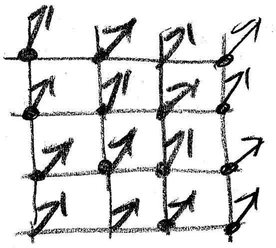
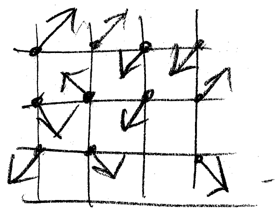
1. Introduction: Spin models

Consider e.g. a ferromagnet:

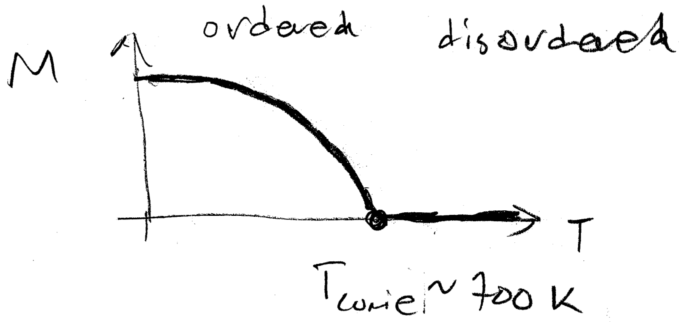




Spins want to align, but thermal energy randomizes!

$T < T_{curie}$ — magnetization $\bar{M} \neq 0$

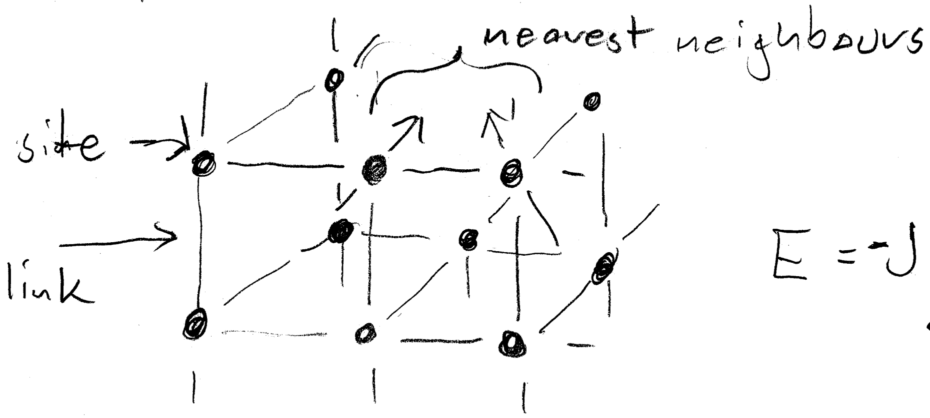
$T > T_{curie}$ — $\bar{M} \simeq 0$



Magnetic spins become disordered at high T

(Note: in real ferromagnets the magnetization happens in domains $\leftrightarrow$ spins)

Model interaction with nearest-neighbour interaction:



3-dim lattice

$$E = -J \sum_{\langle ij \rangle} \bar{S}_i \cdot \bar{S}_j$$

i, j n.n. sites

$J > 0$ for ferromagnet

If the spins are coupled to external magnetic field $\bar{H}$:

$$E = -J \sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j - \gamma \bar{H} \cdot \sum_i \bar{s}_i$$

$\gamma \bar{s}_i$ = magnetic moment of 1 spin

$\bar{H}$ aligns spins $\parallel \bar{H}$.

Thermodynamics

Introduce temperature T. Now the properties of the system are given by the partition function

$$Z = \int [\prod_i ds_i] \, e^{-\frac{1}{kT} E[s]}$$

integral over all values of $\bar{s}_i$

$$= \int [\prod_i ds_i] \, e^{\frac{J}{kT} \sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j + \frac{\gamma}{kT} \bar{H} \cdot \sum_i \bar{s}_i}$$

Use dimensionless quantities $\beta \equiv \frac{J}{kT}$; $\bar{h} \equiv \frac{\gamma}{kT} \bar{H}$

$$Z[\beta, \bar{h}] = \int [\prod_i ds_i] \, e^{\beta \sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j + \bar{h} \cdot \sum_i \bar{s}_i}$$

"Thermodynamic limit": size of the system $\to \infty$ (number of d.o.f's)

Action $S \equiv -\beta \sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j + \bar{h} \cdot \sum \bar{s}_i$, e^{-S}

Note: $\sum_{\langle xy\rangle}' s_x s_y = \sum_x' \sum_{i=1}^{d}{}' s_x s_{x+\hat{e}_i}$

d = dimensionality, $\hat{e}_i$ - unit vector

Models:

