

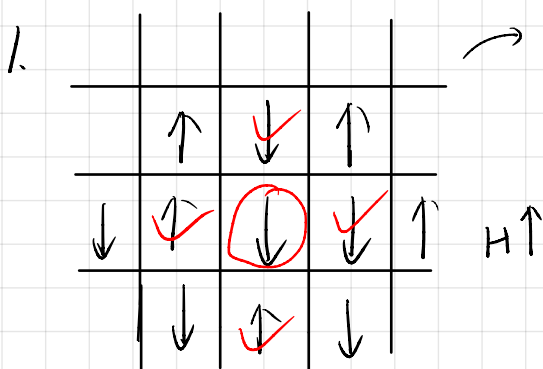
Thermodynamic limit $\rightarrow \begin{matrix} N \rightarrow \infty \\ V \rightarrow \infty \end{matrix} \frac{N}{V} = \rho \sim \text{const.}$

由杨振宁证明, 当我们将 $\beta \rightarrow \beta + i\varepsilon$, 即向复平面延拓, 可以证明, 当 $N \rightarrow \infty$ 时, Q 的零点无限靠近实轴 (奇异性).

(4) Universalrey. class. (普适类).

eg: 幂律. 在临界点附近 $m \sim (\lambda - \lambda_c)^\beta$; 代表一类物质.

§1. Ising 模型. 每一种 $\{s_i\}$ 对应一个能谱, E_ν 只是一个模型而非 Schrödinger 方程的解.



$\rightarrow$ Spin. $s_i = \pm 1 (\mu)$

① ν 态 $\{s_i\}$. ν 态 $\leftrightarrow \{s_i\}$.

② $E_\nu = ?$

$$E_{\nu=\{s_i\}} = - \sum_{i=1}^N \mu H s_i + \sum_{ij} J_{ij} s_i s_j$$

Ising 模型: ① $\sum_{ij} \rightarrow \sum_{\langle ij \rangle}$ (只考虑最近邻)

② $J_{ij} \rightarrow -J$. (认为所有 J 相同, 且自旋倾向相同)

$\downarrow$ (只考虑最近邻)

即: $E_{\nu=\{s_i\}} = - \sum_{i=1}^N \mu H s_i - \sum_{\langle ij \rangle} J s_i s_j$ 即限定了 N, H . 之后热力学函数应取 $G(T, H)$.

对此 (H, M, T) 系统. $M_\nu = (\sum s_i) \rightarrow$ 磁矩.

但此时我们仍需建立 (H, M, T) 系统的热力学关系.

(类似于 (P, V, T) 体系中 $dF = -SdT - PdV + \mu dN = d(-kT \ln Q)$)

2. 热力学描述

① 1st law + 2nd law.

$$(P, V, T): dU = TdS - pdV + \mu dN$$

$$(H, M, T): dU = d\Omega - dw. \quad \left(\begin{array}{l} \text{参考教材: Kubo: Stat. Mech: An} \\ \text{advanced Course with Probe and Solutions} \end{array} \right)$$

$$= TdS + HdM$$

$$\text{即 } (P \leftrightarrow H, V \leftrightarrow -M, T \leftrightarrow T)$$

$$U = U(S, M)$$

通过勒让德变换: $F(T, M) = U(S, M) - TS$ 对磁学体系, 固定 H 是容易的, 但限定 M 是困难的, 因此选取 G 为桥梁.

$$dF = -SdT + HdM$$

$$\star \begin{cases} G(T, H) = F(T, M) - HM \\ dG = -SdT - MdH \end{cases}$$

$$M = - \left(\frac{\partial G(T, H)}{\partial H} \right)_T$$

3. 配分函数与热力学.

