Tutorial on Statistical Physics

- Introduction
- Phase Transitions
- Mean-field Theory
- Disordered Systems: Spin Glass

Equilibrium Statistical Physics

Equilibrium Properties of ``Matter'' consisting of a large number of interacting "objects"

Microscopic variables: $\{\sigma_i\}, i = 1, \ldots, N,$
$N \to \infty$ (Thermodynamic limit).

Hamiltonian (energy function) $\mathcal{H}(\{\sigma_i\})$

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

- A thermodynamic state corresponds to an ensemble of microscopic states
- An ensemble is specified by a set of probabilities {p(n)}
- p(n) is the probability of occurrence of the microscopic state (n) in the ensemble

Thermodynamic (equilibrium) average:

$$\langle \mathcal{O} \rangle \equiv \Sigma_n p(n) \mathcal{O}(n)$$

Canonical Ensemble: $p(n) = \frac{\exp[-\mathcal{H}(n)/T]}{Z}$,

T: Absolute temperature (Boltzmann constant $k_B = 1$)

Partition Function $Z = \Sigma_n \exp[-\mathcal{H}(n)/T]$

Helmholtz Free Energy $F = -T \ln Z$.

Various thermodynamic quantities may be obtained as derivatives of F with respect to appropriate variables.

Internal Energy $E = \Sigma_n p(n)\mathcal{H}(n) = \frac{\partial \beta F}{\partial \beta}$ where $\beta \equiv 1/T$.

Entropy $S = -\Sigma_n p(n) \ln[p(n)] = \frac{\partial F}{\partial T}$

High temperature ($T \to \infty$): $p(n) = 1/N_s$ for all n where N_s is the total number of states $\Rightarrow S = \ln(N_s)$.

$T \to 0$ limit: $p(n)$ is nonzero only for the states corresponding to the global minima of $\mathcal{H}$ [“**Ground States**”] $\Rightarrow S = \ln(N_g)$ where N_g is the number of distinct ground states.

Connection with optimization problems

Local minima of $\mathcal{H}$: states for which any local change increases the energy.

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

States stable under single spin flips:

configurations $|\sigma_1, \sigma_2, \ldots, \sigma_k, \ldots, \sigma_N|$ such that

$\mathcal{H}(\sigma_1, \sigma_2, \ldots, \sigma_k, \ldots, \sigma_N) < \mathcal{H}(\sigma_1, \sigma_2, \ldots, -\sigma_k, \ldots, \sigma_N)$

for all k.

N constraints: $\sigma_i[\Sigma_j J_{ij}\sigma_j] > 0$ for all i.

Connections with constraint satisfaction problems

Local minima of the Hamiltonian play an important role in the dynamics of the system.

The system may "get stuck" at a local minimum at low temperatures

Monte Carlo (Metropolis) Dynamics:

Choose a σ_i at random
Calculate ΔE, the change in energy caused by a change of the sign of σ_i
Change the sign of σ_i if $\Delta E \leq 0$
Change the sign of σ_i with probability $\exp[-\Delta E/T]$ if $\Delta E > 0$.

At T=0, the sign of an Ising variable is changed only if the change decreases the energy.

This dynamics will get stuck at any local minimum of the energy (i.e. any state that is stable under single spin flips).

