{Lecture 1}

Curie - Weiss model of ferromagnetism

N spins $S_i = \{-1, +1\}$.

Hamiltonian:
$$H_N^{\circ}(\vec{S}) = -\frac{1}{2N} \sum_{\substack{i,j \\ i \neq j}} S_i S_j$$
$\vec{S} = \{S_1, \dots, S_N\}$

With external magnetic field h:

$$H_N(\vec{S}) = H_N^{\circ}(\vec{S}) - h \sum_{i=1}^{N} S_i$$

$$P(\vec{S} \mid N, \beta, h) = \frac{e^{-\beta H_N(\vec{S})}}{Z_N(\beta, h)}$$

$\beta = T^{-1}$ $(k_B = 1)$ = inverse temperature

Partition function: $Z_N(\beta, h) = \underbrace{\sum_{\vec{S}}}_{2^N \text{ terms}} e^{-\beta H_N(\vec{S})}$

Introduce magnetization per spin:

$$\underbrace{m}_{\text{r.v.}} = \frac{1}{N} \sum_{i=1}^{N} S_i$$

$$H_N(m) = -N \left[\frac{1}{2} \underbrace{m^2}_{\sum_{i,j} S_i S_j} + h m \right]$$

$\underline{H_N(m) \sim N}$

$\sum_{i,j} S_i S_j$, self-interactions $(i=j)$ included $\Rightarrow$ negligible in the $N \gg 1$ limit

$$m = \left\{-1, -1+\frac{2}{N}, \ldots, 1\right\} \qquad N+1 \text{ terms}$$

Next, consider

$$P(m) = \frac{\Omega(m,N)}{Z_N(\beta,h)} e^{\beta N\left(\frac{m^2}{2}+hm\right)}, \quad \text{where}$$

$\Omega(m,N)$ = # configurations with magnetization m.

$$\text{Consider } \begin{cases} N_+ = \#+1 \text{ spins}, \\ N_- = \#-1 \text{ spins}. \end{cases}$$

$$\begin{cases} N_+ + N_- = N, \\ N_+ - N_- = mN \end{cases} \Rightarrow \begin{cases} N_+ = \frac{N(m+1)}{2}, \\ N_- = \frac{N(1-m)}{2}. \end{cases}$$

$$\text{Thus,} \quad \Omega(m,N) = \frac{N!}{N_+!\,N_-!} = \frac{N!}{\left(\frac{N-Nm}{2}\right)!\left(\frac{N+Nm}{2}\right)!}$$

$$\text{Note that} \quad \sum_{i=0}^{\overset{\#\text{trials}}{n}} \binom{n}{i} p^i (1-p)^{n-i} = 1,$$

$$i=k,\ p=\frac{k}{n}: \quad \binom{n}{k}\left(\frac{k}{n}\right)^k \left(1-\frac{k}{n}\right)^{n-k} < 1, \text{ or}$$

$$H(p) = -p\log p - (1-p)\log(1-p) \qquad \text{entropy}$$

$$e^{nH\left(\frac{k}{n}\right)} = e^{-n\left[\frac{k}{n}\log\frac{k}{n} + \left(1-\frac{k}{n}\right)\log\left(1-\frac{k}{n}\right)\right]} =$$

$$= e^{-\log\left(\frac{k}{n}\right)^k} e^{-\log\left(1-\frac{k}{n}\right)^{n-k}} = \left(\frac{k}{n}\right)^{-k}\left(1-\frac{k}{n}\right)^{k-n}.$$

Then $\binom{n}{k} e^{-nH(\frac{k}{n})} < 1$, or

$$e^{nH(\frac{k}{n})} > \binom{n}{k}.$$

If $p = \frac{k}{n}$, the expected value of 'positive' outcomes is $\frac{k}{n} n = k$ in n trials.

