Approximation theory

* mean-field theory in more detail ⇒ also more general

Convexity inequality

- consider two different density operators

$$D, D_\lambda \Rightarrow D = \frac{e^{-\beta H}}{Z}, \quad D_\lambda = \frac{e^{-\beta H_\lambda}}{Z_\lambda}$$

→ H → Hamiltonian of the system we wish to study, but whose solution is difficult or unknown

→ H_λ → Hamiltonian of an [trial Hamiltonian] auxiliary system → depends on some parameters λ → H_λ is easy (or at least easier than H) to solve

use inequality: $-\mathrm{Tr} D_\lambda \ln D_\lambda \leq -\mathrm{Tr} D_\lambda \ln D$

$$\Downarrow$$

$$-\mathrm{Tr} D_\lambda [-\beta H_\lambda - \ln Z_\lambda] \leq -\mathrm{Tr} D_\lambda [-\beta H - \ln Z]$$

$$\beta \mathrm{Tr} D_\lambda H_\lambda + \ln Z_\lambda \leq \beta \mathrm{Tr} D_\lambda H + \ln Z$$

$$\beta \langle H_\lambda \rangle_\lambda + \ln Z_\lambda \leq \beta \langle H \rangle_\lambda + \ln Z$$

$$\Downarrow$$

$$\boxed{F \leq F_\lambda + \langle H \rangle_\lambda - \langle H_\lambda \rangle_\lambda}$$

$$\Rightarrow \quad F \leq F_\lambda + \langle H \rangle_\lambda - \langle H_\lambda \rangle_\lambda$$

F_λ - free energy of the system described by H_λ

($F_\lambda = -kT \ln Z_\lambda \qquad Z_\lambda = Tr\, e^{-\beta H_\lambda}$)

$\langle H \rangle_\lambda$ - expectation value of the Hamiltonian H over the density matrix $D_\lambda = \dfrac{e^{-\beta H_\lambda}}{Z_\lambda}$

$\langle H_\lambda \rangle_\lambda$ - expectation value of the Hamiltonian H_λ over the density matrix $D_\lambda = \dfrac{e^{-\beta H_\lambda}}{Z_\lambda}$

if H is not easily solvable, but H_λ is

$\Rightarrow$ F we do not know

F_λ, $\langle H \rangle_\lambda$, $\langle H_\lambda \rangle_\lambda$ $\rightarrow$ we can calculate as a function of the parameters λ

$$F \leq \Phi(\lambda) = F_\lambda + \langle H \rangle_\lambda + \langle H_\lambda \rangle_\lambda$$

- we can get an estimate of F by minimizing $\Phi(\lambda)$ in the parameters λ

$$\Rightarrow \quad \frac{\partial \Phi(\lambda)}{\partial \lambda} = 0$$

→ let us use the convexity inequality to derive the mean-field approximation for the Ising model

Ising model:

$$H = -\frac{1}{2}\sum_{ij} J S_i S_j - \mu \sum_i B_i S_i$$

B_i → site-dependent field

auxiliary Hamiltonian: $H_\lambda = -\mu \sum_i \lambda_i S_i$

$$F \leq F_\lambda + \langle H \rangle_\lambda - \langle H_\lambda \rangle_\lambda = \Phi(\lambda)$$

→ evaluate $\Phi(\lambda)$ and minimize

$$F_\lambda = -\frac{1}{\beta}\ln Z_\lambda \qquad Z_\lambda = \sum_{S_1}\dots\sum_{S_N} e^{\beta\mu\sum_i \lambda_i S_i}$$

$$Z_\lambda = \prod_{i=1}^{N}\left[2\cosh\beta\mu\lambda_i\right]$$

$$* \quad F_\lambda = -\frac{1}{\beta}\sum_i \ln 2\cosh\beta\mu\lambda_i$$

magnetization at a particular site i:

$$M_i = -\frac{1}{\mu}\frac{\partial F_\lambda}{\partial \lambda_i} = \tanh(\beta\mu\lambda_i) = \langle S_i \rangle$$

$$\langle H_\lambda \rangle_\lambda = -\mu\sum_i B_i \langle S_i \rangle_\lambda = -\mu\sum_i B_i M_i = -\mu\sum_i B_i \tanh(\beta\mu\lambda_i)$$

$$\langle H \rangle_\lambda = -\frac{1}{2}\sum_{ij} J_{ij}\langle S_i S_j \rangle_\lambda - \mu\sum_i B_i \langle S_i \rangle_\lambda$$

$$\langle S_i S_j \rangle_\lambda = \langle S_i \rangle_\lambda \langle S_j \rangle_\lambda = M_i M_j$$

