Spin Glasses and Related Systems

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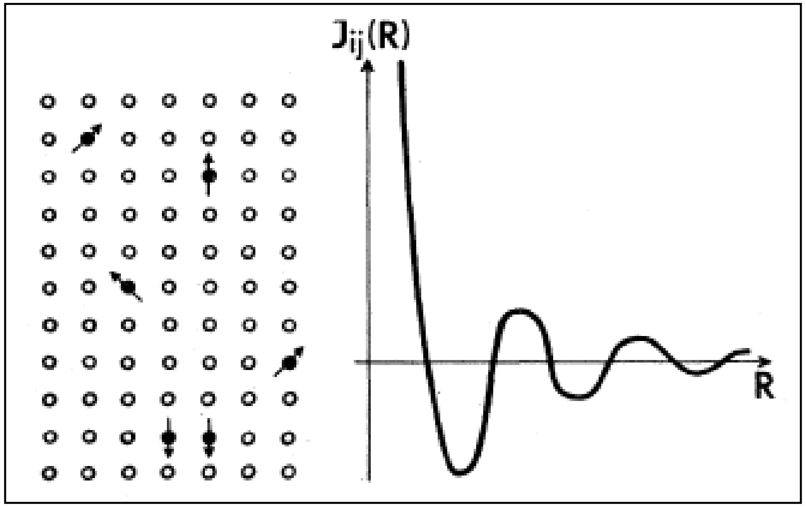
What are Spin Glasses?