$$1) Q(N, \beta, H) = \sum_v e^{-\beta E_v} \longrightarrow G(T, H) = -kT \ln Q(T, H)$$

$$= \sum_{\{S_i = \pm 1\}} e^{+[\beta \mu H \sum_i S_i + \beta J \sum_{ij} S_i S_j]}$$

$$kT \left(\frac{\partial \ln Q}{\partial H} \right)_T = \left(\frac{\partial \ln Q}{\partial (\beta H)} \right)_\beta = \frac{1}{Q} \left(\frac{\partial Q}{\partial (\beta H)} \right)_\beta$$

$$= \frac{1}{Q} \sum_{\{S_i\}} (\mu \sum_i S_i) e^{+[\beta \mu H \sum_i S_i + \beta J \sum_{ij} S_i S_j]}$$

$$\equiv \sum_{\{S_i\}} (\mu \sum_i S_i) \cdot \frac{e^{+[\dots]}}{Q} = \langle \mu \sum_i S_i \rangle = \langle M \rangle$$

由于 $M = - \left(\frac{\partial G(T, H)}{\partial H} \right)_T$, 则 $G(T, H) = -kT \ln Q(\beta, H)$.

响应函数 χ (Susceptibility).

$$\chi = \frac{1}{N} \left(\frac{\partial M}{\partial (\beta H)} \right)_\beta = \frac{1}{N} \left(\frac{\partial^2 \ln Q}{\partial (\beta H)^2} \right)_\beta = \frac{1}{N} \langle \delta M^2 \rangle \quad \delta M = M - \langle M \rangle$$

Proof: $\left(\frac{\partial \langle M \rangle}{\partial (\beta H)} \right)_\beta = \frac{\partial}{\partial h} \left(\frac{1}{Q} \frac{\partial Q}{\partial h} \right) = \frac{1}{Q} \frac{\partial^2 Q}{\partial h^2} - \frac{1}{Q^2} \left(\frac{\partial Q}{\partial h} \right)^2 = \langle \delta M^2 \rangle$
 $(h \sim \beta H)$

4. 相变现象. ($T < T_c, \langle M \rangle \neq 0, H=0$)

1) 一维的 Ising Model 无相变

$$F = G = U - TS$$

eg: 有序态 $\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow\uparrow$ (头尾相连)

N 个位置可以翻转自旋

$\Downarrow$ Kink.

$$\Delta F = \Delta U - T\Delta S \quad \Delta S \sim k \ln N.$$

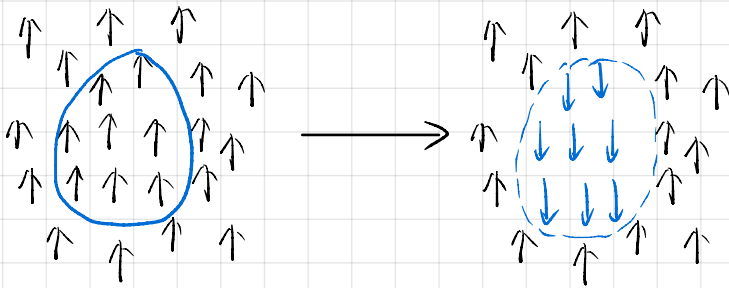
$$= 4J - kT \ln N.$$

$$N \rightarrow \infty, \Delta F < 0.$$

即总是无序态更加稳定, 无相变!

(因为 ΔU 与 N 无关, 但 ΔS 与 N 有关).

考察二维 Model.



产生边界长为 b 的反应“磁畴”

$$\Delta U \sim 2bJ.$$

$$\Delta S \sim k \ln N.$$

($\Omega \sim N^\alpha$, Ω 不可能为 e^N).

$$\Delta F = 2bJ - kT \ln N.$$

但此时 $b \sim N^{\frac{1}{d}}$ (d 维: $b \sim N^{\frac{d-1}{d}}$).

$$\text{即 } \Delta F = 2JN^{\frac{1}{d}} - kT \ln N. \Rightarrow \Delta F_{\text{有序} \rightarrow \text{无序}} \xrightarrow{N \rightarrow \infty} > 0.$$

证明有序态更稳定, 相变可以发生!