⇓

this follows from the fact that H_λ is a non-interacting Hamiltonian

- now we can put $\Phi(\lambda)$ together

$$F \leq \Phi(\lambda) = -\frac{1}{\beta} \sum_i \ln 2\cosh[\beta\mu\lambda_i] - \frac{1}{2}\sum_{ij} J_{ij} M_i M_j - \mu \sum_i B_i M_i$$
$$+ \mu \sum_i \lambda_i M_i$$

- need to minimize in λ_i → but since

$M_i = \tanh(\beta\mu\lambda_i)$ (M_i is a monotonically increasing function of λ_i)

we can also minimize in λ_i ⇒ it is easier

$$\frac{\partial \Phi}{\partial M_i}(M_1 \ldots M_N) = -\frac{1}{\beta} \tanh(\beta\mu\lambda_i)\beta\mu \frac{\partial \lambda_i}{\partial M_i}$$
$$- \sum_j J_{ij} M_j - \mu B_i + \mu\left(\lambda_i + M_i \frac{\partial \lambda_i}{\partial M_i}\right) = 0$$

since $M_i = \tanh(\beta\mu\lambda_i)$

$$\Rightarrow \boxed{-\sum_j J_{ij} M_j - \mu B_i + \mu\lambda_i = 0} \Rightarrow \text{mean-field equations}$$

$$\Leftrightarrow \boxed{\frac{1}{\beta}\tanh^{-1}(M_i) = \sum_j J_{ij} M_j + \mu B_i}$$

→ can also derive an expression for the correlation function

→ differentiate with respect to B_k

$$\frac{1}{\beta}\frac{\partial \tanh^{-1}(M_i)}{\partial B_k} = \sum_j J_{ij}\frac{\partial M_j}{\partial B_k} + \mu\frac{\partial B_i}{\partial B_k}$$

$y = \tanh x \Rightarrow x = \tanh^{-1} y$

$\frac{dy}{dx} = (\cancel{1+\tanh^2 x})\,(1-\tanh^2 x) = (1-y^2)$

$\frac{dx}{dy} = \frac{1}{1-y^2}$ (since $\tanh x$ is monotonically increasing)

y

$$\frac{1}{\beta}\left(\frac{1}{1-M_i^2}\right)\frac{\partial M_i}{\partial B_k} = \sum_j J_{ij}\frac{\partial M_j}{\partial B_k} + \mu\delta_{ik}$$

Since $\frac{\partial M_i}{\partial B_k} = \mu\beta G_{ik}$

$$\Rightarrow \quad \frac{1}{1-M_i^2}G_{ik} = \sum_j J_{ij}G_{jk} + \delta_{ik}$$

→ apply Fourier transform to both sides

→ $\sum_j J_{ij}G_{jk}$ → convolution, its Fourier transform is a product of Fourier transforms → of J_{ij} and G_{ij}

→ also assume that $B_i \to B$ & $M_i \to M$

→ Fourier transform:

$$\frac{1}{1-M^2}\tilde{G}(q) = \tilde{J}(q)\,\tilde{G}(q) + 1$$

what is $\tilde{J}(q)$? ⑥

$J_{ij} \rightarrow \quad J(\vec{r}_i, \vec{r}_0) \rightarrow$ matrix b/w $\vec{r}_i, \vec{r}_j$

$$\int d(\vec{r}_i - \vec{r}_j)\, e^{i\vec{q}\cdot(\vec{r}_i - \vec{r}_j)}\, J(\vec{r}_i, \vec{r}_j)$$

for a model with nearest neighbors only

$J(\vec{r}_i, \vec{r}_j) \rightarrow J$ if $\vec{r}_i$ and $\vec{r}_j$ are nearest neighbors

$$\Downarrow$$

$$J\left[e^{iq_x a} + e^{-iq_x a} + e^{iq_y a} + e^{-iq_y a}\right]$$

$$= 2J\left[\cos q_x a + \cos q_y a\right] \qquad (a \rightarrow \text{lattice constant})$$

$q_x, q_y, q_z \rightarrow$ components of wave-vector $\vec{q}$

$$\Downarrow \qquad \Downarrow \qquad \Downarrow \qquad \Downarrow$$

$$\tilde{G}(\vec{q}) = \frac{1 - M^2}{1 - 2\beta J(1 - M^2) \sum_{\mu = x,y,z} \cos q_\mu} \qquad (\text{in } 3D)$$

long wavelength limit

$$\cos q_x + \cos q_y + \cos q_z = \left(1 - \frac{q_x^2}{2}\right) + \left(1 - \frac{q_y^2}{2}\right) + \left(1 - \frac{q_z^2}{2}\right) + \dots$$

$$= 3 - \frac{\vec{q}^2}{2}$$

more generally: $\sum_\mu \cos q_\mu = D - \frac{q^2}{2}$

$$\Rightarrow \tilde{G}(\vec{q}) \sim \frac{1-M^2}{1-2D\beta J(1-M^2)+\beta J(1-M^2)q^2}$$

