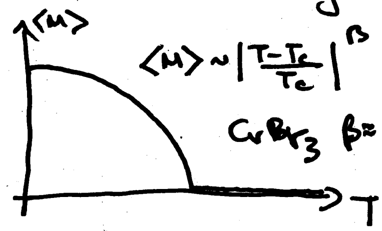
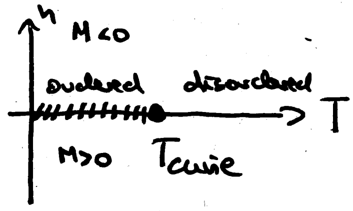
Ising Model (Lenz 1920, Ising 1925)

The first of many discrete spin models used in statistical physics for e.g. the description of magnetism. (See Kogut Rev. Mod. Phys. 51, 4 (1979))

Goal: Behavior of a ferromagnet as function of T, i.e. material may retain ~~spontaneous~~ magnetization if external magn. field is removed. (c.f. paramagnetism: field ∥ external, diamagn. field anti-∥ external)

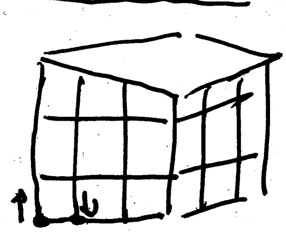
Order parameter magnetization, in 3d we have:





Find simple model to exhibit phase transition

Definition: Assign a "spin" to each spatial site with possible values ± 1. $s_i = \pm 1$. Energy modelled by nearest neighbor interactions:



$s_i \quad s_{i+\hat\mu}$.

$\hat\mu$ unit vector in μ-dir

$$E = \underset{\substack{\text{irrelevant}\\\text{constant from}\\\sum_i (s_i - s_{i+\hat\mu})^2}}{\text{const}} - \tilde{J} \underbrace{\sum_{i,\mu} s_i s_{i+\hat\mu}}_{\text{kinetic term}} + \underset{\text{external magn. field}}{\tilde{h}} \sum_i s_i$$

$J>0$ ferromagnet, $J<0$ antiferromagnet.

[Quantum Ising model $s_i \to \hat\sigma_i$: for $\tilde{J}\sum \hat\sigma_z\hat\sigma_z + \tilde{h}\sum\hat\sigma_z$ reduces to classical but $\tilde{h}\sum\hat\sigma_x$ nontrivial since $[\sigma_z, \sigma_x] \neq 0$ (transverse Ising)]

Thermodynamics: Canonical approach (Contact with heat bath, exchange of energy at fixed T)

Classical probability of microstate $P_s = \dfrac{e^{-\frac{E_s}{kT}}}{\sum_{\{s\}} e^{-\frac{E_s}{kT}}} = \dfrac{1}{Z} e^{-E_s/kT}$

Partition function: $Z(\beta, h, N_{tot}) = \sum_{\{s_i=\pm1\}} \exp\left(+\beta \sum_{i,\mu} s_i s_{i+\hat\mu} + h \sum_i s_i\right)$ $\quad \beta = \frac{\tilde{J}}{kT}$, $h = \frac{\tilde{h}}{kT}$

$\sum_{\{s_i=\pm1\}} = \sum_{s_0=\pm1} \cdots \sum_{s_{N_{tot}-1}=\pm1}$ useful quantity free energy $F = -\frac{1}{kT}\log Z$ (note that only ratio J/T relevant)

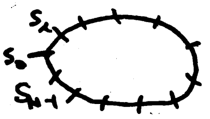
Directly related to observables:

Internal energy: $\langle E\rangle = \frac{1}{Z}\sum_{\{s\}} E_s\, e^{-\beta E_s} = \frac{\partial}{\partial\beta}\sum_{\{s\}} e^{-\beta E_s}/Z = -\frac{\partial}{\partial\beta}\log(Z) = \frac{\partial}{\partial\beta}(\beta F)$

Magnetization: $\langle M\rangle = \frac{1}{N_{tot}}\left\langle \frac{h}{|h|}\sum_i s_i\right\rangle = \frac{1}{N_{tot}}\frac{\partial}{\partial|h|}\log Z = -\frac{1}{N_{tot}}\frac{\partial}{\partial|h|}(\beta F)$

magnetic suscept: $\chi_M = \frac{\partial}{\partial|h|}\langle M\rangle = \frac{\partial^2}{\partial|h|^2}\log Z \frac{1}{N_{tot}} = \langle (M - \langle M\rangle)^2\rangle$

