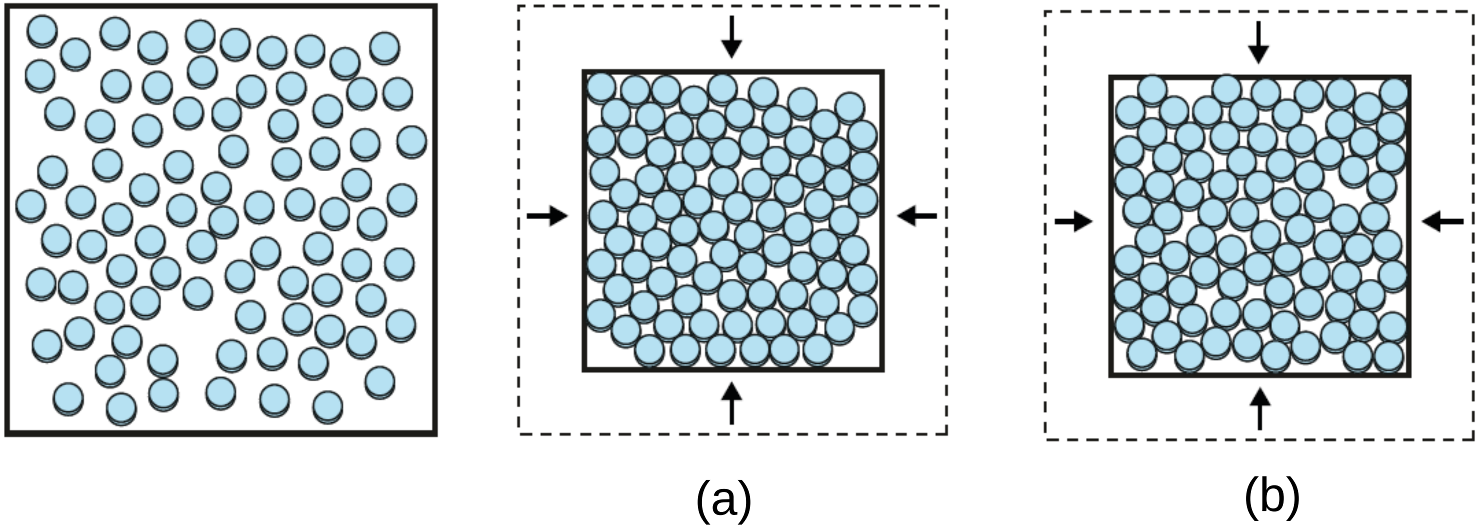
Structure of a glass is similar to that of the high-temperature liquid.

- Very large number of local minima of the potential energy as a function of the coordinates of the constituting particles.
- Mean-field free energy as a functional of the local density exhibits a large number of local minima in the glass phase.
- Very slow dynamics near and below the glass transition temperature.

Talk of Srikanth Sastry

Jamming

Athermal system, compress a collection of hard objects until their freedom of movement is lost



- Force balance: net force on every particle is zero.
- The jammed state depends on the initial configurations and the compression protocol. Different jammed states are obtained for different initial configurations corresponding to the same macroscopic state.

Talk of Francesco Zamponi

Figure from https://www.nobelprize.org/uploads/2021/10/fig5_fy_en_21_disorderedSystems.pdf

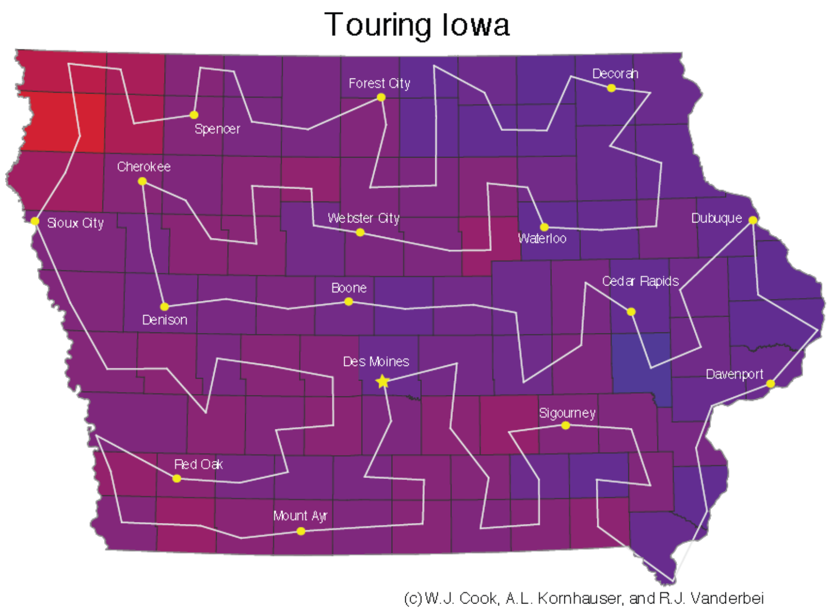
Combinatorial Optimization: The Traveling Salesman Problem

N cities, tour represented as {P(i), i=1,2,….,N} where P(.) is a permutation of the N labels 1,2,…..,N.