Thus, $\binom{n}{k} p^k (1-p)^{n-k}$ is the largest term in the binomial sum:

$$(n+1)\binom{n}{k} \underbrace{p^k (1-p)^{n-k}}_{e^{-nH(\frac{k}{n})}} > 1 \text{, or}$$

$$e^{nH(\frac{k}{n})} < (n+1)\binom{n}{k}.$$

Finally, $\underline{\frac{e^{nH(\frac{k}{n})}}{n+1} < \binom{n}{k} < e^{nH(\frac{k}{n})}}$.

Now, use $p = \frac{m+1}{2}$:

$$H(p) \to H(m) = -\frac{m+1}{2} \log \frac{m+1}{2} - \frac{1-m}{2} \log\left(\frac{1-m}{2}\right).$$

$$1-p = \frac{1-m}{2}$$

$$\frac{n!}{k!(n-k)!} \Rightarrow \frac{N!}{N_+!(N-N_+)!} \text{, yielding}$$

$(n \to N)$ here $\quad k = \frac{N(m+1)}{2}, \quad p = \frac{k}{N} = \frac{m+1}{2}.$

So, $\frac{e^{NH(m)}}{N+1} \leq \Omega(m,N) \leq e^{NH(m)}$.

Next,

$$\frac{e^{NH(m)+\beta N(\frac{m^2}{2}+hm)}}{(N+1)\, Z_N(\beta,h)} \leq P(m) \leq \frac{e^{NH(m)+\beta N(\frac{m^2}{2}+hm)}}{Z_N(\beta,h)}$$

Define $\varphi(m) = H(m) + \frac{\beta m^2}{2} + \beta h m$:

$$\underbrace{\frac{1}{N+1}\frac{e^{N\varphi(m)}}{Z_N} \leq P(m) \leq \frac{e^{N\varphi(m)}}{Z_N}}_{\text{sum over } m}.$$

$$(*) \qquad \sum_m P(m) = 1 \leq \sum_m \frac{e^{N\varphi(m)}}{Z_N} \leq (N+1)\frac{e^{N\varphi(m^*)}}{Z_N},$$

where $m^* \in [-1,1]$ maximizes $\varphi(m)$.
$\quad\quad\;$ " $m^*(\beta,h)$

Take a log of $(*)$:

$$\log Z_N \leq \log(N+1) + N\varphi(m^*), \text{ or}$$

$$\frac{\log Z_N}{N} \leq \varphi(m^*) + \frac{\log(N+1)}{N}.$$

Additionally, $\frac{1}{N+1}\frac{e^{N\varphi(m)}}{Z_N} \leq P(m) \leq 1$, or

$$\log Z_N \geq N\varphi(m) - \log(N+1),$$

$$\frac{\log Z_N}{N} \geq \varphi(m) - \frac{\log(N+1)}{N}.$$

True for $\forall m$, including m^*

For $N \gg 1$, we obtain:

$$\varphi_N(\beta, h) \equiv \frac{\log Z_N(\beta, h)}{N}$$ free entropy density

$$\mathcal{S}(m^*) - \frac{\log(N+1)}{N} \leq \varphi_N \leq \mathcal{S}(m^*) + \frac{\log(N+1)}{N}.$$

Then $$\varphi(\beta, h) = \lim_{N\to\infty} \varphi_N(\beta, h) = \mathcal{S}(m^*).$$

We obtain: $$P(m) \leq \frac{e^{N\mathcal{S}(m)}}{Z_N},$$ or

$$\log P(m) \leq N\mathcal{S}(m) - \log Z_N,$$

(1) $$\frac{\log P(m)}{N} \leq \mathcal{S}(m) - \varphi_N$$

Likewise, $$\log P(m) \geq N\mathcal{S}(m) - \log Z_N - \log(N+1),$$

(2) $$\frac{\log P(m)}{N} \geq \mathcal{S}(m) - \varphi_N - \underbrace{\frac{\log(N+1)}{N}}_{\to 0 \text{ as } N\to\infty}$$

Thus, $$\left[\lim_{N\to\infty} \frac{\log P(m)}{N} = \mathcal{S}(m) - \mathcal{S}(m^*).\right]$$

use (1) & (2)

Note that $\mathcal{S}(m)$ fully characterizes $P(m)$.