§. 1D (2D) Ising 解析解

1. $H=0$ 情形.

$\uparrow \uparrow \uparrow \uparrow \uparrow \dots \uparrow$ 1. N 之间无相互作用. (开放链)
 $i = 1 \quad 2 \quad 3 \quad \dots \quad N$

$$E_N = -J(S_1 S_2 + S_2 S_3 + \dots + S_{N-2} S_{N-1} + S_{N-1} S_N)$$

$$Q(N, \beta, 0) = \sum_{\{S_i = \pm 1\}} e^{\beta J (S_1 S_2 + S_2 S_3 + \dots + S_{N-2} S_{N-1} + S_{N-1} S_N)}$$

$\leftarrow S_1 = \pm 1 \quad S_2 = \pm 1 \quad \dots \quad S_N = \pm 1$

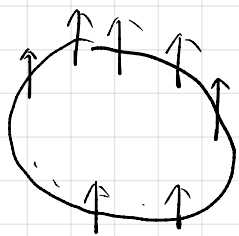
$$Q(N, \beta, 0) = \sum_{S_1, \dots, S_{N-1} = \pm 1} e^{+\beta J (S_1 S_2 + \dots + S_{N-2} S_{N-1})} \left(\sum_{S_N = \pm 1} e^{\beta J S_{N-1} S_N} \right)$$

$$= Q(N-1, \beta, 0) \cdot 2 \cosh(K) \quad (K = \beta J) \quad \left\{ \begin{array}{l} = e^{\beta J S_{N-1}} + e^{-\beta J S_{N-1}} \\ = 2 \cosh \beta J S_{N-1} \end{array} \right.$$

$$\Rightarrow Q(N, \beta, 0) = [2 \cosh(K)]^{N-2} \left(\sum_{S_N} e^{K S_N} \right)$$

$$= 2 \cdot [2 \cosh(K)]^{N-1} \quad \swarrow (2e^K + 2e^{-K})$$

2. 1D Ising (周期链).



$$E_V = -J (S_1 S_2 + S_2 S_3 + \dots + S_N S_1)$$

$$Q = \sum_{\{S_i\}} e^{K(S_1 S_2 + \dots + S_N S_1)}$$

若令 $b_i = S_i S_{i+1}$ 则 $b_i = \pm 1$.

则 $E_V = -J (b_1 + b_2 + \dots + b_N)$ 近似

$Q = \sum_{\{b_i\}} e^{K \sum_i b_i}$ 若 b_i 独立变化, 则 $Q = \left(\sum_{b_1} e^{K b_1} \right) \left(\sum_{b_2} e^{K b_2} \right) \dots \left(\sum_{b_N} e^{K b_N} \right)$

$$= [2 \cosh(K)]^N \quad (N \rightarrow \infty \text{ 时为一个很好的近似})$$

但事实上 b_i 之间有约束: $\prod b_i = 1$

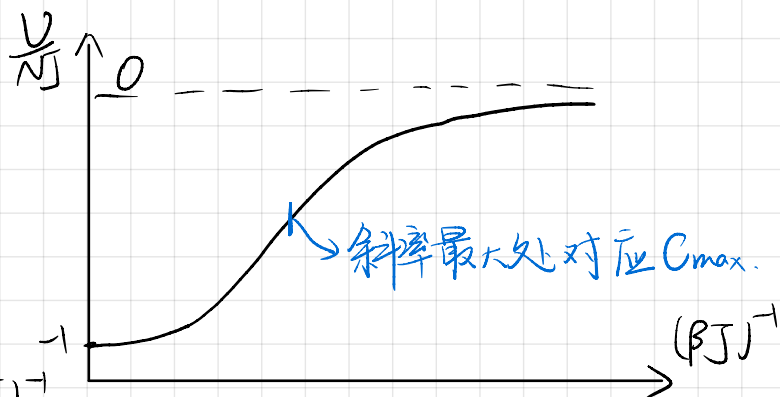
之后我们可以讨论热力学. (利用 b_i 独立变化的近似)