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

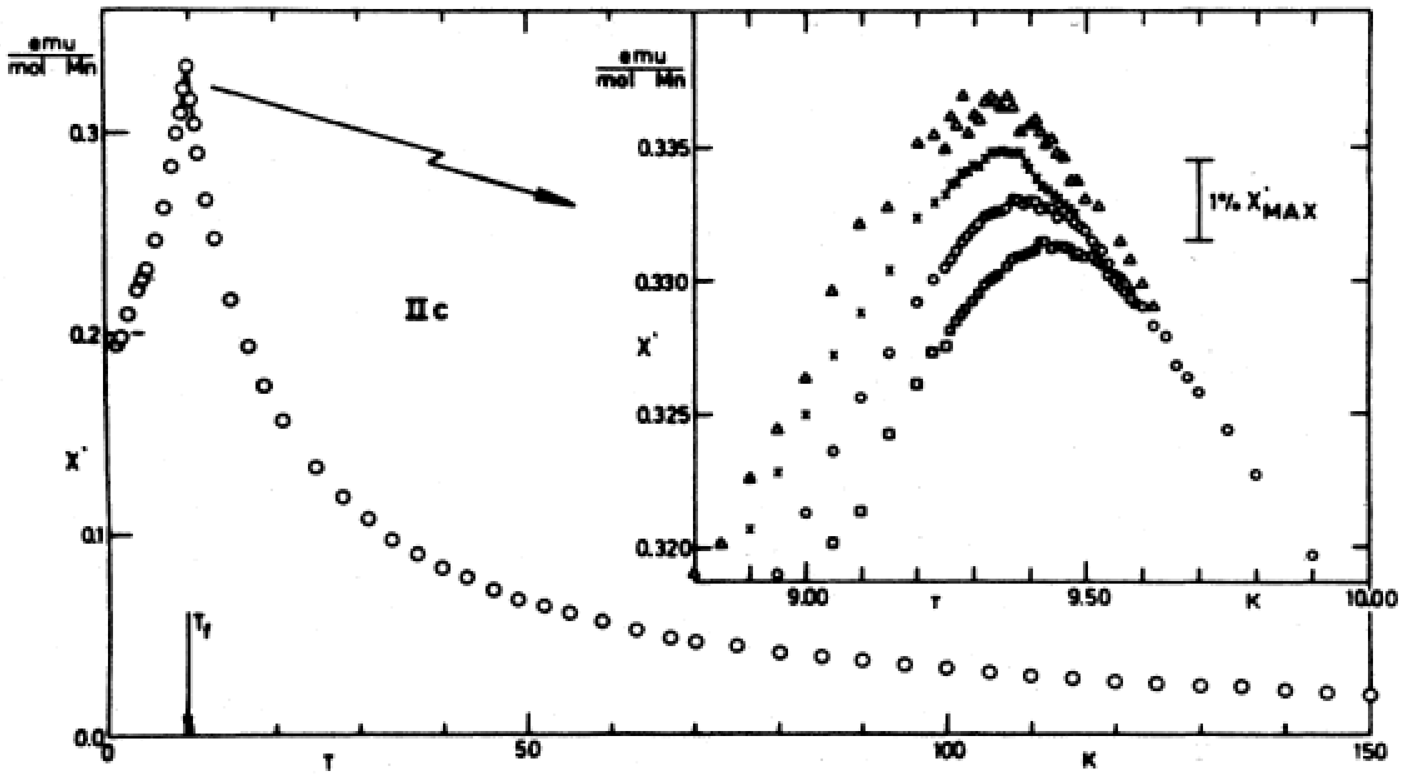
Example: CuMn, AuFe, …

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

RKKY Interaction between localized spins



Experimental results: (1) Cusp in the magnetic susceptibility



Susceptibility of CuMn as a function of temperature

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

Experimental results: (2) Slow dynamics at low temperatures

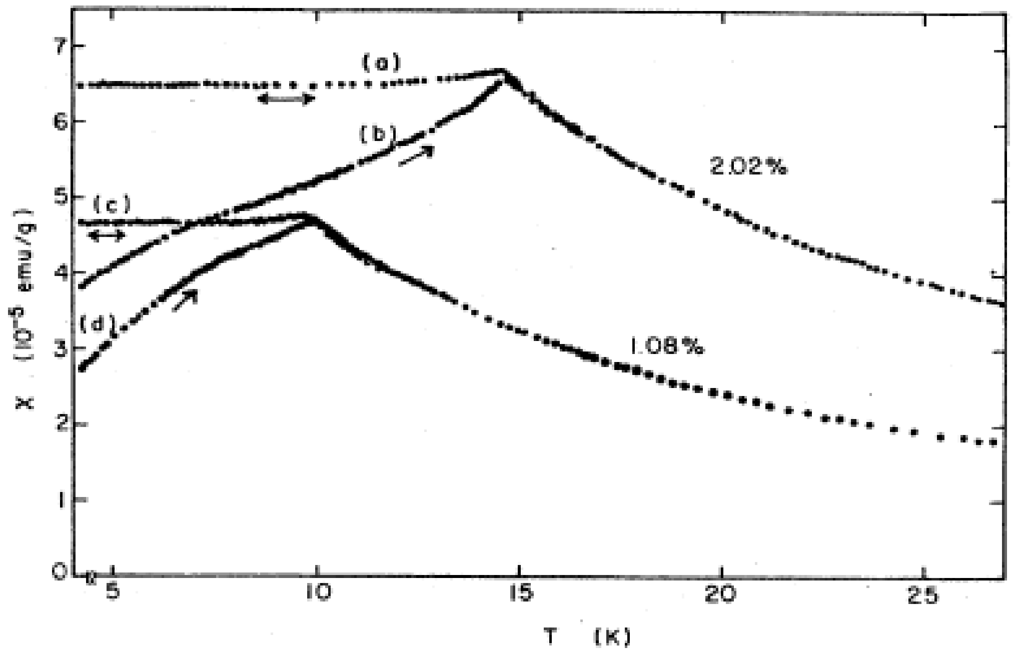
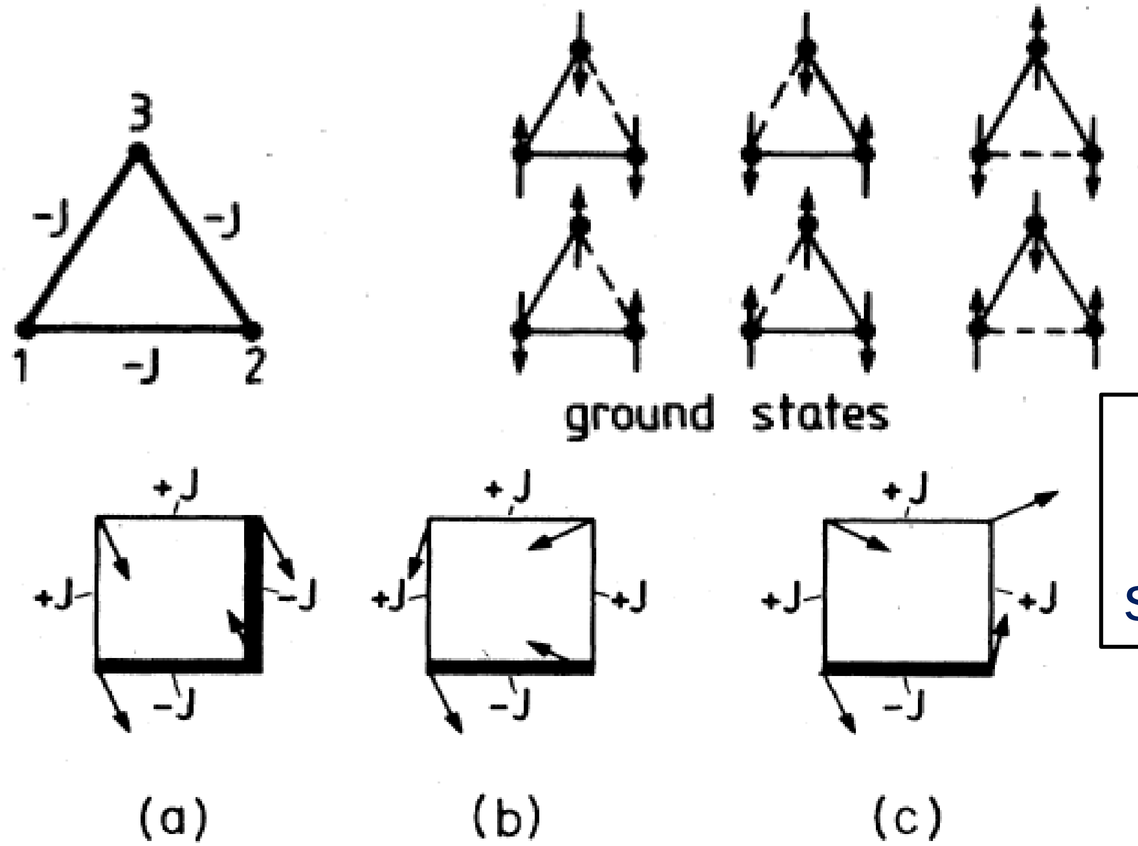


FIG. 7. Static susceptibilities of *Cu*Mn vs temperature for 1.08 and 2.02 at.% Mn. After zero-field cooling ($H < 0.05$ Oe), initial susceptibilities (b) and (d) were taken for increasing temperature in a field of $H = 5.9$ Oe. The susceptibilities (a) and (c) were obtained in the field $H = 5.9$ Oe, 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)

Frustration

All pair interactions can not be satisfied simultaneously



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

FIG. 41. Classical ground state of a set of four spins in the XY model with interactions $\pm J$ (thick bonds are antiferromagnetic, thin bonds are ferromagnetic). (a) Nonfrustrated plaquette; (b) frustrated plaquette, chirality $\tau=+1$; (c) frustrated plaquette, chirality $\tau=-1$.

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

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

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

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

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

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

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

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

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

$\mathcal{H}_{eff}(\{\sigma_i^\alpha\})$ **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

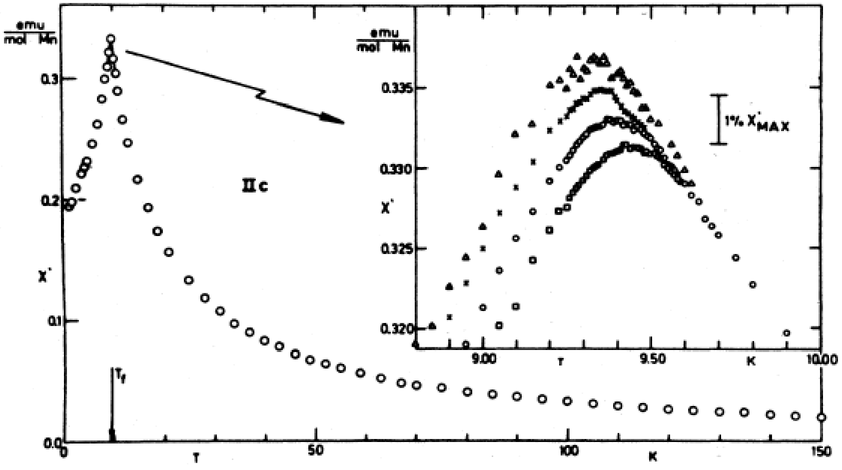
$$\chi(T) = \frac{1}{NT}[\sum_{i,j}(\langle\sigma_i\sigma_j\rangle - \langle\sigma_i\rangle\langle\sigma_j\rangle)]_{av}$$

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

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



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-Stratanovitch Identity:

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

S-K Model (contd.)

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

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

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

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

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

S-K Model (contd.)

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

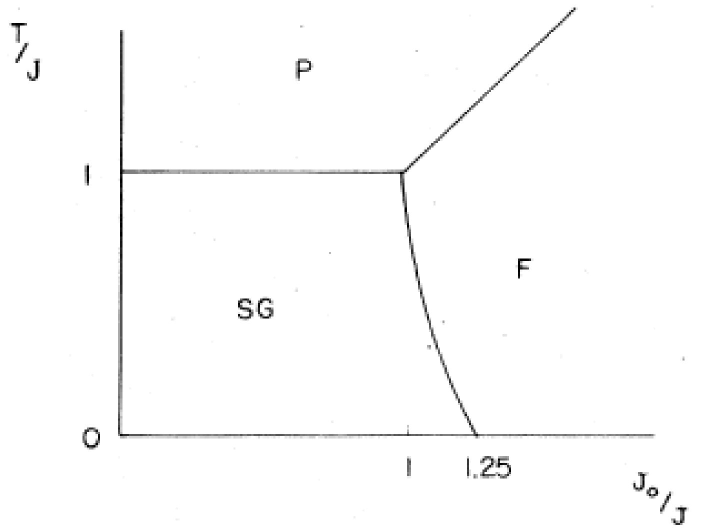
Self-consistency equation:

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

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

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

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

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.)