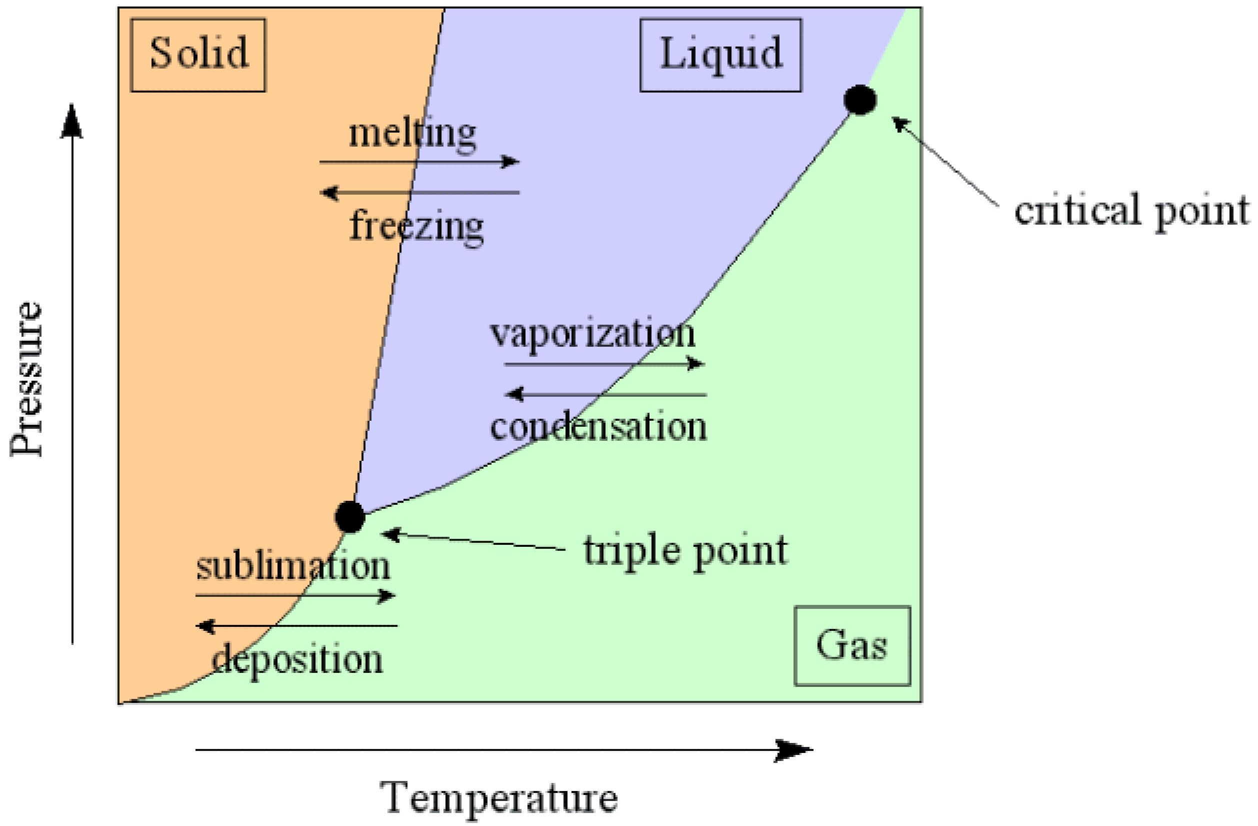
A finite T allows the system to get unstuck.

Simulated Annealing

Phase Transitions

Phase Transition: Drastic change in the thermodynamic properties as a thermodynamic parameter (e.g. temperature, pressure, magnetic field) is changed.

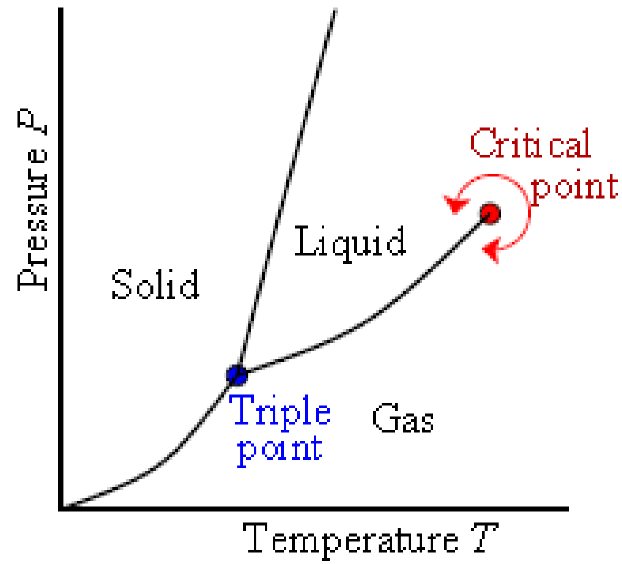
Example: Liquid-gas and Liquid-solid Transitions



First-order Phase Transitions

Volume, entropy, magnetization etc. (first derivatives of the free energy) change discontinuously at the transition.