Find the tour that **minimizes** the **total tour length**

T(P) = d(P(1),P(2))+d(P(2),P(3))+……….+d(P(N-1),P(N)) +d(P(N),P(1)).

Many "**local minima**" of T, corresponding to tours with the property that any **local** change of the sequence in which the cities are visited **increases** the value of T.

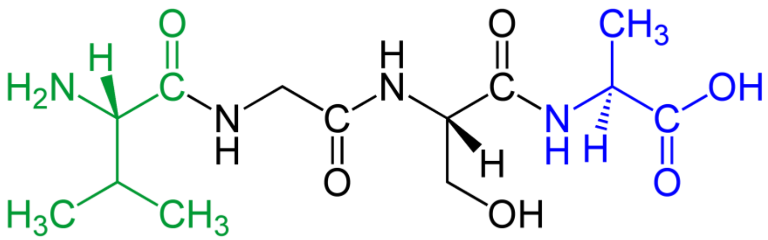


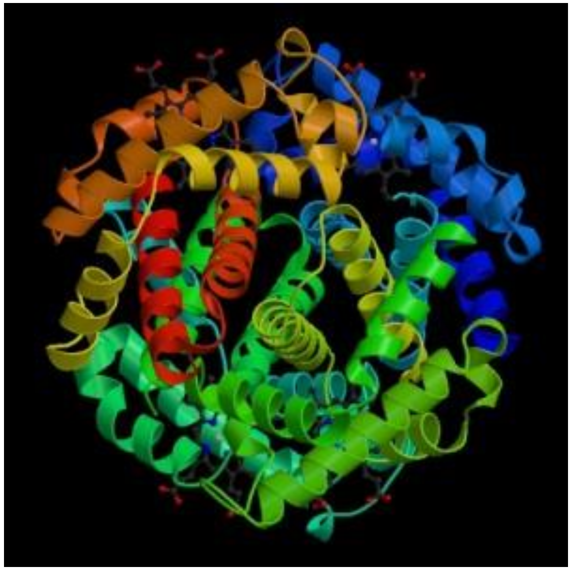
Other Problems in Computer Science: Talk of Marc Mezard

Protein Folding

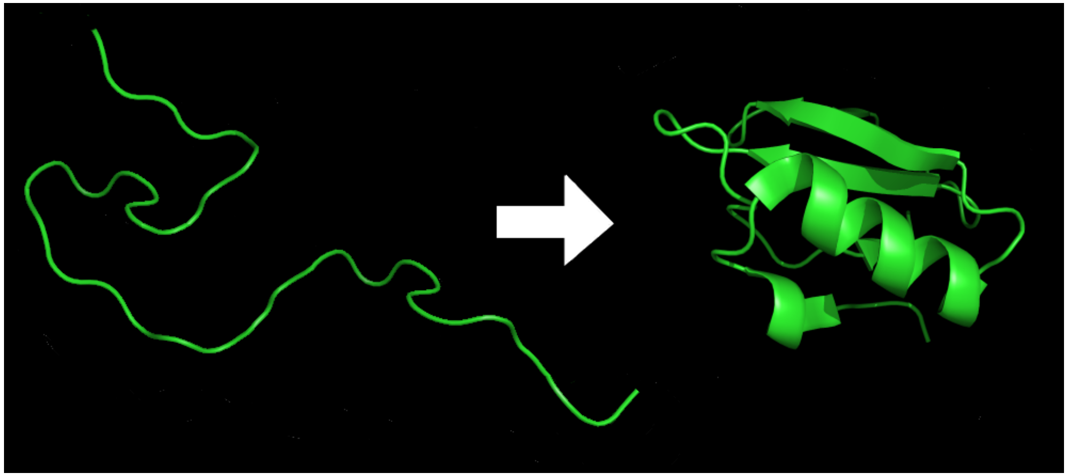
A protein is a polymer consisting of amino acids