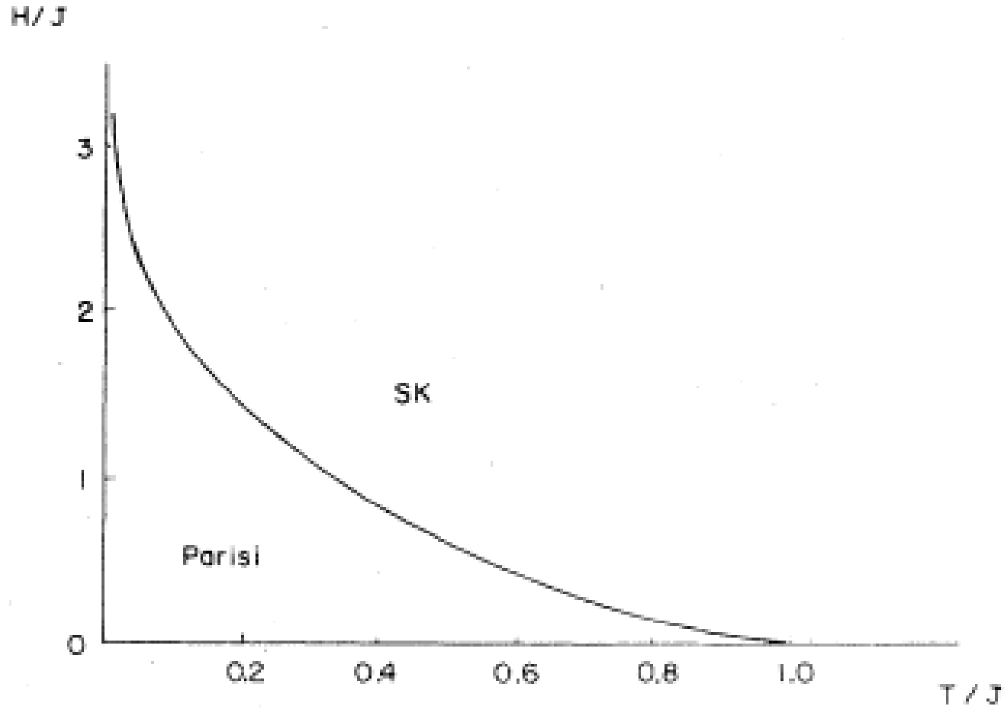
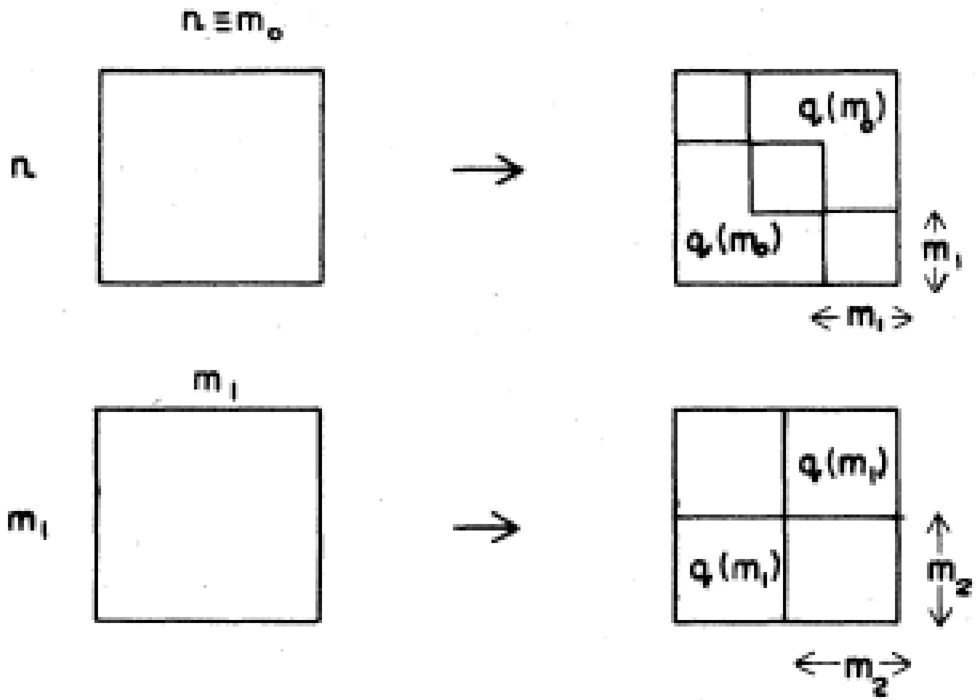


FIG. 48. Plot of the Almeida-Thouless (AT) line for the SK model with $J_0 = 0$. To the right of the line the SK solution with a single order parameter is correct, while to the left of the line the Parisi solution is believed exact. The Parisi solution represents the many-valley structure of phase space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

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

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

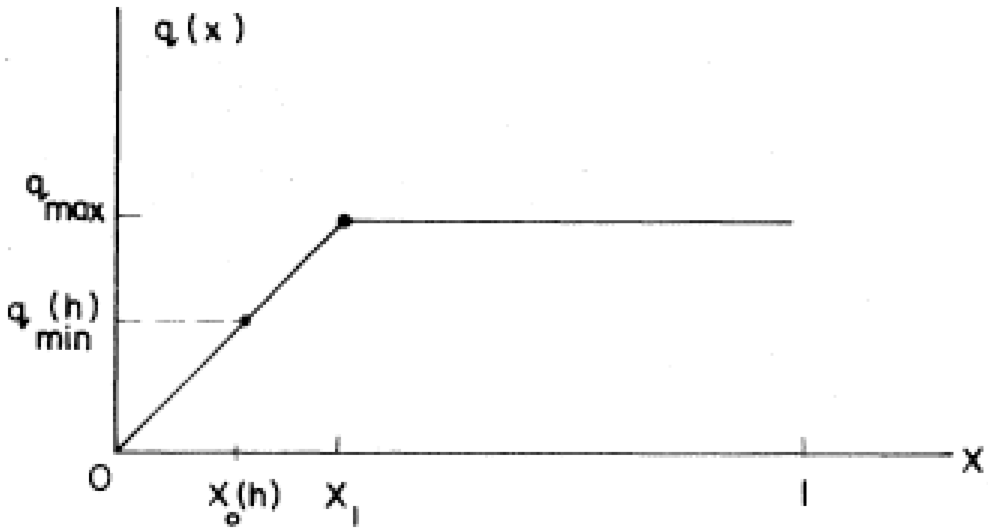
The Parisi Solution (contd.)

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

q(x): Order parameter function

Spin glass order parameter:

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



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

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:

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

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

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]

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

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.)