Metastability (supercooling/superheating)



Continuous Phase Transitions

First derivatives of the free energy are continuous across the transition.

Large fluctuations

Critical point phenomena

Renormalization Group Theory was developed for describing critical point phenomena.

Spontaneous Symmetry Breaking

Phase transitions generally (but not always!) correspond to a change in the symmetry of the thermodynamic state of the system.

The ordered (low-temperature) phase usually breaks one of the symmetries of the underlying Hamiltonian.

Symmetries of the Hamiltonian

Operations under which the Hamiltonian is invariant

System of particles

$$\mathcal{H} = \Sigma_i |\vec{p}_i|^2/(2m) + \frac{1}{2}\Sigma_{i\neq j} V(|\vec{r}_i - \vec{r}_j|)$$

$\mathcal{H}$ is invariant under uniform translation $\vec{r}_i \longrightarrow \vec{r}_i + \vec{r}_0$

Heisenberg model of magnetism

$$\mathcal{H} = \frac{1}{2}\Sigma_{i\neq j} J_{ij} \vec{S}_i \cdot \vec{S}_j$$

$\mathcal{H}$ is invariant under uniform rotation of spin vectors.

Symmetries of a Thermodynamic State

- A thermodynamic state corresponds to an ensemble of microscopic states
- An ensemble is specified by a set of probabilities {p(n)}
- p(n) is the probability of occurrence of the microscopic state (n) in the ensemble

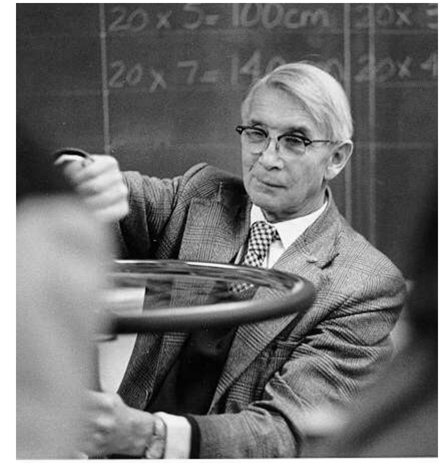
Canonical Ensemble: $p(n) = \frac{\exp[-E(n)/(k_B T)]}{Z}$

Thermodynamic averages: $\langle \mathcal{O} \rangle \equiv \Sigma_n p(n) \mathcal{O}(n)$

Is p(n) **the same** for all microscopic states related to each other by a symmetry operation of the Hamiltonian?

The answer is NO for a thermodynamic state with Spontaneously Broken symmetry.

The Ferromagnetic Ising Model

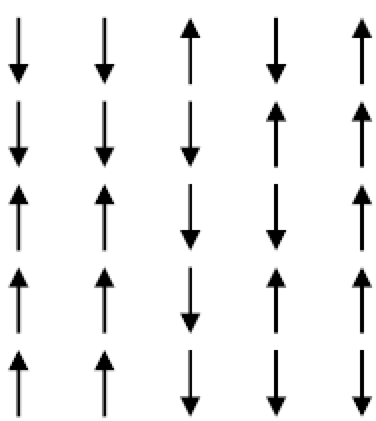


$$\mathcal{H} = -\sum_{i>j} J_{ij}\sigma_i\sigma_j - h\sum_i \sigma_i \quad \sigma_i = \pm 1$$

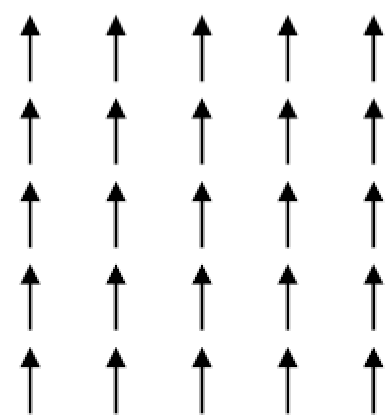
$J_{ij} = J > 0$ if i and j are nearest neighbors