- Ising model : $s_i = \pm 1$, only 2 values

$$Z = \sum_{\{s_i\}}' \exp\left[\beta \sum_{\langle ij\rangle}' s_i s_j + h \sum_i s_i \right]$$

↑ sum over all values of $s_i = \pm 1$, symbolically $= \prod_i \sum_{s_i=-1,+1}'$

solved in 1, 2 (Onsager) dimensions

- q-state Potts model generalization of Ising

$s_i = 1, 2, \dots, q$, q discrete values

$$Z = \sum_{\{s_i\}}' \exp\left[\beta \sum_{\langle ij\rangle}' \delta_{s_i, s_j} + \sum_{\ell=1}^{q} h_\ell \sum_i' \delta_{s_i, \ell}\right]$$

"$\bar{h} \cdot \sum \bar{s}$"

favours like neighbours, if different, interaction = 0. All values "equally distant" from each other

h_ℓ: field pulling to spin value ℓ,

$\bar{h} = (h_1, h_2 \dots h_q)$

$q=2$: Ising model :

In Ising, $\beta s_i s_j = \begin{cases} +\beta & \text{if } s_i = s_j \\ -\beta & s_i \neq s_j \end{cases}$

$= 2\beta \left(\delta_{s_i, s_j} - \frac{1}{2} \right)$

Thus, $\beta \sum_{\langle ij \rangle} s_i s_j = 2\beta \sum_{\langle ij \rangle}' \delta_{s_i, s_j} - \underbrace{\cancel{\beta \sum_{\langle ij \rangle}' 1}}_{\beta \cdot N \cdot d}$ constant, can drop!

number of sites

Redefining $2\beta \to \beta'$ we get Potts.

- In the Ising model, the Curie transition is of 2nd order at $d \geq 2$ (no transition at $d=1$)
- In the Potts model, at $\underline{d=2}$ the transition is of 2nd order at $q = 2, 3, 4$
  1st order at $q \geq 5$

At $d \geq 3$, 2nd order at $q=2$, 1st otherwise

- At $d=2$, the Curie point is at $\underline{\beta_c = \ln(1+\sqrt{q})}$

- O(2) model or XY-model

$\bar{S}_i = (\cos\theta_i, \sin\theta_i)$ - 2-comp. vector w. $|\bar{S}_i| = 1$

$$Z = \prod_i \int_{-\pi}^{\pi} d\theta_i \, e^{\beta \sum_{\langle ij \rangle}' \cos(\theta_i - \theta_j)}$$

$s_i \cdot s_j$

O(2) : 2×2 orthogonal matrix, planar rotations

- $O(3)$: $\bar{s} = (s_x, s_y, s_z)$, $|\bar{s}| = 1$

  Heisenberg model, magnetization

- $O(N)$: $\bar{s}$ N-comp. vector, $|\bar{s}| = 1$.

Observables :

- Expectation value of energy (when $\bar{h} = 0$):

$$\langle E \rangle = \langle -\sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j \rangle = -\frac{\partial}{\partial \beta} \ln Z$$

$$= \frac{1}{Z} \int [ds] \left(-\sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j\right) e^{\beta \sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j}$$

- Magnetization : write $\bar{h} = h \bar{e}_h$, now

$$\langle M \rangle = \langle \bar{e}_h \cdot \sum_i \bar{s}_i \rangle = \frac{\partial}{\partial h} \ln Z$$

- Heat capacity / specific heat

$$\chi = \frac{-1}{N_{tot}} \frac{\partial}{\partial \beta} \langle E \rangle = \frac{1}{N_{tot}} \frac{\partial^2}{\partial \beta^2} \ln Z$$

$$= \frac{1}{N_{tot}} \left(\frac{1}{Z} \int [ds] \left(\sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j\right)\left(\sum_{\langle k\ell \rangle} \bar{s}_k \cdot \bar{s}_\ell\right) e^{\beta \sum_{ij} \bar{s}_i \cdot \bar{s}_j} - \left[\frac{1}{Z} \int [ds] \left(\sum_{\langle ij \rangle} \bar{s}_i \cdot \bar{s}_j\right) e^{\beta \sum \bar{s}_i \bar{s}_j} \right]^2 \right)$$

$$= \frac{1}{N_{tot}} \left(\langle E^2 \rangle - \langle E \rangle^2 \right)$$

$$= \frac{1}{N_{tot}} \left(\langle (E - \langle E \rangle)^2 \rangle \right) = \frac{1}{N_{tot}} \langle \Delta E^2 \rangle$$