In specific cases analytic solution possible (1-dim, 2-dim)

<u>One-dimensional Ising Model</u>: Periodic boundary cond.  $s_N = s_0$

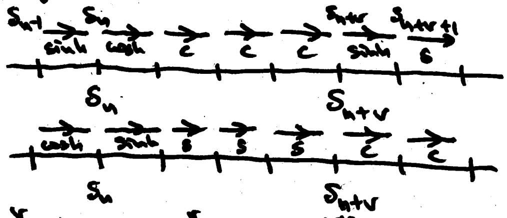
<u>Explicit approach @ h=0</u>: $Z = \sum_{\{s\}} \prod_i e^{\beta s_i s_{i+1}} \overset{\text{trick}}{=} \sum_{\{s\}} \prod_i \left(\cosh(\beta s_i s_{i+1}) + \sinh(\beta s_i s_{i+1})\right)$

$$\overset{\text{symm.}}{=} \sum_{\{s\}} \prod_i \left(\cosh(\beta) + s_i s_{i+1} \sinh(\beta)\right) = 2^N \left(\cosh^N(\beta) + \sinh^N(\beta)\right) \quad \text{mixterms cancel}$$

Correlation function: $\langle s_n s_{n+r} \rangle = \frac{1}{Z} \left[\sum_{\{s\}} s_n s_{n+r} \prod_i \left(\cosh(\beta) + s_i s_{i+1} \sinh(\beta)\right)\right]$

receives contributions from terms with an EVEN number of products of spins

Two possibilities:



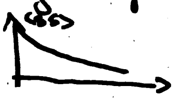
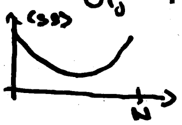
$\cosh^r(\beta)\sinh^{N-r}(\beta)$

$\sinh^r(\beta)\cosh^{N-r}(\beta)$

$$\langle s_n s_{n+r} \rangle = \frac{\cosh^{N-r}(\beta)\sinh^r(\beta) + \cosh^r(\beta)\sinh^{N-r}(\beta)}{\cosh^N(\beta) + \sinh^N(\beta)} = \tanh^r(\beta)\,\frac{1+\tanh^{N-2r}(\beta)}{1+\tanh^N(\beta)}$$

$$\overset{N\to\infty}{=} \tanh^r(\beta) = \exp(-r\underbrace{|\log\tanh(\beta)|}_{\text{mass-gap}}) = \exp(-r/\underset{\substack{\uparrow \\ \text{correlation length}}}{r_0})$$

Even in thermodynamic limit system is always disordered, i.e. NO PHASE TRANSITION. (With long-range interaction $\delta_{ij} \sim |i-j|^{-\alpha}$ $1<\alpha<2$ PT possible)

Note for PBC and finite N:  $\xrightarrow{N<\infty}$ 

<u>Transfer matrix approach @ h≠0</u>

With PBC write explicitly: $Z = \sum_{s_0=\pm1} \dots \sum_{s_{N-1}=\pm1} e^{\beta \sum_i s_i s_{i+1} + \frac{1}{2} h \sum_i (s_i + s_{i+1})}$

$$= \sum_{s_0} \dots \sum_{s_{N-1}} T_{s_0 s_1} \dots T_{s_{N-1} s_0} \quad \text{with} \quad T_{s_i s_j} = \exp\left[\beta s_i s_j + \tfrac{1}{2} h (s_i + s_j)\right]$$

$$= \sum_{s_0=\pm1} (\hat{T} \dots \hat{T})_{s_0 s_0} = \mathrm{Tr}[\hat{T}^N] \quad \text{with} \quad \hat{T} = \begin{pmatrix} e^{\beta+h} & e^{-\beta} \\ e^{-\beta} & e^{\beta-h} \end{pmatrix} = \begin{pmatrix} T_{11} & T_{1-1} \\ T_{-11} & T_{-1-1} \end{pmatrix}$$

Can be solved if EIGENVALUES known: $A = \begin{pmatrix} a & b \\ c & d \end{pmatrix} \to \lambda_\pm = \frac{\mathrm{Tr}(A) \pm \sqrt{\mathrm{Tr}(A)^2 - 4\,\mathrm{Det}(A)}}{2}$,