Tetrapeptide Val-Gly-Ser-Ala



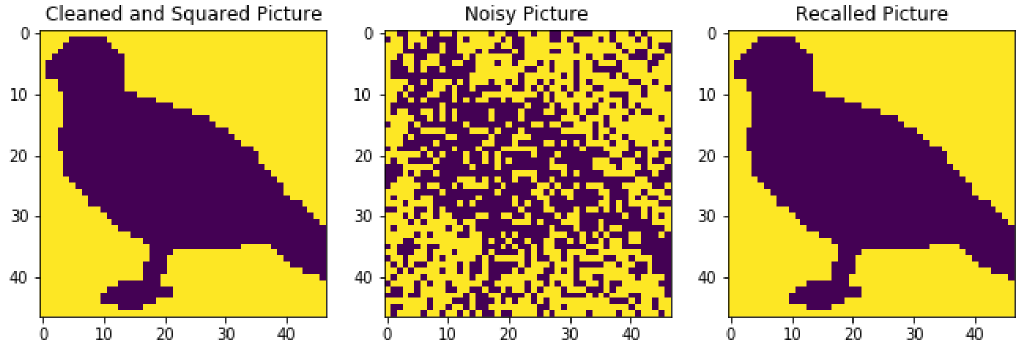


How does a protein reach its low-temperature “native” configuration from the high-temperature “denatured” state as the temperature is decreased?



Associative Memory: Retrieval of stored information from partial knowledge [content addressable memory]

A system acts as associative memory if its dynamics takes initial states close to a stored memory state (partial knowledge) to the memory state itself (complete retrieval of the memory).



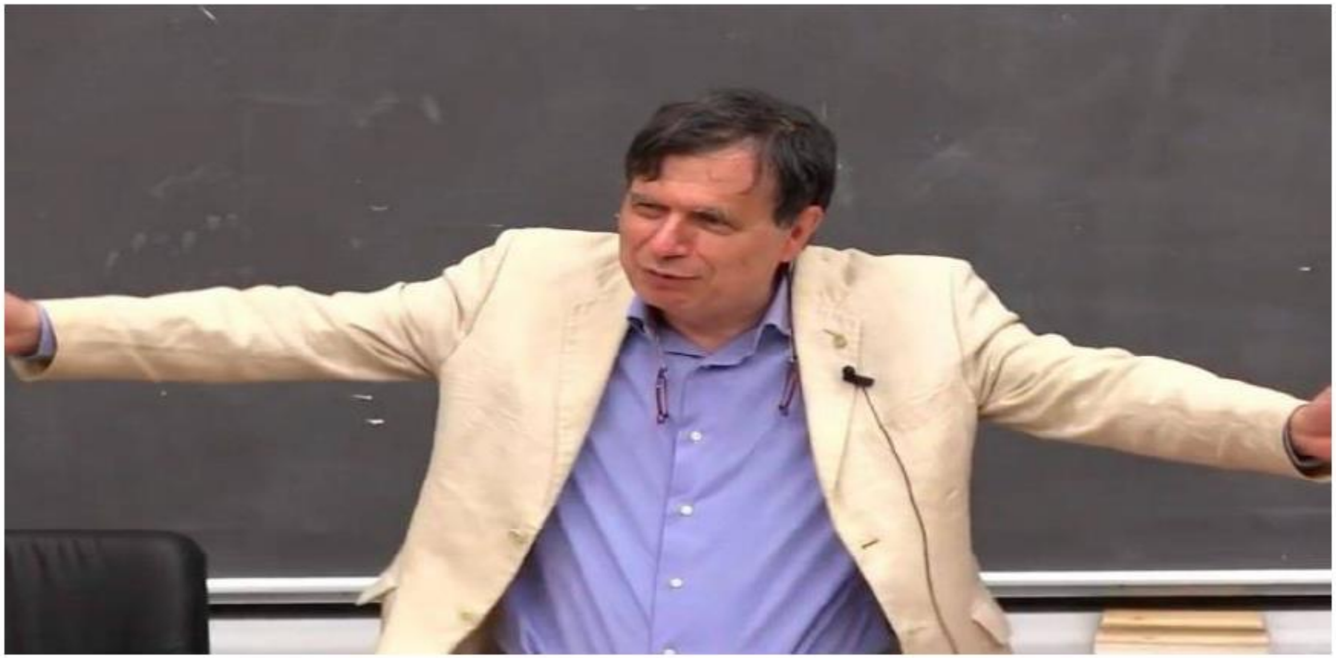
The Hopfield Model [J.J. Hopeld: Proc. Natl. Acad. Sci. USA 79, 2554 (1982)]

Memory states are stored as local minima of the energy.
Dynamics corresponds to changes that decrease the energy.

Figure from https://github.com/nosratullah/hopfieldNeuralNetwork

Congratulations to Giorgio Parisi!

For the Nobel prize in appreciation of his wide ranging contributions to theoretical physics!!



Spin glass

Interfaces

Bird flocks

Climate change

QCD

Glasses

Simulations

Turbulence

Slide from Srikanth Sastry