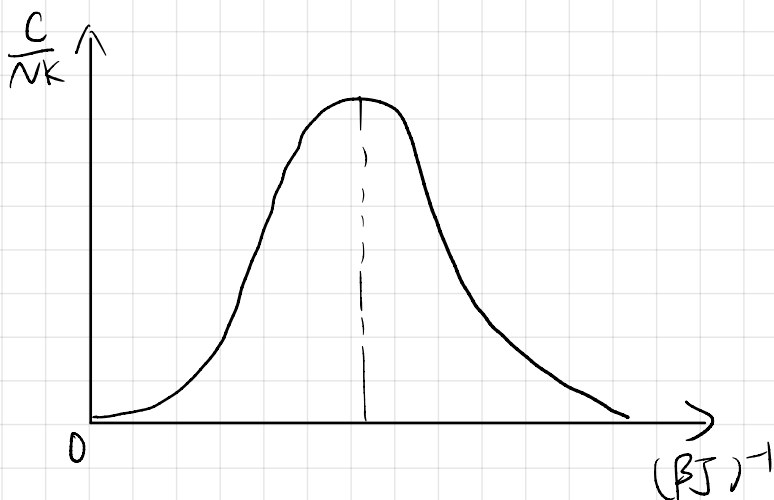
$$F = -kT \ln Q = -NkT \ln [2 \cosh(\beta J)]$$

$$U = -\frac{\partial \ln Q}{\partial \beta} = -NJ \tanh(\beta J) \quad S = -\frac{\partial F}{\partial T} = Nk \{ \ln [2 \cosh(\beta J)] - \beta J \tanh(\beta J) \}$$

$$C = \frac{\partial U}{\partial T} = Nk(\beta J)^2 / \cosh^2(\beta J)$$

$$\begin{cases} \beta J \rightarrow 0, & S = Nk \ln 2 \\ \beta J \rightarrow \infty, & S = 0 \end{cases}$$





3. 转移矩阵法

1) 周期链, ($H=0$)

$$Q(N, \beta, 0) = \sum_{\{S_i\}} e^{k(S_1 S_2 + S_2 S_3 + \dots + S_N S_1)}$$

$$\text{定义 } T(S_i, S_j) = e^{k S_i S_j}$$

$$= \sum_{S_1=\pm 1} \sum_{S_2=\pm 1} \dots \sum_{S_N=\pm 1} \underbrace{T(S_1, S_2) T(S_2, S_3) \dots T(S_N, S_1)}$$

$$\text{类比于 } \sum_j A_{ij} B_{jk} = (AB)_{ik}$$

而 T 代表一个 $\begin{pmatrix} (1,1) & (1,-1) \\ (1,1) & (-1,-1) \end{pmatrix}$ 类似的矩阵.

$$\text{则 } \sum_{S_2=\pm 1} T(S_1, S_2) T(S_2, S_3) = (T^2)_{S_1 S_3}$$

$$\text{原式} = \sum_{S_1=\pm 1} \sum_{S_N=\pm 1} (T^N)_{S_1 S_N} T_{S_N S_1}$$

$$= \sum_{S_1=\pm 1} T^N_{S_1 S_1} = \text{Tr}(T^N) = (\lambda_+)^N + (\lambda_-)^N$$

其中 λ_+, λ_- 为 T 的两个本征值.

$$\text{其中 } T = \begin{pmatrix} e^k & e^{-k} \\ e^{-k} & e^k \end{pmatrix}$$

$$\Rightarrow \lambda_{\pm} = e^k \pm e^{-k} \quad (\lambda_+ > \lambda_-)$$

$$\text{则 } Q = [2 \cosh(k)]^N + [2 \sinh(k)]^N$$

$$\text{当 } N \rightarrow \infty \text{ 时, } Q \approx [2 \cosh(k)]^N \quad (\text{因为 } \cosh(k) > \sinh(k))$$

恰为之前的结果.