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

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

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

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

These predictions have been confirmed from simulations

Correctness of the RSB solution has been established from more rigorous analysis.

What is a “glassy” system?

- ❖No “obvious” long-range order
- ❖Different from “trivial” high-temperature state
- ❖Presence of large number of nearly equivalent metastable states
- ❖Slow dynamics

Most common example is **structural glass**

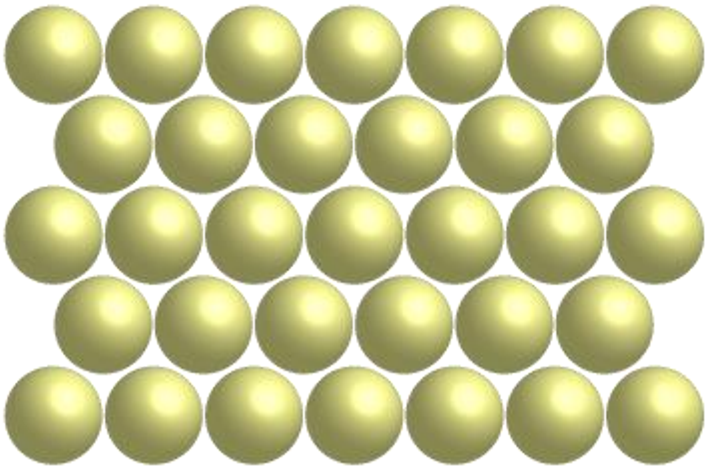
Structural Glass: Disordered solid-like state obtained by rapidly cooling a liquid to a temperature lower than the equilibrium crystallization temperature

The glassy state is metastable

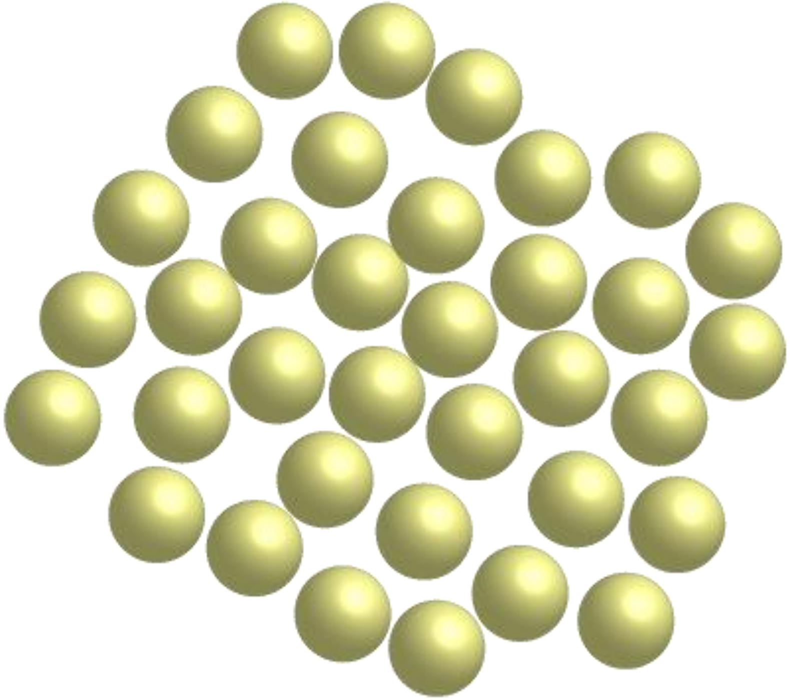
Examples:

- Oxide glasses (silica, Germania glass,….)
- Chalcogenide glasses (GeSbTe, AgInSbTe,…..)
- Metallic glasses (Fe-Cr-Mo-C-B, Mg-Cu-Tb,….)
- Polymer glasses (polystyrene, poly-vinyl-acetate,..)
- Colloidal glasses
- Simple molecular glasses (ortho-terphenyl, salol,..)

Glass: non-crystalline "solid"



Crystalline Structure



Disordered Structure

Viscosity increases by 14-16 orders of magnitude as the temperature of a supercooled liquid is decreased by about 100 degrees

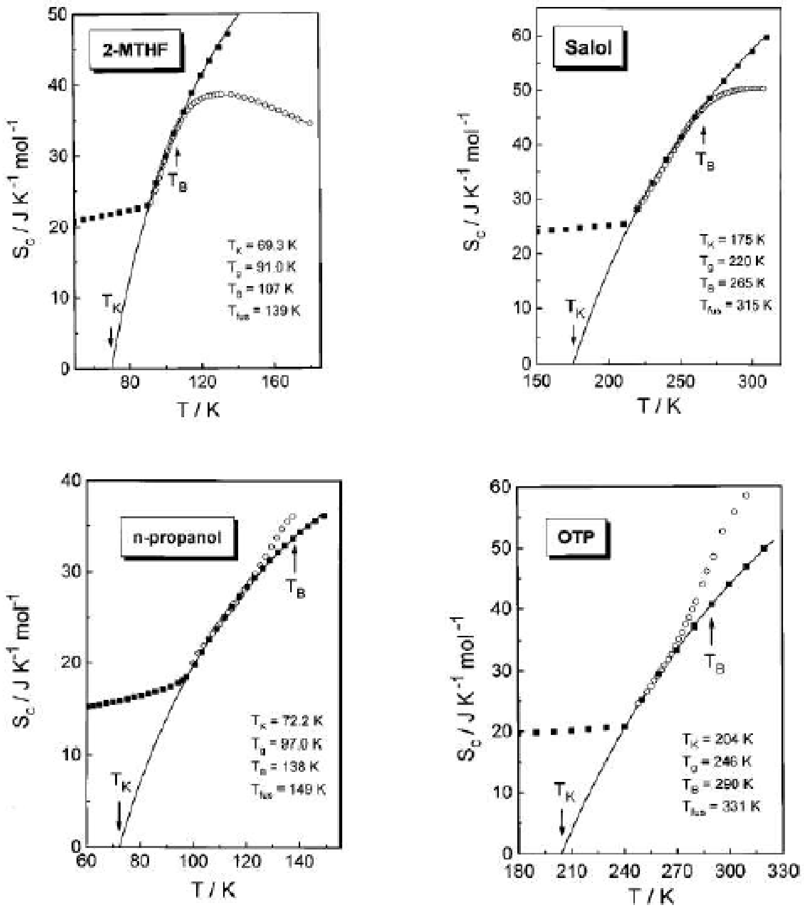
$$\eta(T) \propto \exp[BT_0/(T - T_0)]$$

Vogel-Fulcher-Tammann (VFT) Form
"Fragile" liquid

The "excess entropy", defined as the difference between the entropy of the supercooled liquid and the crystalline solid, extrapolates to zero at the "Kauzmann Temperature" T_K which is close to T_0 .