$J_{ij} = 0$ otherwise

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



Paramagnetic state

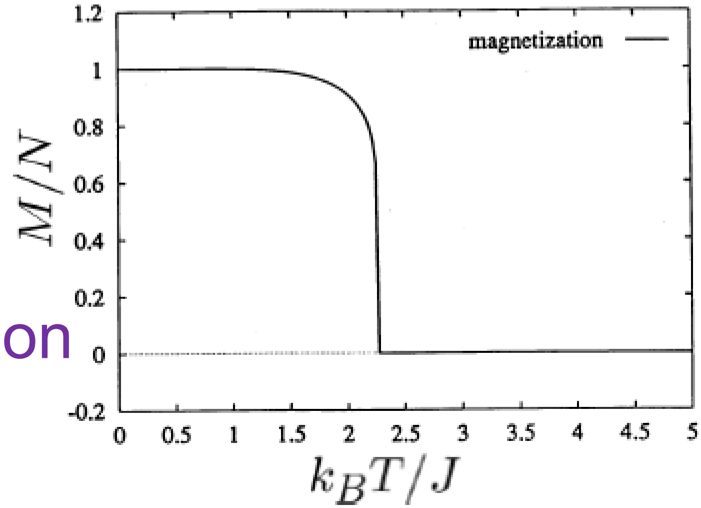


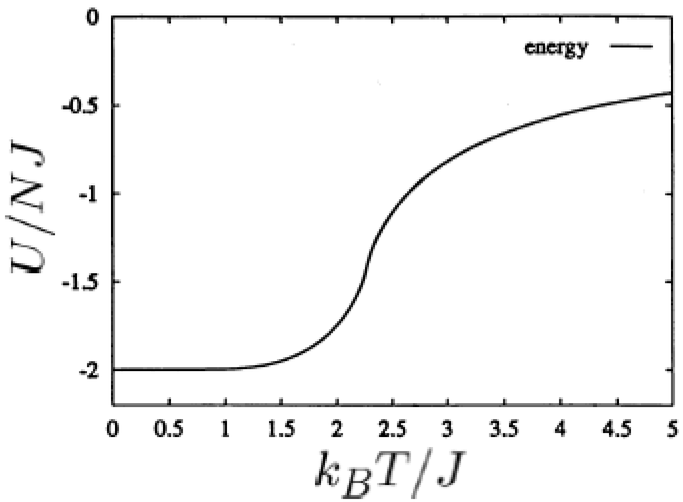
Ferromagnetic state

Exact solution in two dimensions (Onsager)