1D potential

Recall that

$$\left[g(m) = -\frac{m+1}{2}\log\left(\frac{m+1}{2}\right) - \frac{1-m}{2}\log\left(\frac{1-m}{2}\right) + + \frac{\beta m^2}{2} + \beta h m \right].$$

Since $\varphi(\beta, h) = \underbrace{g(m^*)}_{\max\limits_{m\in[-1,1]} g(m)}$, we obtain

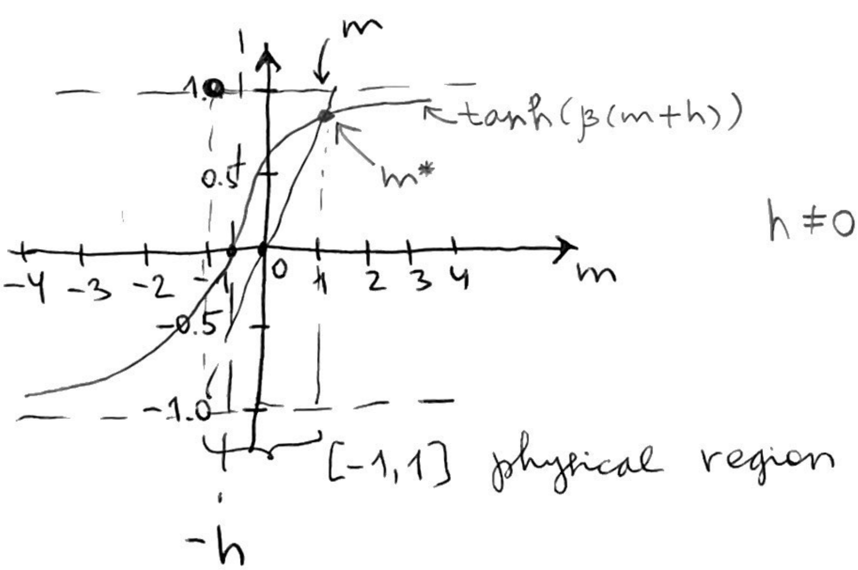
$m^* \to m$ for brevity

$$g'(m) = 0 \Rightarrow -\cancel{\frac{1}{2}} - \frac{1}{2}\log\frac{m+1}{2} + \cancel{\frac{1}{2}} + + \frac{1}{2}\log\frac{1-m}{2} + \beta m + \beta h = 0, \text{ or}$$

$$\beta(m+h) = \frac{1}{2}\log\frac{1+m}{1-m}.$$

Using $\tanh^{-1}(x) = \frac{1}{2}\log\frac{1+x}{1-x}$, we get:

$$m = \tanh[\beta(m+h)]$$



Note that $P(m) \underset{N\to\infty}{\to} e^{N(\varphi(m) - \varphi(m^*))}$.

If m^* is unique, $P(m) \underset{N\to\infty}{\to} 0$ unless $\varphi(m) = \varphi(m^*)$,

so that $\begin{cases} P(m^*) = 1, \\ P(m) = 0, & m \neq m^* \end{cases}$

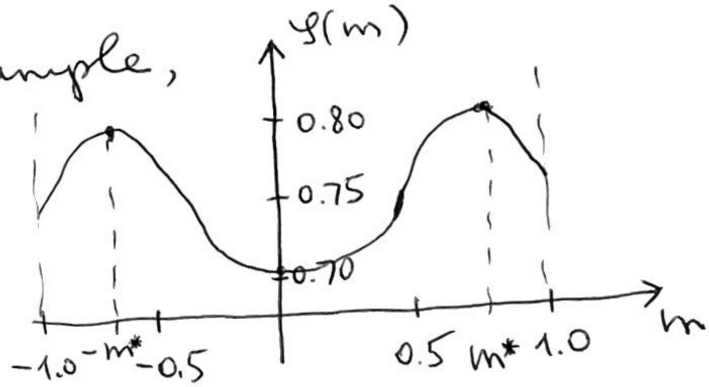
Thus, magnetization becomes deterministic in the thermodynamic limit.