12) $H \neq 0$.

$$\begin{aligned}
 Q(N, \beta, H) &= \sum_{\{S_i = \pm 1\}} e^{K(S_1 S_2 + \dots + S_N S_1) + \sum_i (\beta \mu H) S_i} \\
 &= \sum_{\{S_i = \pm 1\}} e^{K(S_1 S_2 + \dots + S_N S_1) + \underbrace{K'(S_1 + S_2 + \dots + S_N)}_{\substack{\text{令其为 } K' \\ \downarrow}}} \\
 &= \sum_{\{S_i = \pm 1\}} e^{\frac{K'}{2} [(S_1 + S_2) + (S_2 + S_3) + \dots + (S_{N-1} + S_N) + (S_N + S_1)]} \\
 &= \sum_{\{S_i = \pm 1\}} \exp \left\{ \sum_i \left[K S_i S_{i+1} + \frac{K'}{2} (S_i + S_{i+1}) \right] \right\}.
 \end{aligned}$$

同样的, 定义: $T_{S_i S_j} = e^{K S_i S_j + \frac{K'}{2} (S_i + S_j)} \Rightarrow T = \begin{pmatrix} e^{K+K'} & e^{-K} \\ e^{-K} & e^{K-K'} \end{pmatrix}$

则 $Q = \text{Tr}(T^N) = \lambda_+^N + \lambda_-^N$

作业: 5.3 5.21

$$(\lambda_{\pm} = e^K [\cosh(K') \pm \sqrt{\sinh^2(K') + e^{-4K}}])$$

当 $N \rightarrow \infty$ 时, $Q = \lambda_+^N = (\beta, H, N)$

$$\langle M \rangle = + \frac{\partial \ln Q}{\partial (\beta H)} = N K T \frac{1}{\lambda_+} \frac{\partial \lambda_+}{\partial H} \doteq \frac{N \mu \sinh(K')}{\sqrt{\sinh^2(K') + e^{-4K}}} \quad \begin{pmatrix} K' = \beta \mu H \\ K = \beta J \end{pmatrix}$$

① 给定温度 ($\beta < \infty$), $H \rightarrow 0$, $\langle M \rangle \rightarrow 0$. (无相变)

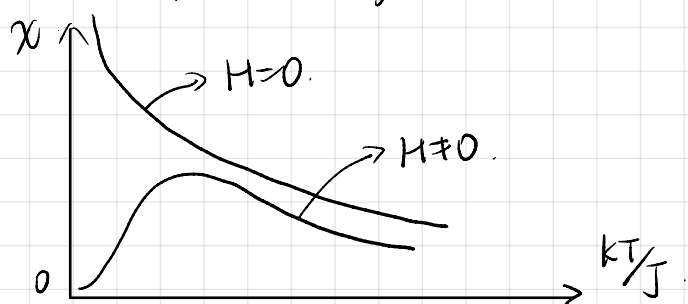
② $\beta \rightarrow \infty$ ($T \rightarrow 0$), 使得 $\sinh^2(K') \gg e^{-4\beta J}$. $\langle M \rangle \rightarrow \pm N \mu$.

即只要 $T \rightarrow 0$, 发生无序 $\rightarrow$ 有序相变 (有外场).

$$\langle E \rangle \rightarrow N J$$

③ $\chi = \frac{1}{N} \frac{\partial M}{\partial (\beta H)} = \mu^2 \frac{\cosh(\beta \mu H) e^{-4\beta J}}{(\sinh^2(\beta \mu H) + e^{-4\beta J})^{\frac{3}{2}}}$ 注: $\chi = \frac{1}{N} \langle \delta M^2 \rangle \sim \mu^2$

$$\begin{aligned}
 &= \int \beta \rightarrow \infty (T \rightarrow 0) \sim \begin{cases} \mu^2 e^{2\beta J} & (H=0) \\ \mu^2 e^{-2K'-4K} & (H \neq 0) \end{cases} \\
 &\quad \beta \rightarrow 0 \sim \mu^2.
 \end{aligned}$$



