# Mean field solutions to Ising model

## 1 Bragg – Willams approximation

$$H = -J\sum_{\langle ij\rangle}\sigma_i\sigma_j - h\sum_i \sigma_i, \text{ and } Z=\sum_{\{\sigma_i\}} e^{-\beta H} .$$

mean field method: find a single site problem within a molecular field + external field. Molecular field is an averaged effect from inter site interactio[n]

define $\langle\sigma_i\rangle = M$, $\Rightarrow$ For site $i$, $H_i = -(zJM+h)\,\sigma_i = -(h+h_{mol})\,\sigma_i$.

$z$ coordination number

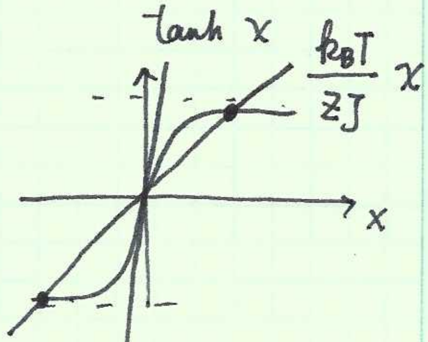
Then
$$\langle\sigma_i\rangle = \frac{e^{(h+h_{mol})\beta} - e^{-(h+h_{mol})\beta}}{e^{(h+h_{mol})\beta} + e^{-(h+h_{mol})\beta}} = \tanh\left(\frac{h+h_{mol}}{k_BT}\right).$$

we need Self-consistency:

$$h_{mol} = zJ\langle\sigma\rangle \Rightarrow \boxed{\tanh\left(\beta(h+h_{mol})\right) = \frac{h_{mol}}{zJ}} .$$

Define $x = \beta(h_{mol}+h)$, then the self-consistent Eq becomes

$$\tanh x = \frac{k_BT}{zJ}x - \frac{h}{zJ} .$$




1 at $h=0$, at

$\frac{k_BT}{zJ} < 1$, we have nonzero solution

and thus mean field $k_BT_c = zJ$. For square lattice

$$\boxed{\frac{k_BT_c}{J} = 4} \leftarrow \text{BW.}$$

② as $T \to T_c + 0^-$: the relation of $M \sim T$.

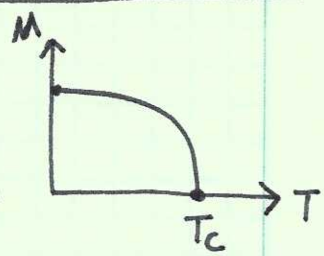
exercise
$M \simeq 1 - 2e^{-2T_c/T}$
at $T \to 0$

$$\tanh x \simeq \frac{x + x^3/6}{1 + x^2/2} = x - \frac{x^3}{3}. \Rightarrow x - \frac{x^3}{3} = \frac{T}{T_c} x$$

$$\Rightarrow \quad x = \sqrt{3}\left(1 - \frac{T}{T_c}\right)^{1/2}. \quad \leftarrow \quad M = \frac{k_B T}{zJ} x$$

$$\Rightarrow \quad \boxed{M \sim \left(1 - \frac{T}{T_c}\right)^{\beta}},$$

$\beta = 1/2$ for BW
$= 1/8$ exact: onsager, C.N. Yang




③ magnetic susceptibility at $T \to T_c + 0^+$

$$\tanh x = \frac{k_B T}{zJ} x - \frac{h}{zJ} = x + \frac{x k_B (T - T_c) - h}{zJ} \simeq x$$

$$\Rightarrow \quad x \simeq \frac{h}{k_B (T - T_c)} \quad \leftarrow \quad M = \frac{1}{zJ}\left[k_B T x - h\right]$$

$$M \simeq \frac{k_B T}{k_B (T - T_c)} \frac{x}{zJ} + \dots \Rightarrow \quad \chi_{sus} \sim \frac{1}{zJ\left(1 - \frac{T_c}{T}\right)}$$

c.f. $\boxed{\chi \sim \frac{1}{(T - T_c)^{\gamma}}}$

$\gamma = 1$ at mean field
$7/4$ exact solution

④ $M \sim h$ realation at $T = T_c$.

$$\tanh x = x - \frac{x^3}{3} = x - \frac{h}{zJ} \quad \Rightarrow \quad x = \left(\frac{3h}{zJ}\right)^{1/3}$$

$$M = \frac{1}{zJ}\left[k_B T x - h\right] \underset{T = T_c}{\simeq} \frac{k_B T_c}{(zJ)^{4/3}} 3^{1/3} h^{1/3} + \dots$$

c.f. $M \sim h^{1/\delta}$. $\delta = 3$ at B-W
$= 15$ : (exact)

⑤ specific heat

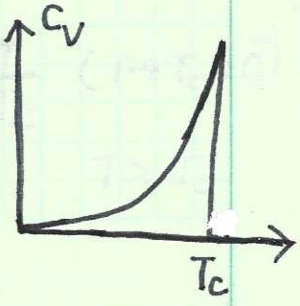
$U = \frac{N}{2} z \sum_i \langle \ H_i \rangle$ at mean field level. ($\frac{1}{2}$-factor is to reduce the double counting).