However, the global max m^* is <u>not</u> always unique: consider $h=0$, s.t.

$m = \tanh(\beta m)$.

Then $m^* = 0$ is always a solution, but for $\beta > 1$ we have two more: $m = \pm m^*$ (note that $\varphi(m) = \varphi(-m)$ if $h=0$).

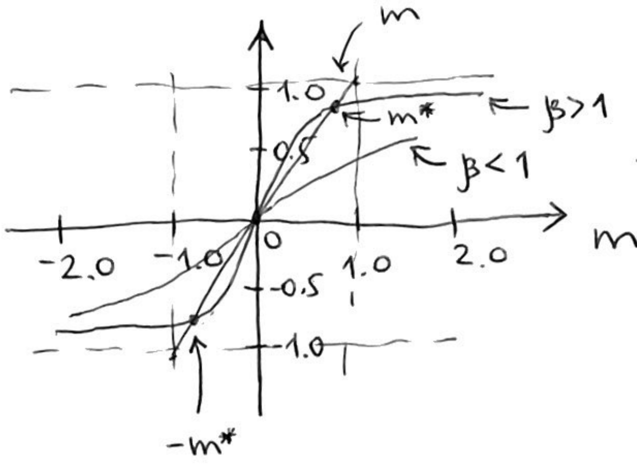
For example,

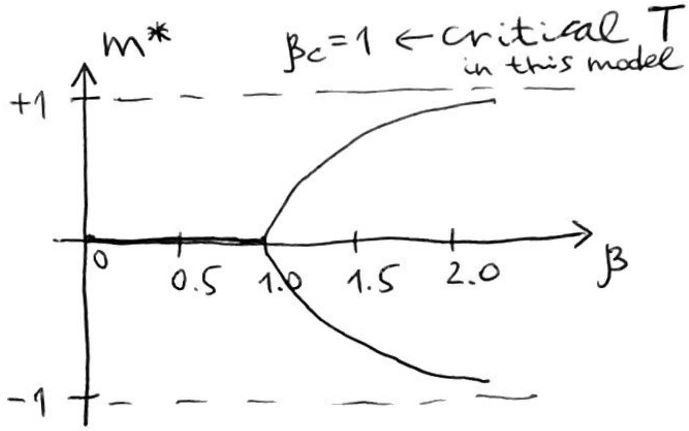


$m=0$ is actually a min, <u>not</u> a max

$\begin{cases} m = 0 \leftarrow \text{paramagnetic (disordered) phase} \\ m = \pm m^* \leftarrow \text{ferromagnetic phases} \end{cases}$

as $\beta \to \infty$ $(T \to 0)$, $m^* \to 1$ (fully ordered phase)





$\underline{\beta > 1}$:

$$\begin{cases} P(m^*) = \frac{1}{2}, \\ P(-m^*) = \frac{1}{2} \end{cases}$$

$(h = 0)$

phase co-existence

For $h \neq 0$, $\exists$ global max of $\varphi(m) \Rightarrow$ single phase ; h breaks the $\pm m^*$ symmetry.

$\Phi(\beta, h)$ is a key quantity in this framework. It is basically <u>free energy</u>:

$$f_N(\beta, h) = -\frac{1}{\beta} \Phi_N(\beta, h),$$

$$f(\beta, h) = \lim_{N\to\infty} f_N(\beta, h) = \min_{m \in [-1,1]} f(m, \beta, h),$$

where $f(m, \beta, h) = -\frac{1}{\beta}\varphi(m) = -\frac{m^2}{2} - hm - \frac{H(m)}{\beta}$

Recall that

$$Z_N(\beta,h) = \sum_{\{\vec{s}\}} e^{-\beta H_N^{\circ} + \beta N h m}.$$

Then

$$\frac{1}{\beta}\frac{\partial}{\partial h}\varphi_N(\beta,h) = \frac{1}{\beta N}\frac{\partial}{\partial h}\log Z_N(\beta,h) =$$