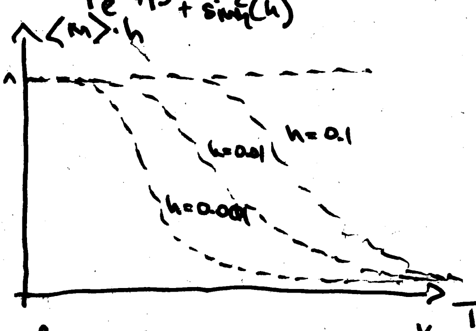
in our case $t_\pm = e^\beta \left(\cosh(h) \pm \sqrt{\sinh^2(h) + \exp(-4\beta)}\right)$

$$\log Z = \log \mathrm{Tr}[\hat{T}^N] = \log \mathrm{Tr}\begin{bmatrix} t_+^N & \\ & t_-^N \end{bmatrix} = \log\left(t_+^N \left(1 + \left(\tfrac{t_-}{t_+}\right)^N\right)\right) \underset{t_+>t_-}{\overset{N\to\infty}{=}} N \log t_+$$

$\Rightarrow$ Magnetization: $\langle M \rangle = \frac{1}{N} \frac{\partial}{\partial h} \log Z = \frac{\partial}{\partial h} \log t_+ = \frac{\sinh(h)}{\sqrt{e^{-4\beta} + \sinh^2(h)}}$

For all $T \neq 0$; $h \to 0$ vanishing magnetization

at $T=0$; $h \to 0$ $\langle M \rangle_h = 1$



Now toward <u>two-dimensional Ising model</u>

Still exactly solvable (Onsager 1944) and good testing ground for approximate methods

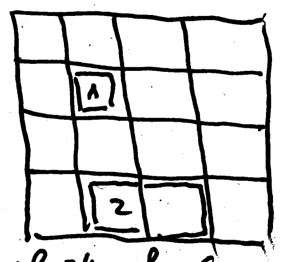
(see also: Mattis, Lieb Rev. Mod. Phys. 36, 856 (1964))

$\beta_c = 0{,}4407$ $\langle M \rangle \sim (\beta - \beta_c)^{1/8}$

① Strong coupling expansion / High T expansion (see hopping expansion ROTHE p. 151 (170))

$\beta \ll 1 \quad V = N_x N_x \quad Z = \sum_{\{s_i\}} \prod_{i,\mu} e^{\beta s_i s_{i+\hat\mu}} = \cosh(\beta)^{2V} \sum_{\{s_i\}} \prod_{i,\mu} (1 + \tanh(\beta s_i s_{i+\mu}))$

Two links $\langle ij \rangle$ emanate from each site. Need to identify the contributing terms: Only even powers of the involved spins survive and $\tanh(\beta)$ term couples neighbours → only closed loops relevant, its lines may not cross. ($\ell \hat{=}$ lattice length = factors of $\tanh(\beta)$)



$\ell_1 = 4 \quad \ell_2 = 6$

For each loop sum over all 2^V possible spin configs.

$Z = 2^V \cosh(\beta)^{2V} \left(1 + V(\tanh\beta)^4 + 2V(\tanh(\beta))^6 + \dots\right)$ loops can start anywhere thus V possibilities

Since $\beta \ll 1$ we can expand: $\cosh(\beta) \approx 1 + \beta^2/2$, $\tanh(\beta) \approx \beta - \beta^3/3$

$\approx 2^V (1 + V\beta^4 + \dots)$ ⇒ For correlations $\langle s_n s_{n+r} \rangle = \frac{1}{Z} \cosh(\beta)^{2V} \sum_s \prod_{i,\mu} (1 + \tanh(\beta s_i s_{i+\hat\mu})) s_n s_{n+r}$

only graphs that connect s_n and s_{n+r} with length $\ell = r, r+2, r+4 \dots$

$\langle s_n s_{n+r} \rangle \propto \sum_s \prod_{i,\mu} s_n s_{n+r} (\tanh^r(\beta) s_n s_{n+r} + \underbrace{r(r-1)}_{\text{exercise!}} \tanh^{r+2}(\beta) s_n s_{n+r} + \dots)$

all other s_i's quadratic

$\propto e^{-r |\log \tanh(\beta)|} (1 + r(r-1)\tanh^2(\beta) + \dots)$ single exponential is modified, mass-gap may vanish!