N_{tot} = number of sites, intensive quantity

• Magnetic susceptibility

$$\chi_M \equiv \frac{1}{N_{tot}} \frac{\partial}{\partial h} \langle M \rangle = \frac{1}{N_{tot}} \frac{\partial^2}{\partial h^2} \ln Z$$

$$= \frac{1}{N_{tot}} \left(\langle M^2 \rangle - \langle M^2 \rangle \right) = \frac{1}{N_{tot}} \langle \Delta M^2 \rangle$$

Correlation function

$$C(\bar{x}-\bar{y}) = \langle s_{\bar{x}} s_{\bar{y}} \rangle - \langle s_{\bar{x}} \rangle \langle s_{\bar{y}} \rangle \rightarrow e^{-|\bar{x}-\bar{y}|/\xi}, \quad |\bar{x}-\bar{y}| \to \infty$$

ξ = correlation length

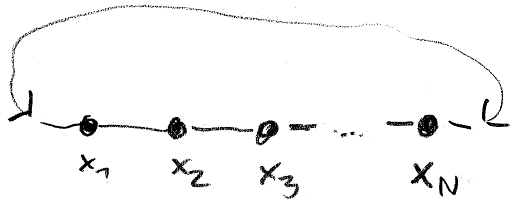
Can be derived from Z by introducing $\bar{x}$-dep. source (field) $h_{\bar{x}}$:

$$Z = \int [ds] \, e^{\beta \sum s_x s_y + \sum_x h_x s_x}$$

$$C(\bar{x}-\bar{y}) = \frac{\partial}{\partial h_{\bar{x}}} \frac{\partial}{\partial h_{\bar{y}}} \ln Z \Big|_{h=0}$$

Example of an exact solution: 1-d Ising

($d=2$: Onsager 1944, $h=0$; Yang 52 for $h \neq 0$)



periodic b.c. :: neighbour of x_N is x_1; $X_{N+1} \equiv X_1$

$$\beta \sum_{i=1}^{N} s_i s_{i+1} + h \sum_{i=1}^{N} s_i = \sum_{i=1}^{N} \left(\beta s_i s_{i+1} + \tfrac{1}{2} h (s_i + s_{i+1}) \right)$$

(here $s_i \equiv s_{x_i}$). Define 2×2 transfer matrix

$$T_{ss'} = \exp\left[\beta s s' + \tfrac{1}{2} h (s + s') \right]$$

Now

$$Z = \sum_{\{s_i\}} T_{s_1 s_2} T_{s_2 s_3} \cdots T_{s_{N-1} s_N} T_{s_N s_1} = \sum_{s_1} (T^N)_{s_1 s_1}$$

$$= \operatorname{Tr} T^N .$$

Explicitly, $T = \begin{pmatrix} e^{\beta+h} & e^{-\beta} \\ e^{-\beta} & e^{\beta-h} \end{pmatrix}$

Trace can be evaluated by diagonalizing:

Eigenvalues $\lambda_\pm$: $\operatorname{Det} \begin{pmatrix} e^{\beta+h} - \lambda & e^{-\beta} \\ e^{-\beta} & e^{\beta-h} - \lambda \end{pmatrix} = (e^{\beta+h} - \lambda)(e^{\beta-h} - \lambda) - e^{-2\beta} = 0$

$$\Rightarrow \lambda_\pm = e^{\beta} \left[\cosh(h) \pm \sqrt{\sinh^2(h) + e^{-4\beta}} \right]$$

$$\ln Z = \ln \operatorname{Tr} \begin{pmatrix} \lambda_+ & \\ & \lambda_- \end{pmatrix}^N = \ln(\lambda_+^N + \lambda_-^N)$$

$$= \ln\left(\lambda_+^N \left(1 + \left(\tfrac{\lambda_-}{\lambda_+}\right)^N\right)\right) = \ln \lambda_+^N + \ln\left(1 + \left(\tfrac{\lambda_-}{\lambda_+}\right)^N\right)$$

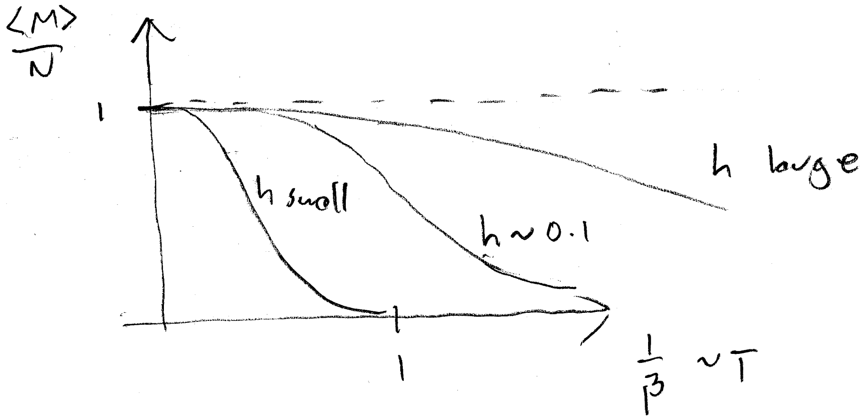
In the limit $N \to \infty$, $\lambda_- / \lambda_+ \to 0$,