$$\tau(T) \propto \exp[A/\{TS_{ex}(T)\}]$$

Adam-Gibbs Relation

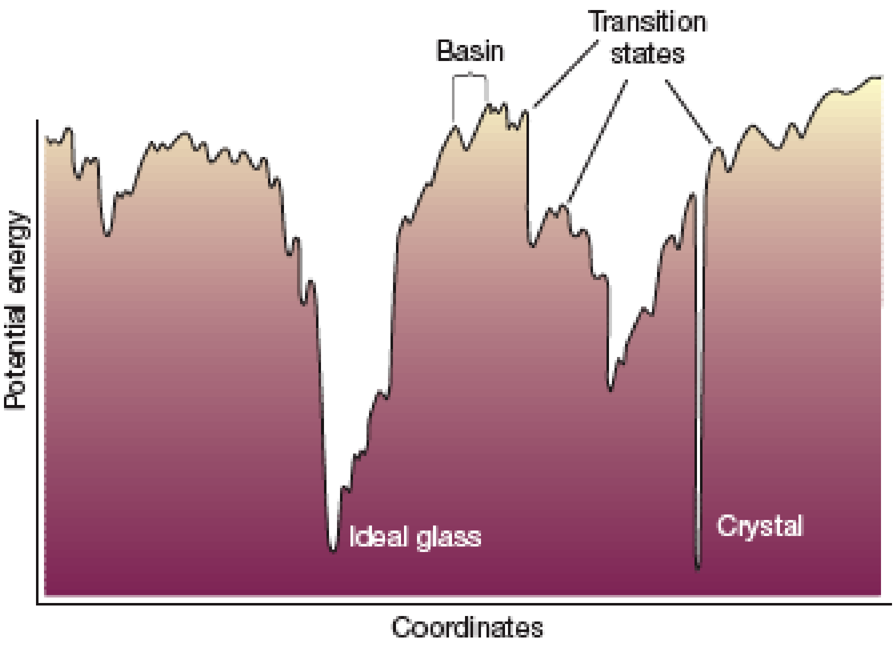


Kauzmann "Paradox": Experimental data

From: R. Richert and C. A. Angell, J. Chem. Phys. **108,** 9016 (1998)

Energy landscape picture

- Disordered liquid structure implies many local energy minima.
- Lowering temperature, the local minima sampled get deeper, and it gets harder to go from one to the other.
- Increasing viscosity.
- Configurational entropy ~ logarithm of number of sampled local energy minima



From Srikanth Sastry

Partition Function $Q(N, \rho, T)$

$$= \int d\Phi \Omega(\Phi) \exp[-\beta(\Phi + F_{bas}(\Phi, T))]$$

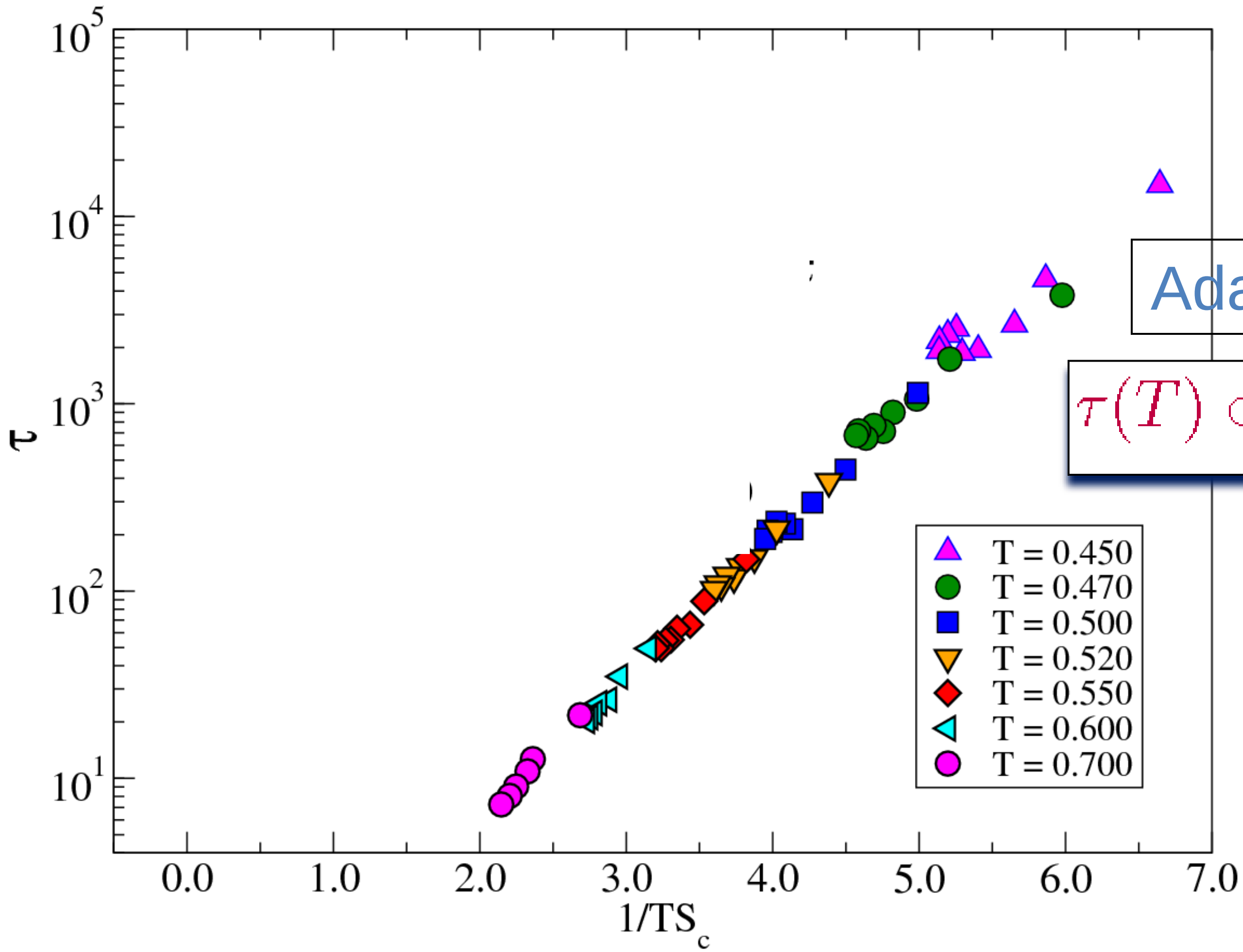
[Exclude IS's with large crystallites]

$S_c(\Phi) \equiv k_B \ln \Omega(\Phi)$ **is the configurational entropy of inherent structures at energy** Φ**.**

$$S_c(T) = \int d\Phi S_c(\Phi) P(\Phi, T)$$

$S_c(\Phi)$ **and** $S_c(T)$ **can be determined numerically by appropriate sampling methods**

- **Numerically determined** $S_c(T)$ **extrapolates to zero at** $T = T_K \simeq T_0$ **extracted from VFT fits to dynamical data**
- **Adam-Gibbs relation is satisfied within numerical accuracy**



Adam-Gibbs Relation

$$\tau(T) \propto \exp[A/\{TS_{ex}(T)\}]$$

The dependence of the α relaxation time on both T and N is well described by the Adam-Gibbs relation

[Karmakar, CD, Sastry, PNAS **106**, 3675 (2009)]

Entropic nucleation and "mosaic structure"

Extensive configurational entropy $S_c(T)$ provides an entropic mechanism for the formation of a "mosaic" structure consisting of "droplets" of different "phases".