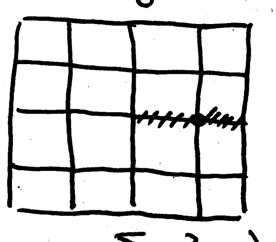
② Dimerization (see also Worm algorithm, Wolff NPB 810 491)

Reinterpret the partition function in terms of new d.o.f. may lead to new simulation algorithms, physics insight. (Fisher J. Math. Phys. 7 1776 (1966)) Kasteleyn 4 287 (1963))

$Z = \cosh(\beta)^{2V} \sum_{\{s\}} \prod_{i,\mu} (1 + \tanh(\beta) s_i s_{i+\hat\mu})$ @ each site $(1 + \tanh(\beta) s_i s_{i+\mu}) = \sum_{n_{i,\mu}=0,1} (\tanh\beta\, s_i s_{i+\mu})^{n_{i,\mu}}$

$= \cosh(\beta)^{2V} \sum_{\{s\}} \sum_{\{n_i\}} \prod_{i,\mu} (\tanh\beta\, s_i s_{i+\mu})^{n_{i,\mu}}$

Now reinterpret the $n_{i,\mu}$ as the degrees of freedom; i.e. for a given configuration of "links" $n_{i,\mu}$ carry out the spin sum.



$= \cosh(\beta)^{2V} \sum_{n_{i,\mu}=0,1} \tanh(\beta)^{\sum_{i,\mu} n_{i,\mu}} \sum_{\{s\}} \prod_{i,\mu} (s_i s_{i+\mu})^{n_{i,\mu}}$

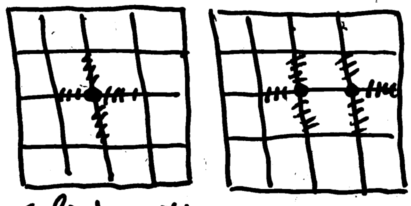
We have $\sum_{\{s\}} \prod_{i,\mu} (s_i s_{i+\hat\mu})^{n_{i,\mu}} = \sum_{\{s\}} \prod_i s_i^{b_i} \quad b_i = \sum_\mu n_{i,\mu} \quad (\sum_{\{s\}} s_i = 0,\ \sum_{\{s\}} s_i^2 = 1)$

$= \begin{cases} 0 & \text{for any odd } b_i \\ 2^V & \text{for } b_i \text{ even} \end{cases}$ → only those configs $n_{i,\mu}$ contribute where an even number of links emanates from each site.

$\Rightarrow Z = 2^V (\cosh(\beta))^{2V} \sum_{\{n_{i,\mu}\}} (\tanh(\beta))^{\sum_{i,\mu} n_{i,\mu}} \prod_i (b_i \bmod 2)$ constrained system!

③ Low temperature expansion / Weak coupling (see lattice perturbation theory hep-lat/0211036)

Intuition: At $T=0$ ground state is fully ordered $s_i = \pm 1$ $E_0 = -2V$ and the first excitation is a single spin flip.



≡ links with opposing spins

Enumerate the possible states:

$$Z = e^{\beta 2V} + V e^{\beta(2V-4) - \beta 4} + \dots$$

$$= e^{2V\beta}\left(1 + V e^{-8\beta} + \dots\right) \quad \text{with } \beta \gg 1$$

Kramers-Wannier Duality (Phys. Rev. 60, 252 (1941))

There exists a subtle connection between the $\beta \gg 1$ and $\beta \ll 1$ representation of the Ising model.

$$\log Z_{\beta \ll 1} = \log(2^V) + \log(\cosh \beta^{2V}) + \log(1 + V \tanh^4 \beta)$$

$$\log Z_{\beta \gg 1} = \log(e^{2V\beta^*}) + \log(1 + V e^{-8\beta^*}) \quad \left[\text{introduce } \beta^* = -\tfrac{1}{2}\log\tanh(\beta)\right]$$

$$= \log(\tanh(\beta)^{-V}) + \log(1 + V\tanh^4(\beta)) \quad \left[\tanh(\beta)^{-V} = \sinh^{-V}\beta \cosh^{V}\beta = 2\sinh(2\beta)^{-V}\cosh^{2V}\beta\right]$$

$$= \log(2^V) + \log(\sinh^{-V}(2\beta)) + \log(\cosh^{2V}\beta) + \log(1 + V\tanh^4(\beta))$$

$$\Rightarrow \beta \gg 1 \equiv \beta \ll 1 \text{ if } \sinh(2\beta) = 1$$

$\Rightarrow \beta_{crit} = 0.4407$ at phase transition both descriptions may cross.
Confirmed by Onsager's exact solution.