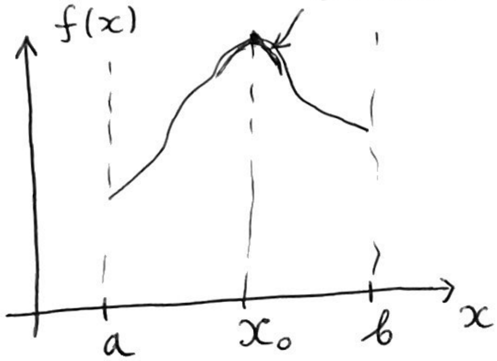
$$= \frac{1}{Z_N(\beta,h)}\sum_{\{\vec{s}\}} m e^{-\beta H_N^{\bullet}} = \underbrace{\langle m\rangle_N}_{\text{average magnetization}}$$

Likewise, $\frac{1}{\beta}\frac{\partial^2}{\partial h^2}\varphi_N(\beta,h) =$

$$= \frac{\partial}{\partial h}\sum_{\{\vec{s}\}}\frac{m e^{-\beta H_N}}{Z_N} = N\beta\left[\langle m^2\rangle_N - \langle m\rangle_N^2\right] \geq 0.$$

Thus, φ_N is convex.

Laplace approximation



$f'(x_0) = 0$

$$\begin{cases} f(x_0) = \max\limits_{x \in [a,b]} f(x), \\ f''(x_0) < 0 \end{cases}$$

Then $$\int_a^b dx\, e^{nf(x)} \underset{n\to\infty}{\rightarrow} e^{nf(x_0)} \sqrt{\frac{2\pi}{n(-f''(x_0))}} .$$

$$f(x) \simeq f(x_0) + \frac{1}{2} f''(x_0)(x-x_0)^2$$

Consequently,

$$\frac{1}{n} \log \int_a^b dx\, e^{nf(x)} \underset{n\to\infty}{\rightarrow} f(x_0) + \Theta\left(\frac{\log n}{n}\right)$$

Now, define $$P(m|h=0) \underset{N\to\infty}{\rightarrow} e^{-N \underbrace{I_0^*(m)}_{\text{large deviation rate, } h=0}}$$

Then $$Z_N(\beta,h) \underset{N\to\infty}{\rightarrow} \int_{-1}^{1} dm\, P(m|h=0)\, Z_N(\beta,0)\, e^{N\beta hm} =$$

$$= \sum_{m\in S_N} e^{N\beta hm} \Big[\overbrace{\Big(\sum_{\{\vec{s}\}} e^{-\beta H_N^0} \Big)}^{Z_N(\beta,0)} P(m|h=0) \Big]$$

$$P(m|h=0) = \frac{\sum_{\{\vec{s}\}} e^{-\beta H_N^0}\, \mathbb{1}(m)}{\sum_{\{\vec{s}\}} e^{-\beta H_N^0}}$$

$$\stackrel{\circ}{=} \int_{-1}^{1} dm\, e^{-N I_0^*(m)}\, e^{N \varphi_N(\beta,0)}\, e^{N\beta h m}.$$

Thus $\varphi_N(\beta,h) = \dfrac{\log Z_N(\beta,h)}{N} \underset{N\to\infty}{\to}$

$$\underset{N\to\infty}{\to} \max_{m\in[-1,1]} \Big\{ \underbrace{\varphi_N(\beta,0)}_{\text{indep. of } m} + \beta h m - I_0^*(m) \Big\}, \text{ or}$$

$$\varphi(\beta,h) - \varphi(\beta,0) = \underbrace{\max_m \{\beta h m - I_0^*(m)\}}_{m\to h \text{ Legendre transform of } I_0^*(m)}.$$

Inverse transform:

$$I_0(m) = \varphi(\beta,0) + \max_h \{\beta h m - \varphi(\beta,h)\}$$