Free energy cost of nucleating a "droplet" of *any possible* phase $\mathcal{B} \neq \mathcal{A}$ in phase $\mathcal{A}$ is given by

$$\Delta F = -TS_C r^d/V + \sigma r^\theta$$

where r is the size of the droplet, V is the volume, σ is a generalized surface tension, and $\theta \leq d - 1$.

The barrier $(\Delta F)_{max}$ for nucleation of a different phase is the maximum of ΔF as a function of r, and the relaxation time is assumed to be proportional to $\exp[(\Delta F)^{\psi}_{max}/(k_B T)]$, with $\psi \leq 1$.

Random First Order Transition (RFOT) Theory

[Wolynes, Kirkpatrick, Thirumalai, Biroli, Bouchaud, ….]

“Mosaic scale” of RFOT / “Point-to-set” length scale:

$$\xi(T) \propto 1/[TS_c(T)]^{1/(d-\theta)}$$

$$\ln\tau(T) = \ln\tau(\infty) + \frac{A\xi^{\psi}}{k_B T}$$

$$= \ln\tau(\infty) + \frac{A}{k_B T}\left(\frac{Y}{TS_c}\right)^{\frac{\psi}{D-\theta}}$$

ψ: “Barrier height” exponent

θ : “Surface free-energy” exponent

Other “Glassy” Systems

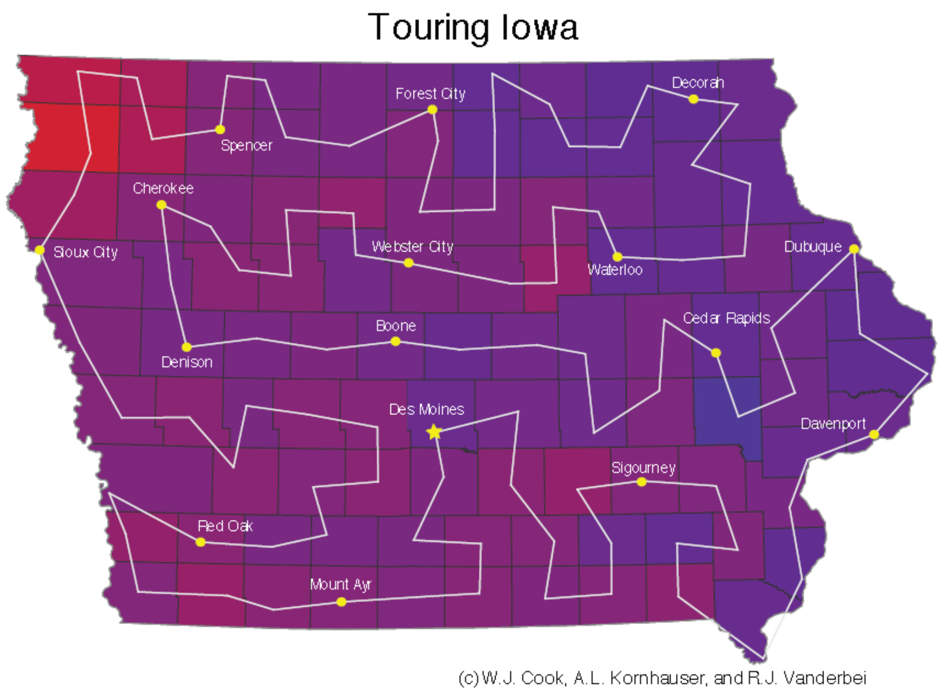
Combinatorial Optimization: The Traveling Salesman Problem

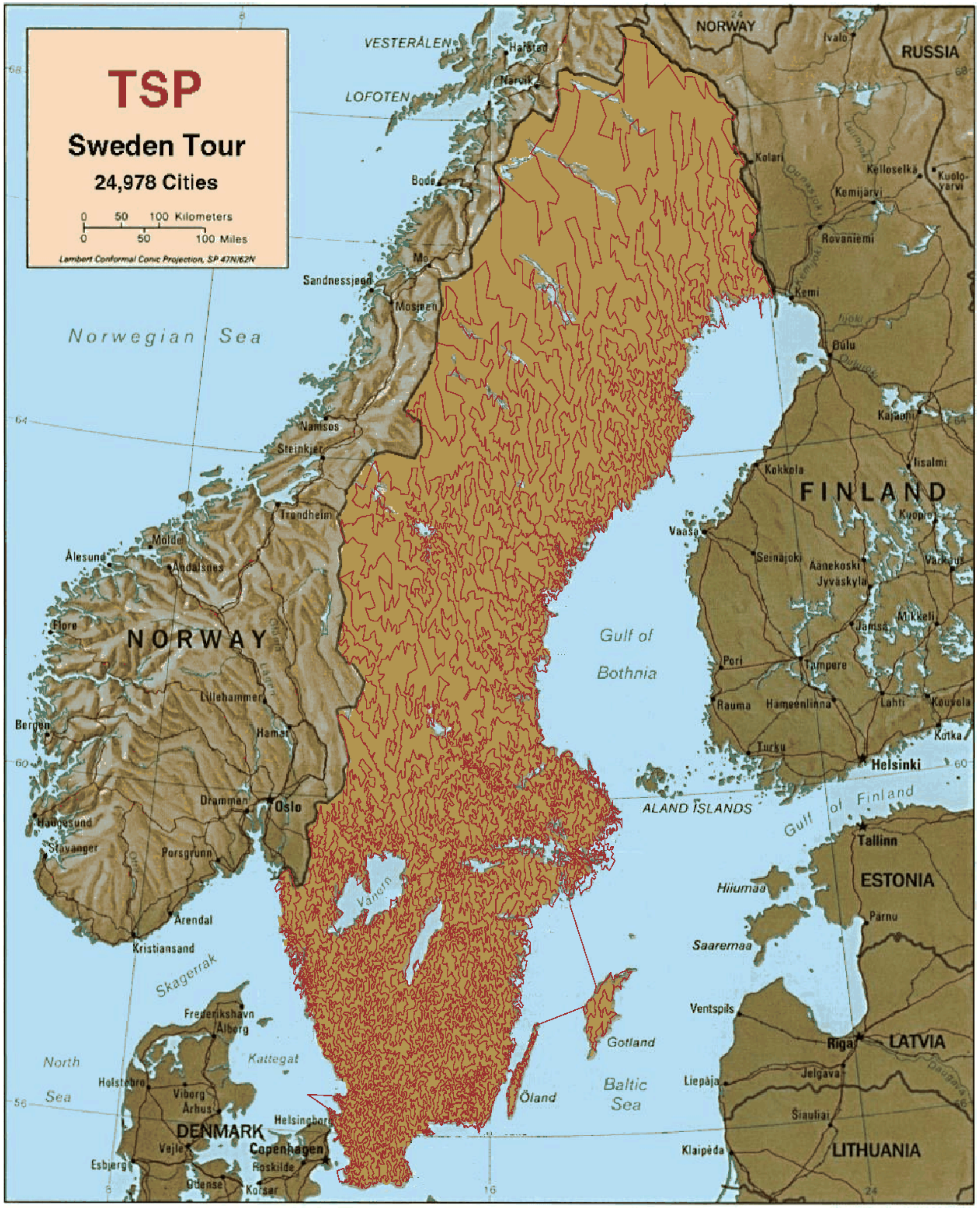
N cities, tour represented as {P(i), i=1,2,….,N} where P(.) is a permutation of the N labels 1,2,…..,N.