Other models of interest: Nature of spins different

q-state Potts model: spin in plane pointing to one of equally spaced directions (Wu, Rev. Mod. Phys. 54 235 (1982)) given by the angle $\theta_n = 2\pi n / q$

O(n) model: unit length, n-component, continuous spins (XY model = O(2)) with global symmetry:

- $\vec{s}_i \vec{s}_{i+\hat\mu} \to \sum_k (s_i)_k (s_{i+\hat\mu})_k = \sum_{l,j,k} M_{lj} M_{lk} (s_i)_j (s_{i+\hat\mu})_k = \sum_{j,k} (s_i)_j [M^T M]_{jk} (s_{i+\hat\mu})_k$

  if $M^T M = \mathbb{1}$ orthogonal matrix.

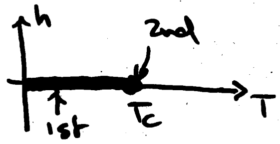
- $\vec{h} \cdot \vec{s}_i \to \sum_{jk} h_j M_{jk} (s_i)_k \Rightarrow$ not invariant

- Measure $\sum_{\{s\}} \to \int_{S^{N-1}} d\vec{s}_i = \int_{|\vec{s}|=1} d^N s_k \to \int_{|\vec{s}'|=1} d^N s'_k = |\det M| \int_{|\vec{s}|=1} d^N s_k \Rightarrow$ invariant

Global O(N) symmetry if $h = 0$

Phase Transition examples: (see Hohenberg, Halperin Rev. Mod. Phys 49, 435 (1977))

- $d=1$ Ising-Model : No phase transition
- $d=2$ Ising: 2nd-order PT @ $\beta_c = \frac{1}{2}\log(1+\sqrt{2})$
  magnetization breaks discrete $\mathbb{Z}(2)$ symmetry
- $d=2$ $O(N)$ model with $N \geq 2$. Not a genuine phase transition due to Mermin-Wagner-Coleman theorem which prohibits breaking of continuous symmetries in $d=2$
  But in XY model there is the Kosterlitz-Thouless transition. (2016 Nobel)
- $d=3$ $O(N)$ second order phase transition



- $d=2$ Potts : 2nd order for $q \leq 4$
  1st order for $q \geq 5$

  $d=3$ 2nd order for $q=2$

- $d \geq 4$ $O(N)$ 2nd order PT with critical exponents correctly given by the mean-field approximation

$\Rightarrow$ MEAN-FIELD approximation in the TUTORIAL

Form of the partition function : Normalization of the density matrix of states!

Need density matrix that fulfills principle of maximum entropy under two constraints:

$$\sum_i \rho_i = 1 \quad \text{(probabilities add up to 1)}$$

$$\langle E \rangle = \sum_i \rho_i E_i \equiv U \quad \text{fixed}$$

$$\mathcal{L} = \left(-k_B \sum_i \rho_i \log(\rho_i)\right) + \lambda_i \left(\sum_i \rho_i - 1\right) + \lambda_2 \left(\sum_i \rho_i E_i - U\right)$$

① $$0 = \frac{\partial \mathcal{L}}{\partial \rho_i} = -k_B \log(\rho_i) - k_B + \lambda_i + \lambda_2 E_i$$

$$\Rightarrow \rho_i = \exp\left(\frac{-k_B + \lambda_1 + \lambda_2 E_i}{k_B}\right)$$

② ① $\rightarrow \sum_i \rho_i = 1 \Rightarrow 1 = \exp\left(\frac{-k_B + \lambda_1}{k_B}\right) Z$ with $Z = \sum_i \exp\left(\frac{\lambda_2}{k_B} E_i\right)$

$$\Rightarrow \rho_i = \frac{1}{Z} \exp\left(\frac{\lambda_2}{k_B} E_i\right)$$

③ $S = -k_B \sum_i \rho_i \log \rho_i = -\lambda_2 U + k_B \log(Z)$ $\quad \frac{\partial S}{\partial U} = -\lambda_2 = \frac{1}{T}$

$\Rightarrow Z = \sum_i e^{-\beta E_i}$ with $\beta = \frac{1}{k_B T}$ $\Rightarrow \rho_i = \frac{e^{-\beta E_i}}{Z}$