3. 关联函数. $C_{ij} = \langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle$

毫无关联时 $\langle S_i S_j \rangle = \langle S_i \rangle \langle S_j \rangle \Rightarrow C_{ij} = 0$

$$\chi = \frac{1}{N} \langle (\delta M)^2 \rangle \quad \delta M = M - \langle M \rangle = \sum_i (S_i - \langle S_i \rangle)$$

$$\begin{aligned} \langle (\delta M)^2 \rangle &= \sum_i \sum_j \langle (S_i - \langle S_i \rangle) (S_j - \langle S_j \rangle) \rangle \\ &= \sum_{ij} (\langle S_i S_j \rangle - \langle S_i \rangle \langle S_j \rangle) \\ &= \sum_{ij} C_{ij} \end{aligned}$$

$$\text{即 } \chi = \frac{1}{N} \sum_{ij} C_{ij} = \frac{1}{N} \sum_i \left(\sum_{j=1}^N C_{ij} \right) = \sum_{j=1}^N C_{ij}$$

$\sum_{j=1}^N C_{ij}$ 是其它 spin 与 "i" 的关联.

$\Rightarrow \chi$ 的发散 $\rightarrow$ 长程关联 ("巨" 涨落)

相变往往伴随巨大的涨落与长程的关联.

* 1D 链关联函数. ($H=0$, 开放链) $\uparrow \uparrow \downarrow \dots \downarrow \uparrow \downarrow \dots$ $\langle S_i \rangle = \langle S_{i+j} \rangle = 0$

$$\langle S_i S_{i+j} \rangle = \frac{1}{Q} \sum_{\nu} e^{-\beta E_{\nu}} S_i S_{i+j}$$

$$= \frac{1}{Q} \sum_{\nu} S_i S_{i+j} \exp \left[\beta \sum_{l=1}^{N-1} \underbrace{J_l S_l S_{l+1}}_{\text{最后再令 } J_L = J} \right]$$

$$\textcircled{1} Q_N = 2 \prod_{l=1}^N [2 \cosh(\beta J_l)]$$

$$\textcircled{2} S_i S_{i+j} = (S_i S_{i+1}) (S_{i+1} S_{i+2}) \dots (S_{i+j-1} S_{i+j})$$

$$\textcircled{3} S_i S_{i+1} = \frac{\partial}{\partial J_i} \left(\sum_{l=1}^{N-1} J_l S_l S_{l+1} \right)$$

$$\textcircled{4} \langle S_i S_{i+j} \rangle = \frac{1}{Q_N} \frac{\partial^j Q_N(J_i, J_{i+1}, \dots, J_{i+j})}{\partial J_i \partial J_{i+1} \dots \partial J_{i+j-1}} \cdot \frac{1}{\beta J} \quad \text{代入 } Q_N \text{ 的表达式可得}$$

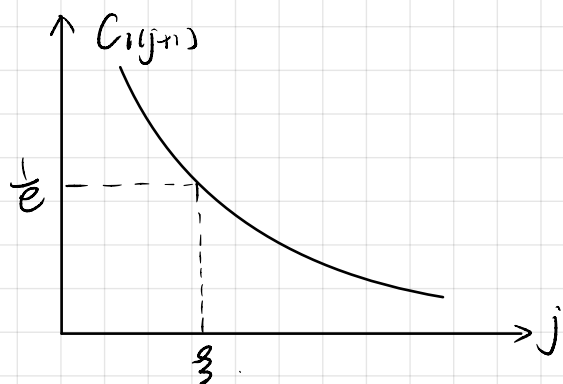
$$\textcircled{5} \langle S_i S_{i+j} \rangle = [\tanh(\beta J)]^j \sim e^{-j/\xi} \quad \xi = -\left\{ \ln [\tanh(\beta J)] \right\}^{-1}$$

* $\beta J \rightarrow \infty$ ($T \rightarrow 0$).