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.



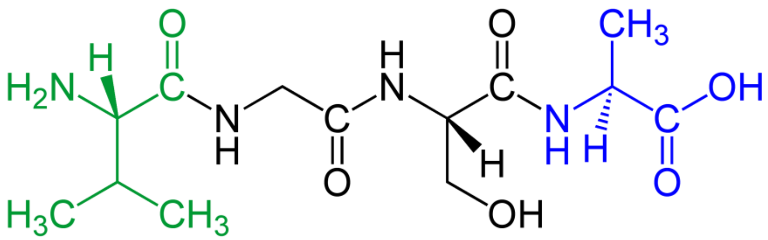


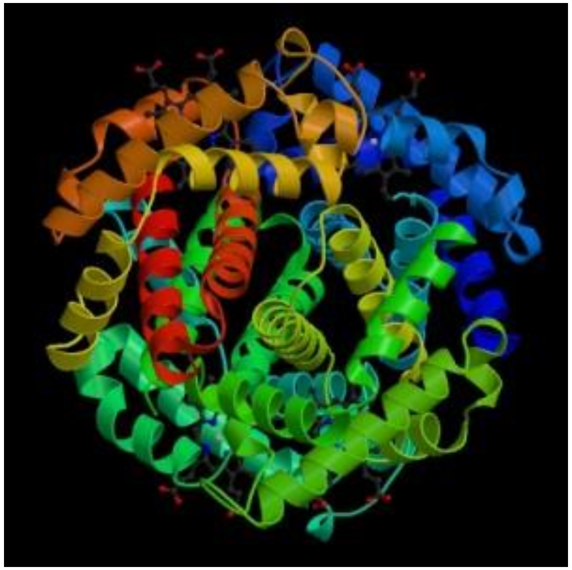
Simulated Annealing: Method of obtaining near-optimal solutions, based on an analogy with annealing of glasses

Protein Folding

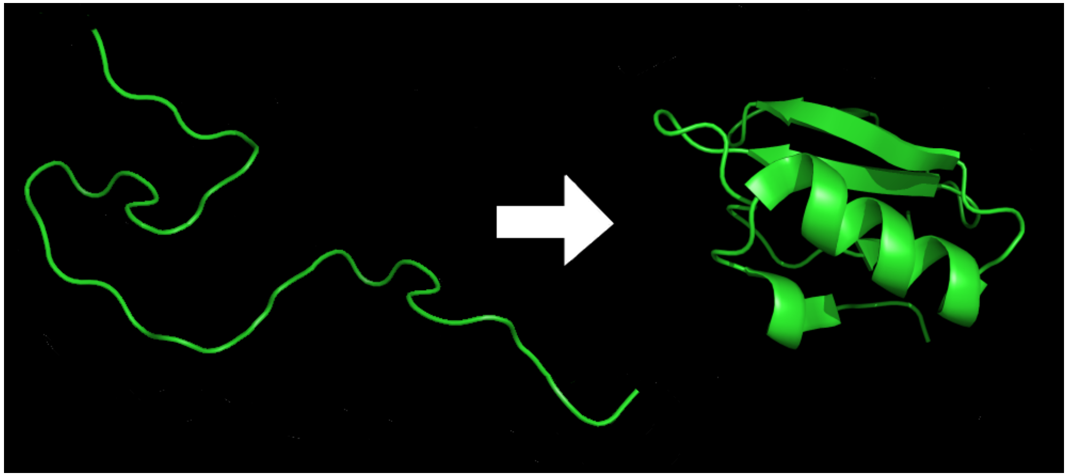
A protein is a polymer consisting of amino acids

Tetrapeptide Val-Gly-Ser-Ala

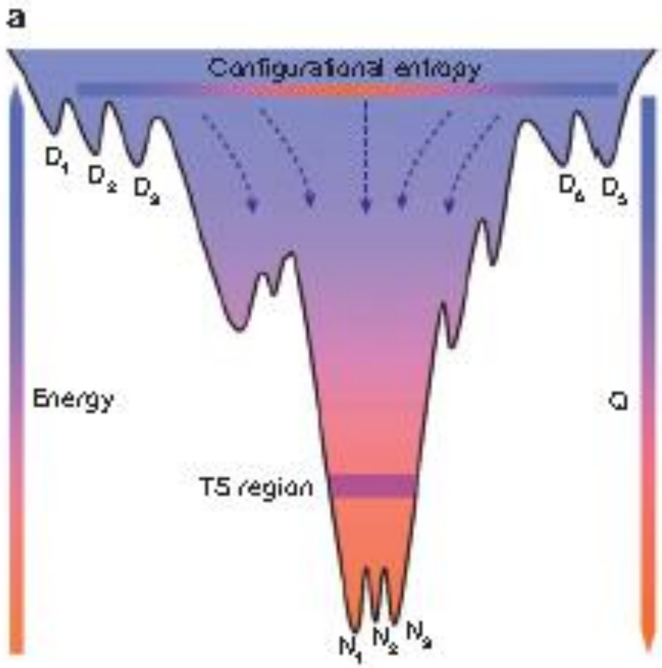




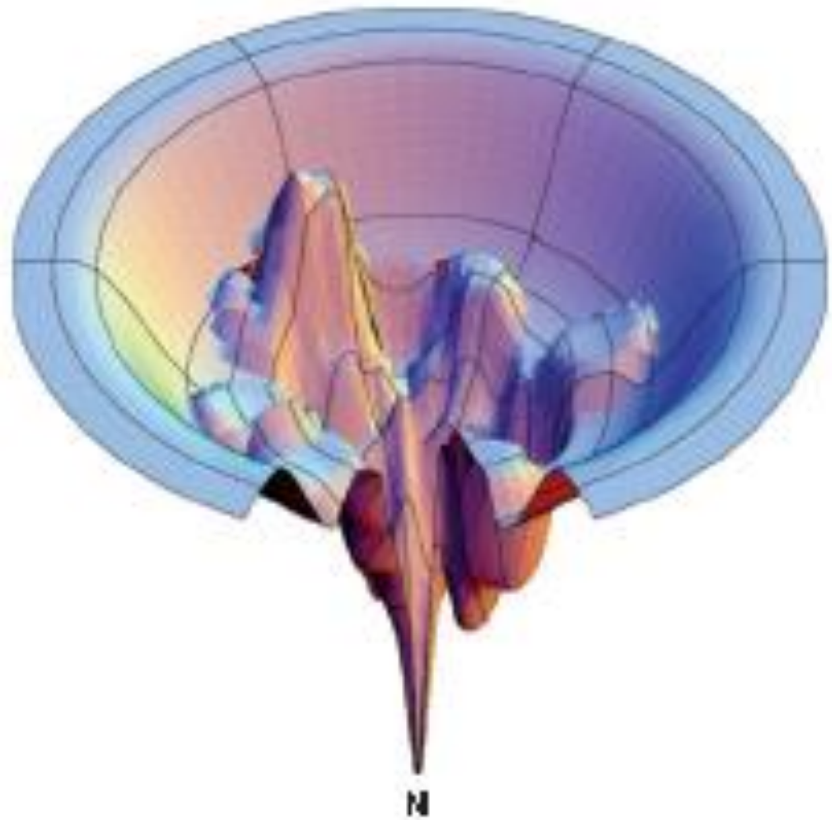
How does a protein reach its low-temperature “native” configuration from the high-temperature “denatured” state as the temperature is decreased?