and
$$\ln Z = N \left(\ln \left(\cosh(h) + \sqrt{\sinh^2(h) + e^{-4\beta}} \right) + \beta \right)$$

Now magnetization

$$\langle M \rangle = \frac{1}{N} \frac{\partial}{\partial h} \ln Z = \frac{\sinh(h) + \frac{\cosh(h)\sinh(h)}{\sqrt{\sinh^2 + e^{-4\beta}}}}{\cosh(h) + \sqrt{\sinh^2 + e^{-4\beta}}}$$

$$= \frac{\sinh(h)}{\sqrt{\sinh^2(h) + e^{-4\beta}}} \qquad (\text{using } 1 + \sinh^2 = \cosh^2)$$



no phase transition (singularity)

$h = 0 \to \langle M \rangle = 0$, no ferromagnetism.

(Homework: calculate magnetization in 1d 3-state Potts model. For simplicity, use only h to 1-direction $h \sum_x \delta_{s_x, 1}$)

Symmetries (global)

$$S = -\beta \sum_{\langle ij \rangle}{}' s_i \cdot s_j - h \cdot \sum_i s_i \qquad \text{action}$$

Partition function

$$Z = \int [ds_i]\, e^{-S}$$

$$= \int \prod_i ds_i\, e^{-S[} \qquad \text{for e.g. } O(N) \text{ models}$$

$$= \prod_i \sum_{s_i=+1,-1} e^{-S} \qquad \text{for Ising, Potts}$$

System has a <u>global symmetry</u>, if we can transform $s \to s' = Ms$ so that $S[s]$ and $[ds]$ are invariant!

- Ising: $s_i \to -s_i$, if $h = 0$!
- O(N)-model:

$s \to s' = Ms$, where M is $N \times N$ matrix.

$$s_i \cdot s_j = (s_i)_\alpha (s_j)_\alpha \to$$

$$(s_i')_\alpha (s_j')_\alpha = M_{\alpha\beta} M_{\alpha\gamma} (s_i)_\beta (s_j)_\gamma$$

is invariant if $M_{\alpha\beta} M_{\alpha\gamma} = \delta_{\beta\gamma}$ or

$MM^T = \mathbb{1} \Rightarrow M$ orthogonal, $M^T = M^{-1}$,

and $M \in O(N)$ (group of orthogonal $N \times N$)

$$h \cdot s_i \to h_\alpha M_{\alpha\beta} (s_i)_\beta$$ not invariant if $h \neq 0$!

$$\int ds_i = \int_{|s_i|=1} d^N s_i = \int d^N s_i \, \delta(|s_i|-1)$$

$$\to \int d^N s_i' \, \delta(|s_i'|-1)$$

$$= \int d^N s_i \, \left\| \frac{ds'}{ds} \right\| \delta(|M s_i| - 1)$$

$$\left\| \frac{ds'}{ds} \right\| = \text{Jacobi}, = |\det M|$$

because $M^T M = \mathbb{1} \Rightarrow \det M = \pm 1$

$$\Rightarrow |M s_i| = |s_i|$$

Thus, also measure is invariant.

Theory is $O(N)$ symmetric if $h=0$.

Symmetry breaking

Consider $h=0$, N finite.

$$\langle M \rangle = \frac{\int [d\sigma] \left(\sum_i s_i\right) e^{-S}}{Z}$$

Because system has ($O(N)$) symmetry, it is symmetric under $s \to M s = -\mathbb{I} s$ $\quad (-\mathbb{I} \in O(N))$

However, $\langle M \rangle \to -\langle M \rangle$; M is not symmetri[c]

and $\underline{\langle M \rangle = 0}$.

- Symmetry restored, disordered phase.
- $\underline{h \neq 0}$: symmetry is explicitly broken.
- What happens if $N \to \infty$ (thermodynamic limit?)