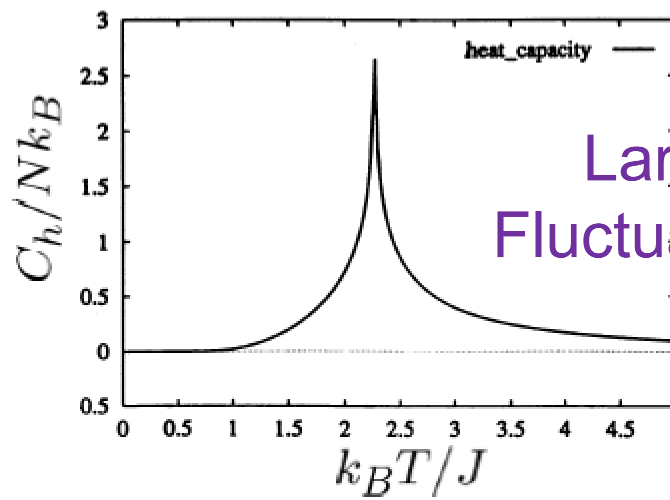
Magnetization →

Continuous Transition





Internal Energy



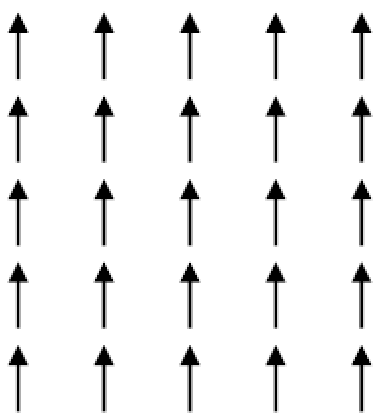
Large Fluctuations

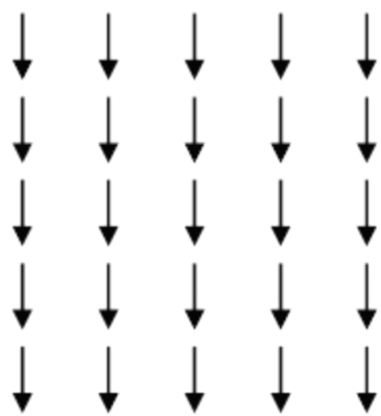
Specific Heat

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

For h=0, the Hamiltonian is invariant under $\sigma_i \rightarrow -\sigma_i$ for all i
i.e., $E(\{\sigma_i\}) = E(\{-\sigma_i\})$

However, $p(\{\sigma_i\}) \neq p(\{-\sigma_i\})$ in the ordered phase!



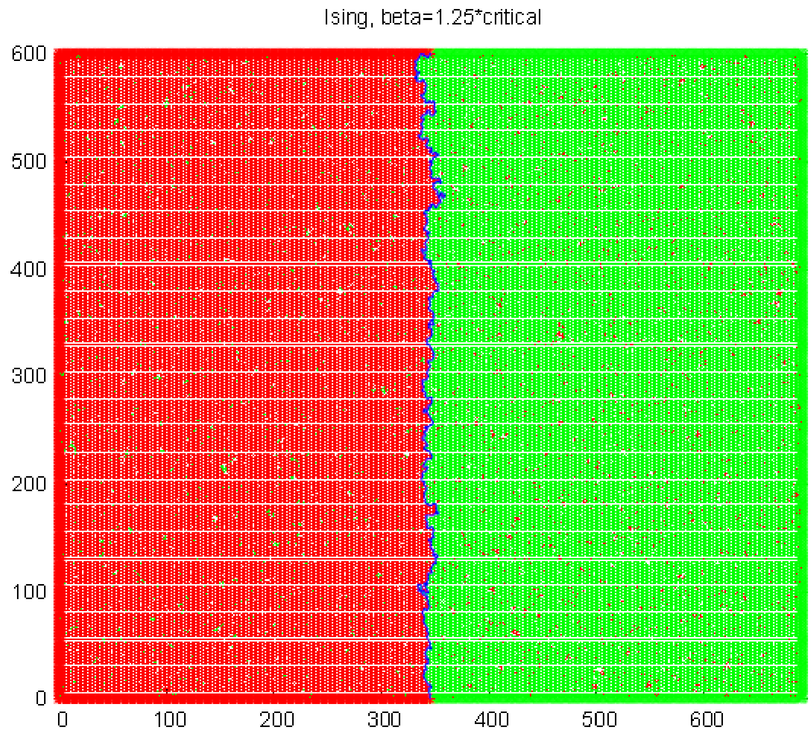


These two states have the same energy.

The state with down spins does not appear in the ensemble for the ordered state with m > 0.

The up-down symmetry of the paramagnetic phase (and also of the underlying Hamiltonian) is spontaneously broken in the ferromagnetic phase.

This is possible only in the thermodynamic limit



System has to go through a domain-wall state in order to explore ordered states with positive and negative magnetization.

Energy of a domain wall ~ 2JL where L is the system size.

This energy **diverges** in the thermodynamic limit.

Typically, (order-disorder) phase transitions occur due to a competition between energy and entropy.

Equilibrium state minimizes the free energy F = E - TS

At high temperatures, the entropy S is dominant => F is minimized by ~ maximizing the entropy => the system is in the disordered phase.

At low temperatures, the energy E is dominant => F is minimized by ~ minimizing the energy => the system is In the ordered phase.