$\xi \rightarrow \infty$. 即 $T \rightarrow 0$ 时长程关联.

ξ 关联长度.

若 $\xi \rightarrow \infty$, 则为长程关联.



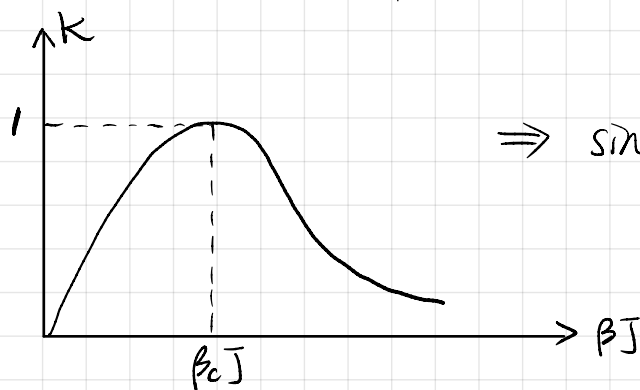
2D Ising 模型解.

$$Q(N, \beta, 0) = [2 \cosh(2\beta J) e^I]^N$$

$$I = (2\pi)^{-1} \int_0^{2\pi} d\phi \ln \left\{ \frac{1}{2} [1 + (1 - K^2 \sin^2 \phi)^{\frac{1}{2}}] \right\}$$

$$\text{其中 } K(J) = 2 \sinh(2\beta J) / \cosh^2(2\beta J)$$

* $K \rightarrow 1$, 会出现奇异性.



$$\Rightarrow \sinh(2\beta_c J) = 1 \Rightarrow K T_c = 2.269 J$$

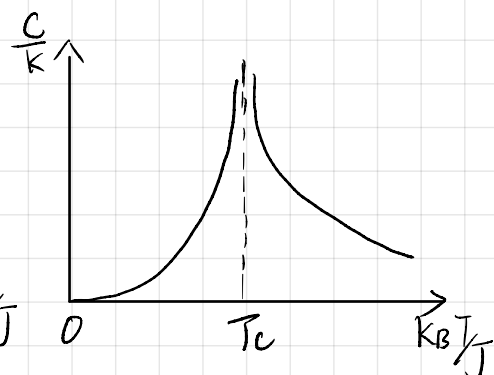
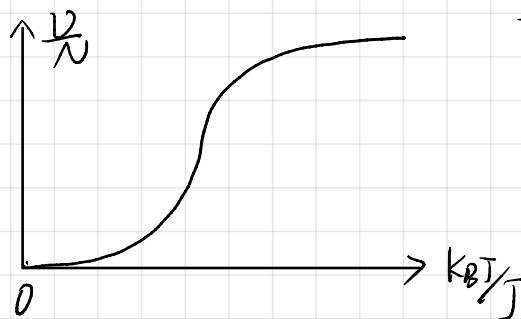
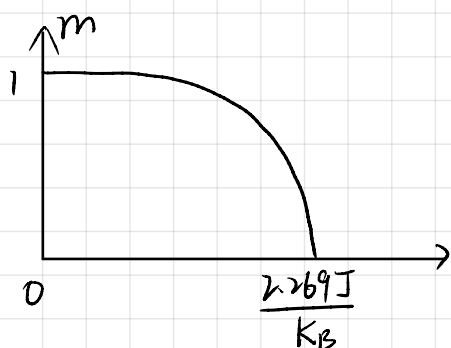
$$U = -\frac{\partial}{\partial \beta} (\ln Q) \quad C = \left(\frac{\partial U}{\partial T} \right)_{N \rightarrow \infty}$$