Symmetry is spontaneously broken, if

$$\lim_{h \to 0} \left[\lim_{N \to \infty} \frac{\langle M \rangle}{N} \right] \neq 0$$

(note order of limits)

- 1d Ising: symmetry $s \to -s$ not spontaneously broken:

$$\lim_{N \to \infty} \frac{\langle M \rangle}{N} = \operatorname{sign}(h) \times \frac{\sinh(h)}{\sqrt{\sinh^2(h) + e^{-4\beta}}}$$

Phase transition:

at $h=0$ some models have e.g.

- broken symmetry if $\beta > \beta_c$
- restored symmetry if $\beta < \beta_c$

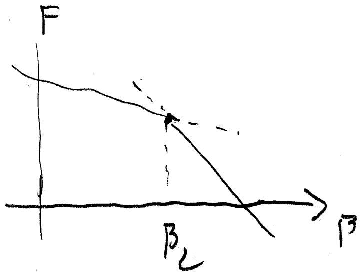
$\Rightarrow$ phase transition at $\beta = \beta_c$

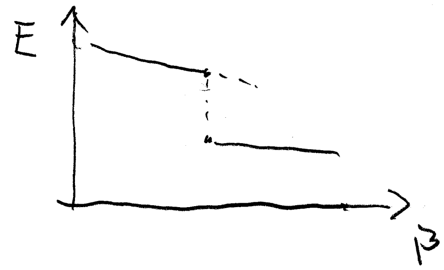
* First order phase transition

"Free energy" $F = -\ln Z$ continuous,

but its 1st derivatives not:

$\langle E \rangle = \frac{\partial}{\partial \beta} F$, $\langle M \rangle = \frac{\partial}{\partial h} F$ discontinuous





$\frac{1}{N} \Delta E$ = latent heat

$$= \left(\lim_{\beta \to \beta_-} \langle E \rangle - \lim_{\beta \to \beta_+} \langle E \rangle \right) \frac{1}{N} = \frac{E_- - E_+}{N}$$

$$\chi = \frac{1}{N} \langle (E - \langle E \rangle)^2 \rangle \simeq \frac{1}{N} \frac{\Delta E^2}{4} = N \frac{1}{4} \left(\frac{\Delta E}{N} \right)^2 \propto N$$

at β_c, $E \simeq E_+$ or E_-,
but $\langle E \rangle = \frac{1}{2}(E_+ + E_-)$

physically: at β_c (T_c), two phases can coexist (ice/water)

* <u>2nd order</u> p.t.

F' continuous, F'' discontinuous

- <u>Critical phenomena</u>: correlation length diverges $\xi \to \infty$, structure of all scales

Let $\tau = \beta - \beta_c$:

$$\chi \propto |\tau|^{-\alpha}$$

$$\chi_M \propto |\tau|^{-\gamma}$$

$$\xi \propto |\tau|^{-\nu}$$

$$\frac{\langle M \rangle}{N} = 0, \quad \beta < \beta_c \; ; \quad \frac{\langle M \rangle}{N} \propto |\tau|^{\delta} \quad \beta > \beta_c$$

Critical exponents - characteristic for the dimensionality $\underline{d}$ and symmetry

- $d=2$ Potts (Ising) has p.t. at $\beta = \ln(1+\sqrt{q})$ 2nd order for $q \leq 4$, otherwise 1st.

This is a <u>discrete</u> symmetry

- $d=2$ $O(N)$ models do not have symmetry breaking transitions:
  Mermin-Wagner-Coleman theorem:
  2d continuous symmetries do not break.

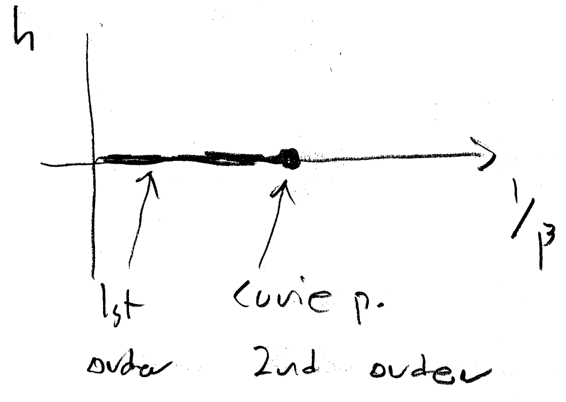
  - 2d XY ($O(2)$) has a special ∞-order p.t., Kosterlitz-Thouless. Symmetry restored on both sides

- $d=3$ $O(N)$ have 2nd order p.t.
  critical exponents have been numerically determined.

- $d=3$ $q\geq 3$ Potts 1st order; Ising 2nd.

- $d\geq 4$ $O(N)$ models have 2nd order P.T. with mean field exponents (computable analytically)

Note: e.g. in Ising or $O(N)$



If we fix $\beta > \beta_c$ and change h, 1st order transition (line)