Mean Field Theory

Mean field theory

Ferromagnetic Ising model $\mathcal{H} = -J \sum_{<ij>} \sigma_i \sigma_j$

Order parameter $m =< \sigma_i >$

fluctuation $\delta\sigma_i = \sigma_i - m$

$$\sigma_i \sigma_j = (m + \delta\sigma_i)(m + \delta\sigma_j) \approx m^2 + m(\delta\sigma_i + \delta\sigma_j)$$

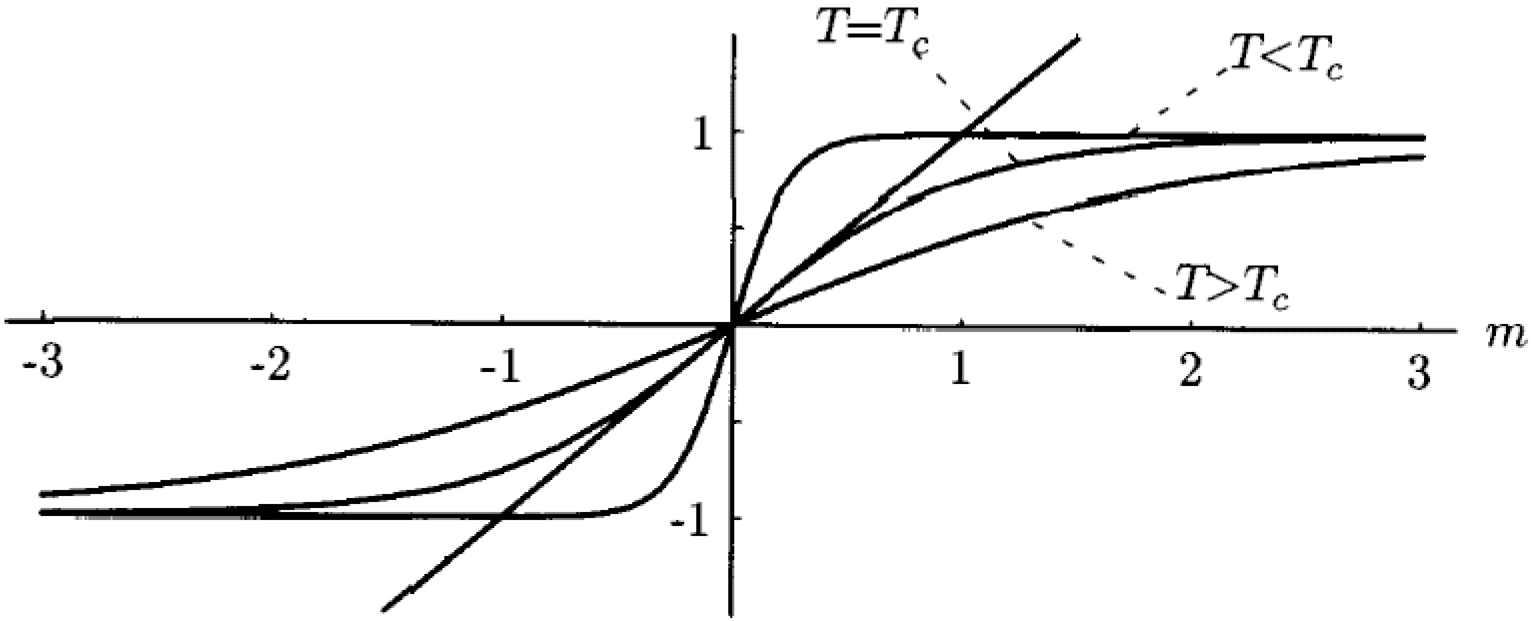
$$= m(\sigma_i + \sigma_j) - m^2$$

$$\mathcal{H} = -J \sum_{<ij>} \sigma_i \sigma_j \approx -Jzm \sum_i \sigma_i$$

z is the number of neighbours

$$m =< \sigma_i >= \tanh[\beta J z m]$$

Phase transition at $T_c = Jz$.