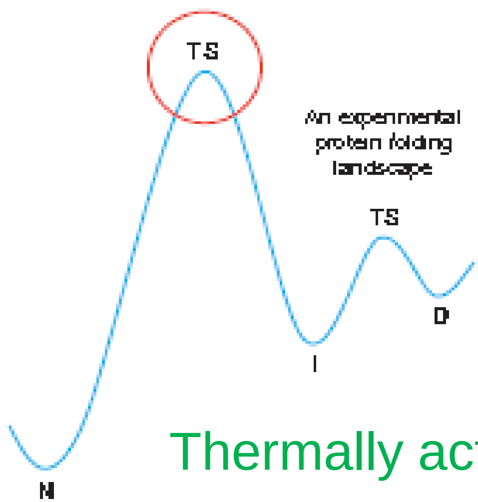


Cross-section of the energy landscape



The Energy Landscape

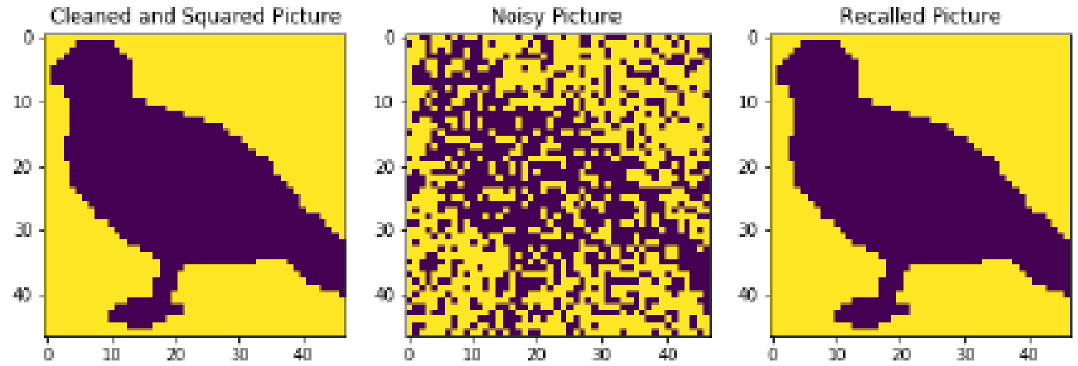




Thermally activated transitions

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)]

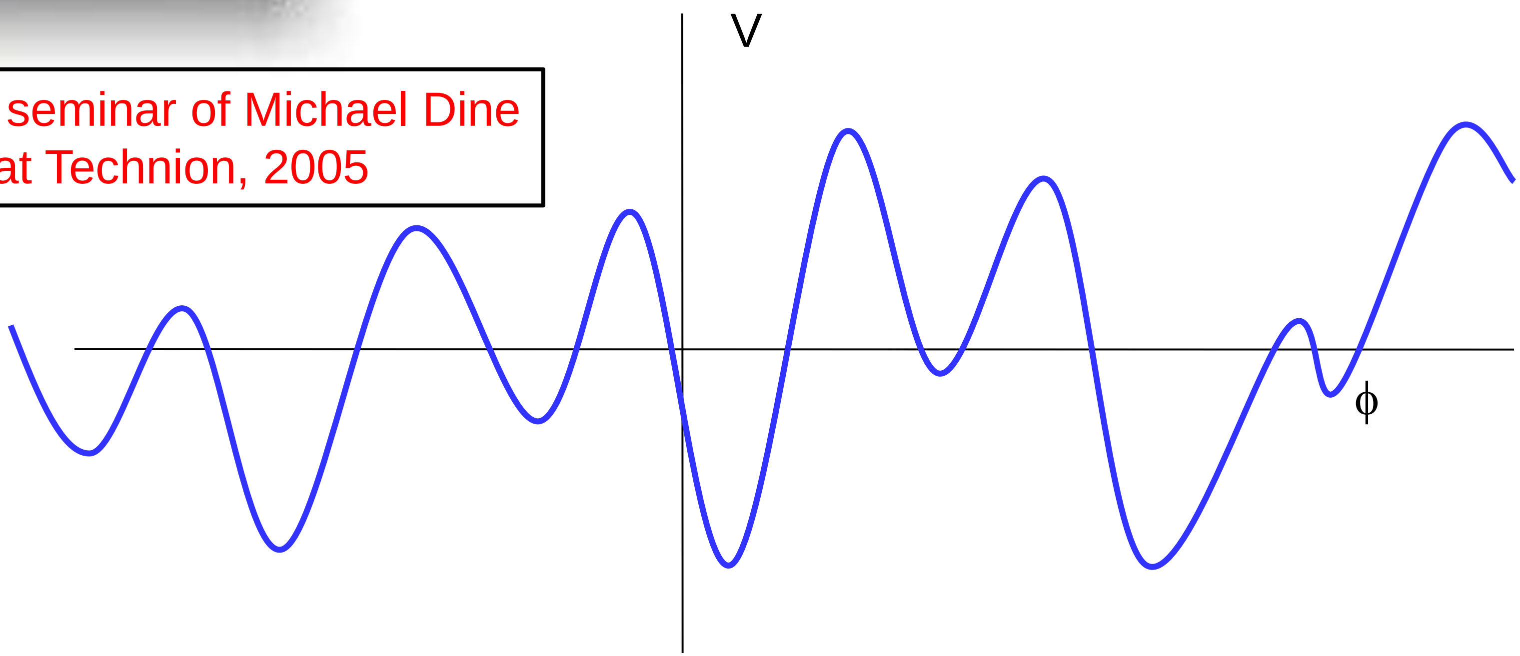
Memory states are stored as local minima of the energy.
Dynamics corresponds to changes that decrease the energy.

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

The String Theory Landscape

Vast array of vacuum states. A discretuum of values of the cosmological constant (Bousso, Polchinski; Banks, Dine, Seiberg).

From a seminar of Michael Dine at Technion, 2005



Summary

- Statistical mechanics and dynamics of glassy systems pose many interesting questions.

- In spite of extensive studies over several decades, some of these questions remain unanswered.

- Concepts and techniques developed in studies of glassy systems are useful in many other areas.