$$\frac{U}{N} = -\frac{zJ}{2} \langle \sigma \rangle^2 = -\frac{zJ}{2} \left(\frac{k_B T}{zJ}\right)^2 \chi^2(T)$$

at $T < T_c$, $\chi^2 \simeq 3\left(1 - \frac{T}{T_c}\right)$, thus

$$\Rightarrow \qquad \frac{U}{N} = -\frac{3 k_B T^2}{2 \, T_c} \left(1 - \frac{T}{T_c}\right) \Rightarrow$$

$$\frac{C_V}{N} = -3 k_B \frac{T}{T_c} + \frac{9}{2} k_B \frac{T^2}{T_c} \simeq \frac{3}{2} k_B + 6 k_B \frac{T - T_c}{T_c}$$




specific heat is discontinous at $T_c$.

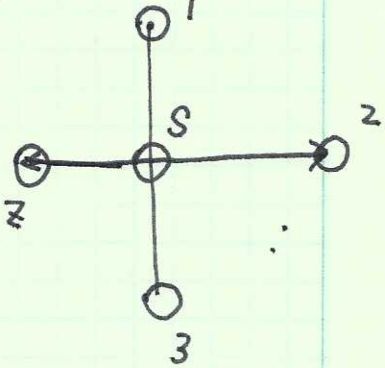
Exact results is logrithimic divergence.

(at $T > T_c$, BW method gives rise to $C_V = 0$. This is certainly unreasonable because it completely neglect the correlation even between neighboring sites)!

how to improve?

② Bethe-approximation (cluster method) ← input correlation

we only consider a site with all its nearest neighbors, (the coordination number is $z$).




$P(+1, n)$: probility of the central site is spin up, and there're $n$ site spin up and $z - n$ spin down among its neighbors.

$P(-1, n)$ : probility of the central site spin down, and its neighbors: $n$ sites spin up and $z - n$ spin down.

$$\begin{cases} P(+1, n) = \frac{1}{q}\binom{z}{n} e^{\beta J(2n-z)} \cdot g^n \\ P(-1, n) = \frac{1}{q}\binom{z}{n} e^{\beta J(z-2n)} \cdot g^n \end{cases}$$

① $g$: represents the effect from the background of other lattice sites. If in the disordered states, the background has no preference of spin ↑ and ↓, and thus $g = 1$. But in the ordered state, there's a preference, and thus $g \neq 1$. $g$ is similar to fugacity, and this is called quasi-chemical method.

② $q$ is for normalization.

$$\sum_{S, n=1}^{z} P(S, n) = 1 \Rightarrow q = \sum_{n=0}^{z} \binom{z}{n}\left[\left(g e^{2\beta J}\right)^n e^{-\beta J z} + \left(g e^{-2\beta J}\right)^n e^{\beta J z}\right]$$

$$= \left(e^{\beta J} + g e^{-\beta J}\right)^z + \left(g e^{\beta J} + e^{-\beta J}\right)^z$$

⇒ Probability of finding an up spin at the center : $\sum_{n=0}^{z} P(1, n)$.

equal

Probability of finding an up spin in the neighbors $\frac{1}{z}\sum_{n=0}^{z} n\left(P(1,n) + P(-1,n)\right)$

$$\Rightarrow \sum_{n=0}^{z} P(+1, n) = \frac{1}{z}\sum_{n=0}^{z} n\left(P(+1,n) + P(-1,n)\right)$$

$$\left(e^{-\beta J} + g e^{\beta J}\right)^z = \frac{1}{z} g \frac{\partial}{\partial g}\left[\left(e^{-\beta J} + g e^{\beta J}\right)^z + \left(e^{\beta J} + g e^{-\beta J}\right)^z\right]$$

$$= g\left[\left(e^{-\beta J} + g e^{\beta J}\right)^{z-1} e^{\beta J} + \left(e^{\beta J} + g e^{-\beta J}\right)^{z-1} e^{-\beta J}\right]$$

$$e^{-\beta J} + \cancel{g e^{\beta J}} = \cancel{g e^{\beta J}} + g\left(\frac{e^{\beta J} + g e^{-\beta J}}{e^{-\beta J} + g e^{\beta J}}\right)^{z-1} e^{-\beta J}$$

$$\Rightarrow \boxed{g = \left(\frac{1 + g e^{2\beta J}}{g + e^{2\beta J}}\right)^{z-1}}$$

if $g$ is a solution the $1/g$ is also a solution

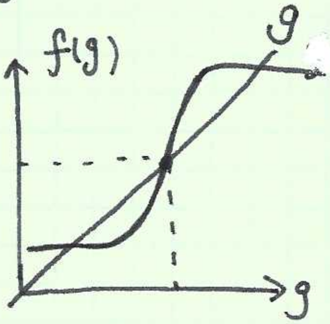
The magnetization $M = \frac{N_\uparrow - N_\downarrow}{N} = \sum_{n=0}^{\gamma} P(1,n) - P(-1,n)$