From: Chaikin and Lubensky

Mean field theory is exact for systems with infinite range interactions

$$\mathcal{H} = -\frac{J}{N}\sum_{i>j}\sigma_i\sigma_j$$

In a state with magnetization m, $N_+ = N(1+m)/2$ σ_is have value $+1$ and $N_- = N(1-m)/2$ σ_is have value -1.

$$\text{Internal Energy } E = -\frac{J}{N}[N_+^2/2 + N_-^2/2 - N_+N_-]$$
$$= -\frac{1}{2}NJm^2$$

Number of microstates with magnetization m is $\mathcal{N}(m) = \dfrac{N!}{N_+!N_-!}$

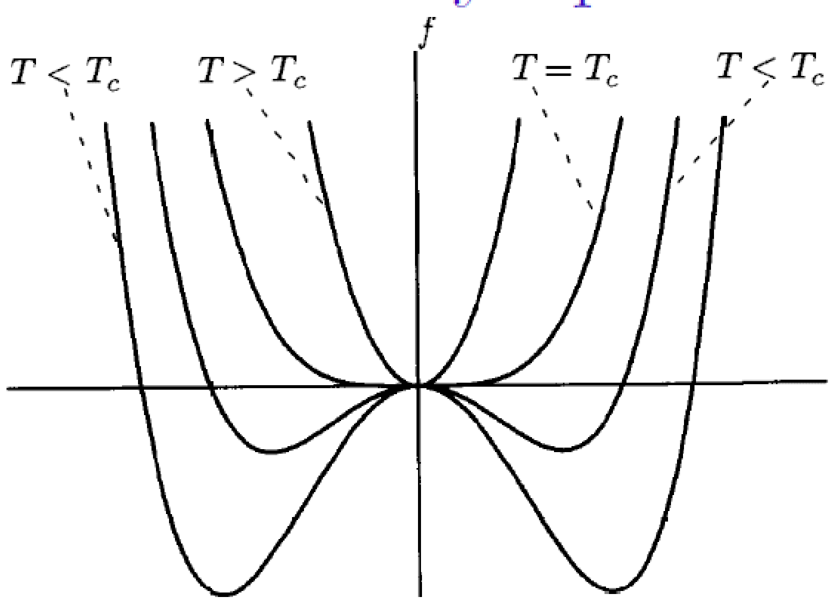
Entropy $S = \ln \mathcal{N}(m)$

$$= -N[\tfrac{1+m}{2}\ln(\tfrac{1+m}{2}) + \tfrac{1-m}{2}\ln(\tfrac{1-m}{2})]$$

Free energy $F = E - TS =$

$$-\tfrac{1}{2}NJm^2 + TN[\tfrac{1+m}{2}\ln(\tfrac{1+m}{2}) + \tfrac{1-m}{2}\ln(\tfrac{1-m}{2})]$$

Minimizing F with respect to m yields the mean-field self-consistency equation $m = \tanh[\beta J m]$.



Disordered Systems

$\mathcal{H}$ is different in different parts of the system
The system is not translationally invariant