if $T > T_c \Rightarrow M = 0$

$$\tilde{G}(\vec{q}) \sim \frac{\cancel{1-M^2}\ 1}{1-2D\beta J+\beta J q^2}$$

$$= \frac{1}{1+\beta J(q^2-2D)}$$

$$= \frac{1}{1-2DJ\beta+\beta J q^2}$$

Broken symmetry

uniform magnetic field B

$$\frac{1}{\beta}\tanh^{-1}(M_i) = \sum_j J_{ij} M_j + \mu B_i$$

$$B_i \rightarrow B$$

$$\frac{1}{\beta}\tanh(M) = 2DJM + \mu B$$

consider function $\frac{1}{\beta}\tanh^{-1}(M) - 2DJM =$

$$= \frac{g(M)}{\beta}$$

as $M \rightarrow 0$

$$\cancel{\frac{1}{\beta}}\tanh^{-1}(M) - 2DJ\beta M \rightarrow (1-2DJ\beta)M$$

$\Rightarrow$ $g'(M) > 0$ if $(1-2DJ\beta) > 0$

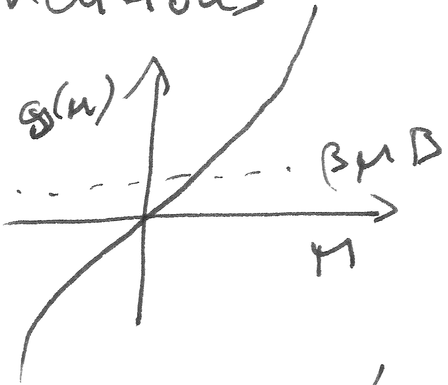
$g'(M) < 0$ if $(1-2DJ\beta) < 0$

remember that $1-2J\beta_c = 0 \Rightarrow$ definition of T_c

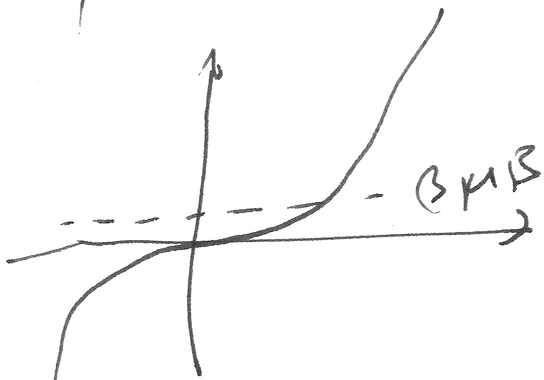
8

g(M) is an odd function of M
- under these conditions ~~(B=0)~~

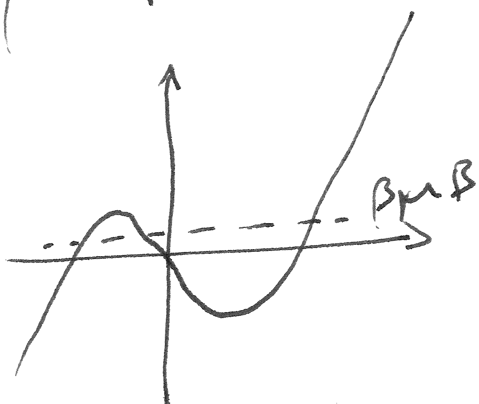
$1-2DJ\beta > 0 \rightarrow$



$1-2DJ\beta = 0 \rightarrow$



$1-2DJ\beta < 0$



1st case: $g(M) = \beta\mu B$ can have only one solution

2nd case $g(M) = \beta\mu B$ can have only one solution

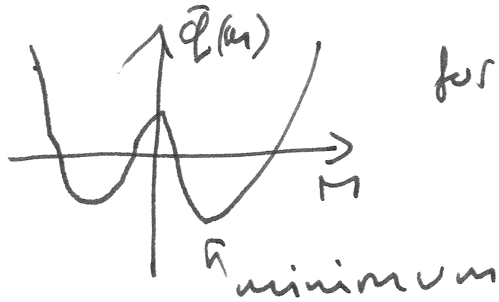
3rd case $g(M) = \beta\mu B$ can have three solutions