$$\rightarrow \frac{C}{N} \sim (\beta_c J)^2 \ln |1 - \frac{T}{T_c}| + \text{const} \sim |T - T_c|^{-\alpha} \rightarrow \alpha = 0$$

$$\text{但此方法无法求 } \langle M \rangle = \frac{\partial \ln Q}{\partial (\beta H)}$$

$$\text{杨振宁证明出 } m = \frac{\langle M \rangle}{N} = \{1 - \sinh^{-4}(2\beta J)\}^{\frac{1}{8}}$$

$$T \rightarrow T_c \quad m(T) \sim (T_c - T)^{\frac{1}{8}}$$



* 对称破缺 (Symmetry Break).

以 $H=0$ 为例. $e^{-\beta E_0} = e^{\beta J (\sum_{ij} S_i S_j)}$

若所有 $S_i \rightarrow -S_i$ $e^{-\beta E'_0} = e^{\beta J (\sum_{ij} S_i S_j)}$ 即 $e^{-\beta E_0} = e^{-\beta E'_0}$

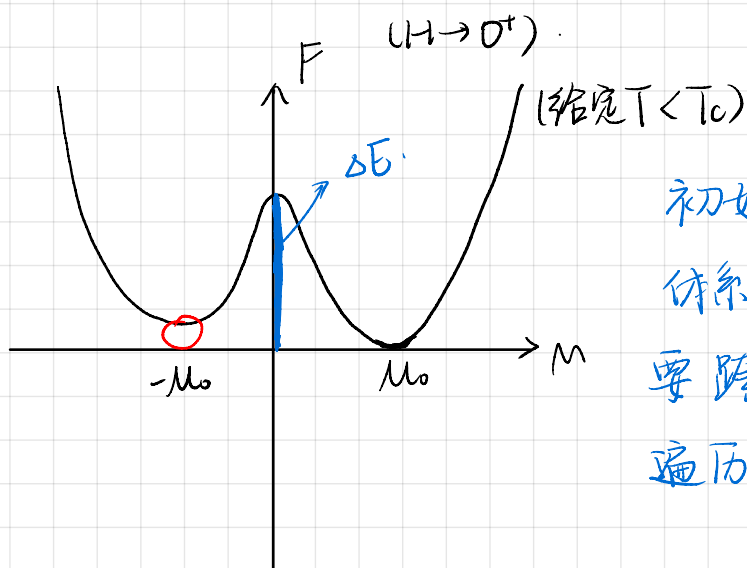
但 $M_0 = \sum_i S_i = -M'_0$

$\langle M \rangle = \sum_{\alpha} M_{\alpha} e^{-\beta E_{\alpha}} = 0!$ (因为 $e^{-\beta E_{\alpha}}$ 对称, M_{α} 反对称).

但 $T < T_c$ 时 $\langle M \rangle \neq 0$, 即状态的对称性低于哈密顿量允许的对
称性 $\Rightarrow$ 对称性破缺.

$H=0$, 固定 M , $F(T, M)$ 极小对应于平衡态

$Q(M) = \sum_{\nu} \delta(M - M_{\nu}) e^{-\beta E_{\nu}}$



初始制备初态时 $H \rightarrow 0^+$, 此时
体系偏向于 $+M_0$, 之后由于从 $M_0 \rightarrow -M_0$
要跨越 ΔE 的能垒, 使 $-M_0$ 无法被
遍历, 出现对称性的破缺.

即 $\langle M \rangle = \lim_{H \rightarrow 0} \left(\lim_{N \rightarrow \infty} \left[- \left(\frac{\partial F}{\partial h} \right)_{\beta} \right] \right) \neq 0$
 $\hookrightarrow$ 后 $\hookrightarrow$ 先 $\hookrightarrow$

$\langle M \rangle = \lim_{N \rightarrow \infty} \left(\lim_{h \rightarrow 0} \left[- \left(\frac{\partial F}{\partial h} \right)_{\beta} \right] \right) = 0$