Example: Dilute Ising Ferromagnet

$$\mathcal{H} = -J \sum_{<ij>} n_i n_j \sigma_i \sigma_j$$

$n_i = 1$ Site i is occupied

$n_i = 0$ Site i is not occupied

n_i : Quenched Random Variable

$$p(n_i) = c\delta(n_i - 1) + (1-c)\delta(n_i)$$

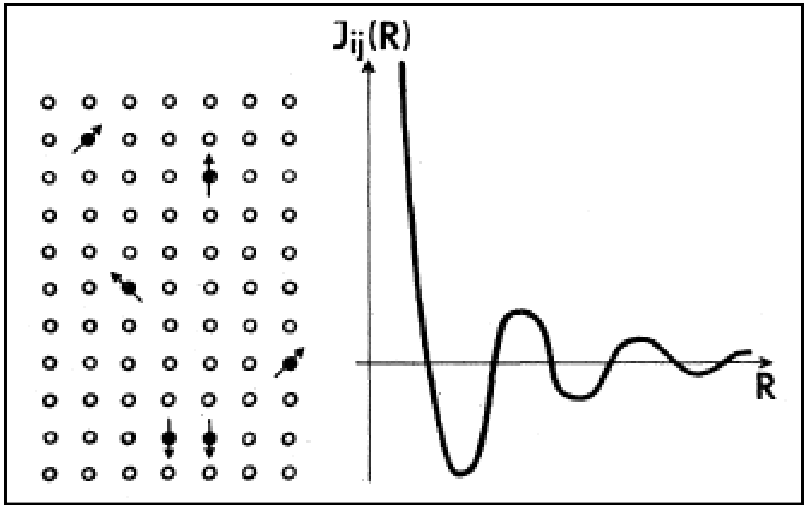
Spin Glasses

- 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



Frustration

All pair interactions can not be satisfied simultaneously

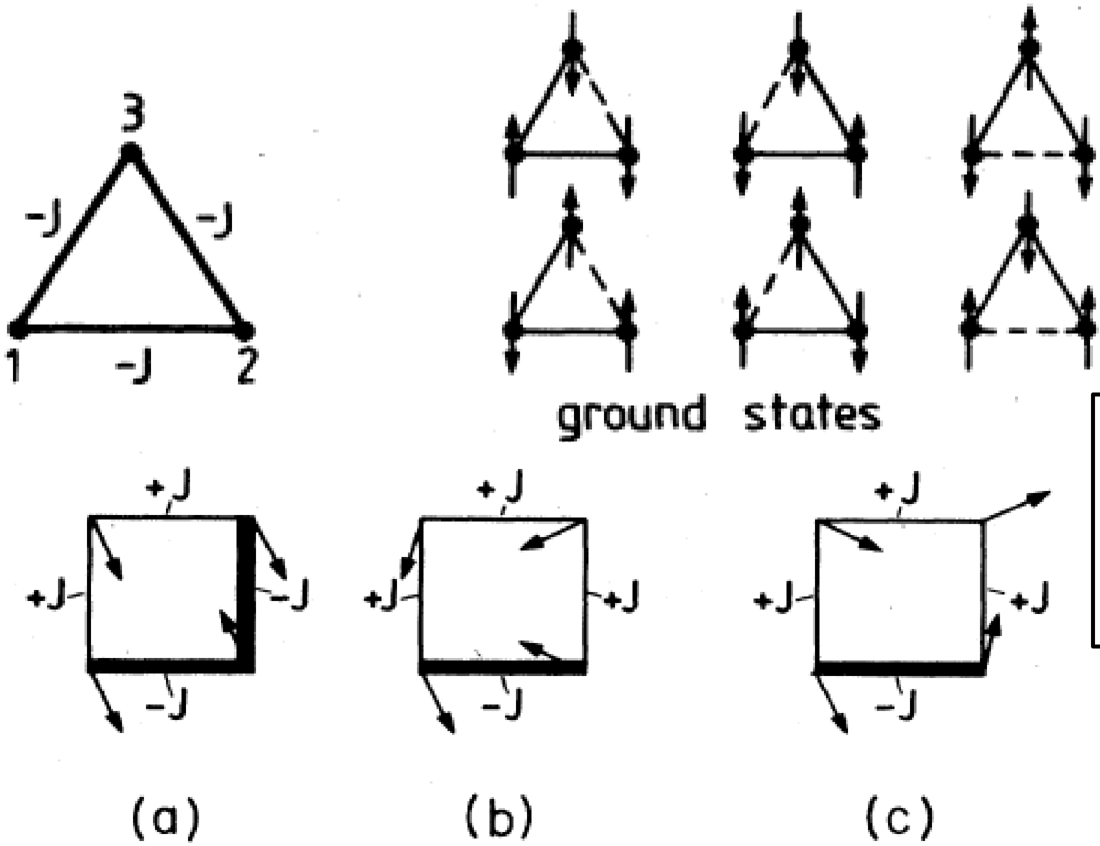


FIG. 41. Classical ground state of a set of four spins in the XY model with interactions $\pm J$ (thick bonds are antiferromagnetic, thin bonds are ferromagnetic). (a) Nonfrustrated plaquette; (b) frustrated plaquette, chirality $\tau = +1$; (c) frustrated plaquette, chirality $\tau = -1$.

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

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

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

Temporal autocorrelation function

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

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

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

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

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

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

The Sherrington-Kirkpatrick Model

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

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

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

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

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

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

The overlap distribution function $P(q)$ plays an important role in the interpretation of “replica symmetry breaking”.