$\Rightarrow$ in this case free energy will be a minimum at 2, maximum at 1

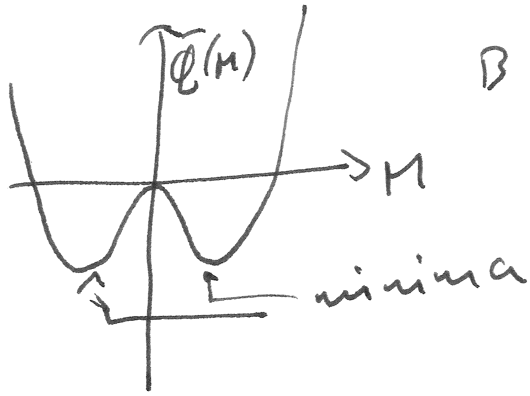
free energy is given by $\Rightarrow$ $F_\lambda + \langle H \rangle_\lambda - \langle H_\lambda \rangle_\lambda$

free energy → can be calculated explicitly as a function of M for finite B

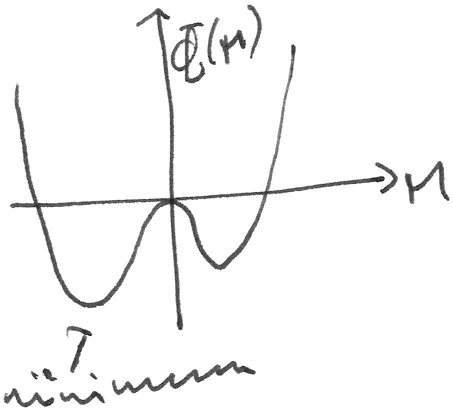
$T < T_c$ for $B > 0$



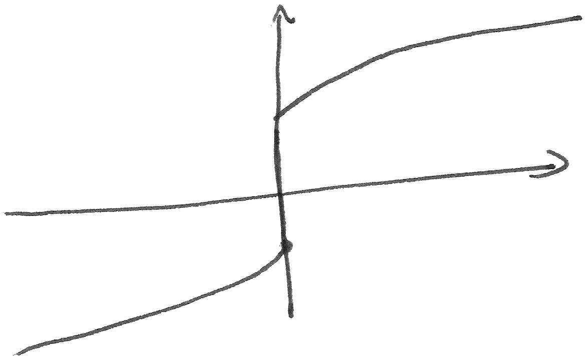
$T < T_c$ $B = 0$



$T < T_c$ $B < 0$



⇒ magnetization as a function of B



⇒ phenomenon of symmetry breaking is thus ~~obtained~~ reproduced from mean-field theory can also obtain critical exponents from mean-field theory ($T_c = \frac{2DJ}{k}$)

→ use $\tanh^{-1}(M) = M + \frac{M^3}{3}$

$\Rightarrow \quad M + \frac{M^3}{3} = \mu B \beta + 2DJ\beta M$

at $T_c \Rightarrow 2DJ\beta = 1$

$\Rightarrow \quad \frac{M^3}{3} \sim \mu B \beta \Rightarrow M \sim B^{1/\delta}$ at T_c

$\boxed{\delta = 3}$

$\Rightarrow \quad (1 - 2DJ\beta) M \sim -\frac{M^3}{3}$

$(1 - \frac{T_c}{T}) M \sim -\frac{M^3}{3}$

$\left[\frac{T - T_c}{T}\right] \cancel{M} \sim -\frac{M^2}{3}$

$\frac{T_c - T}{T} \sim -M^2 \Rightarrow M \sim |T - T_c|^{\beta}$

$\boxed{\beta = 1/2}$

$\Rightarrow \quad (1 - \frac{T_c}{T}) M \sim \frac{\mu B}{kT}$

$M = \frac{\mu B}{T - T_c} \Rightarrow M = \chi B$

$\chi \sim (T - T_c)^{-\gamma}$

$\boxed{\gamma = 1}$

$\Rightarrow \quad C \sim (T - T_c)^{-\alpha} \qquad B = 0$

$E = -\frac{1}{2} K J N M_0^2 = \frac{3}{2} k N (T - T_c) \Rightarrow \boxed{\alpha = 0}$

can also determine ν, η from

$$\tilde{G}(q) = \frac{1}{1 - 2DJ\beta + \beta J q^2} = \frac{1}{q^2\left[\beta J + \frac{1-2DJ\beta}{q^2}\right]}$$

recall that $\tilde{G}(q) = \frac{f(q\xi)}{q^{2-\eta}}$

$$\Rightarrow \boxed{\eta = 0} \qquad f(q\xi) = \frac{1}{\beta J + \left(\frac{1-2DJ\beta}{q^2}\right)}$$

$$\Downarrow$$

$$q^2\xi^2 = \frac{q^2}{(1-2DJ\beta)} = \frac{q^2}{\left(1-\frac{T_c}{T}\right)} = \frac{q^2}{\left(\frac{T-T_c}{T}\right)}$$

$$\xi^2 \sim \frac{1}{|T-T_c|} \Rightarrow \xi \sim (T-T_c)^{-1/2}$$

$$\boxed{\nu = 1/2}$$

SUMMARY OF MEAN-FIELD THEORY:

* independent of dimension D → this is wrong for 1D (no transition for Ising-model), but gets better for large D
* reproduces symmetry breaking
* produces critical exponents which are not in agreement with experiment
* one must know the nature of the ordered phase before applying MFT