$$= \frac{(e^{-\beta J} + g e^{\beta J})^z - (e^{\beta J} + g e^{-\beta J})^z}{(e^{-\beta J} + g e^{\beta J})^z + (e^{\beta J} + g e^{-\beta J})^z} = \frac{\left(\frac{e^{-\beta J} + g e^{\beta J}}{e^{\beta J} + g e^{-\beta J}}\right)^z - 1}{\left(\frac{e^{-\beta J} + g e^{\beta J}}{e^{\beta J} + g e^{-\beta J}}\right)^z + 1}$$

$$= \frac{g^y - 1}{g^y + 1} \quad \text{where } y = \frac{z}{z-1}.$$

Thus $g \neq 1$ represents spontaneous magnetization. Replacing $g$ with $g^{-1}$ changes the sign of $M$. The solution of $g$ can be obtained graphically

$$f(g) = \left(\frac{1 + g e^{2\beta J}}{g + e^{2\beta J}}\right)^{z-1}$$




① $g=1$ is always a solution but a trivial one.

② slope of $f(g)$ at $g=1$: $c = (z-1)\left(\frac{1+ge^{2\beta J}}{g+e^{2\beta J}}\right)^{z-2} \left[\frac{e^{2\beta J}}{g+e^{2\beta J}}\Big|_{g=1} - \frac{1+ge^{2\beta J}}{(g+e^{2\beta J})^2}\Big|_{g=1}\right]$

The $T_c$ is determined by

$C = 1$

$$= \frac{(z-1)(e^{4\beta J} - 1)}{(1 + e^{2\beta J})^2} = (z-1)\frac{e^{2\beta J} - 1}{e^{2\beta J} + 1}$$

$\Rightarrow$

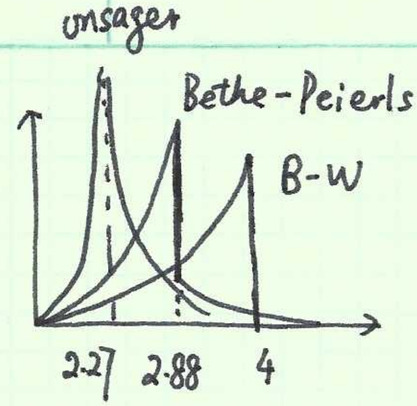
$$\frac{e^{2\beta J} - 1}{e^{2\beta J} + 1} = \frac{1}{z-1} \Rightarrow \boxed{e^{2\beta J} = \frac{z}{z-2} \text{ and } kT_c = \frac{2J}{\ln[z/(z-2)]}}.$$

for 2D square lattice $kT_c = \frac{2J}{\ln 2} \approx 2.88J = \frac{J}{\ln\sqrt{2}}$

Exact onsager: $kT_c = \frac{J}{\ln(\sqrt{2}-1)^{-1}} = \frac{J}{\ln(\sqrt{2}+1)} \simeq 2.27J$

BW $\quad kT_c = 4J$.

we can also work out specific heat




$$\frac{C(T>T_c)}{N} = \frac{2ZJ^2}{(kT)^2} \frac{e^{\beta 2J}}{(1+e^{2\beta J})^2}$$

no-longer zero.

onsager

$$C(T\sim T_c) \approx \frac{2}{\pi}\left(\frac{2J}{k_B T_c}\right)^2 \ln \frac{1}{|1-T/T_c|}$$

Summary of 2D Ising model results (square lattice)

① free energy per site

$$f(T,0) = \frac{F(T,0)}{N} = \frac{1}{\beta}\left[\frac{1}{2}\ln(2\sinh 2\beta J) + \frac{1}{2\pi}\int_0^{\pi}\gamma(\omega)\,d\omega\right]$$

$$\cosh\gamma(\omega) = \cosh 2\phi\cos 2\theta - \cos\omega\sinh 2\phi\sinh 2\theta$$

$$\phi = \beta J, \qquad \theta = \tanh^{-1} e^{-2\beta J}$$

② internal energy

$$u(T,0) = -J\coth 2\beta J\left[1 + \frac{2}{\pi} m' K_1(m)\right]$$

where $K_1(m) = \int_0^{\pi/2}\frac{d\phi}{\sqrt{1-m^2\sin^2\phi}}$, $\quad m' = 2\tanh^2 2\beta J - 1$

$$m = \frac{2\sinh 2\beta J}{\cosh^2 2\beta J}$$

$k_B T_c$ is determined by $m = 1$

i.e. $\left.\begin{array}{l} e^{-J\beta_c} = \sqrt{2}-1, \\ \text{or } \sinh 2\beta J = 1 \end{array}\right\} \Rightarrow k_B T_c = 2.27J.$

③ $$\frac{1}{Nk_B}C(T,0) \simeq -0.495\ln\left|1-\frac{T}{T_c}\right| + \text{const}$$

④ $$\frac{M(T,0)}{N} = \begin{cases} 0 & T > T_c \\ \left[1-(\sinh 2\beta J)^{-4}\right]^{1/8} & T \le T_c \sim 1.224\left(1-\frac{T}{T_c}\right)^{1/8} \end{cases}$$