第十六讲

- $S=\frac{1}{2}$ XY chain

考虑 $$\boxed{\hat{H} = \sum_i \left[-t\cos(\hat{\varphi}_{i+1}-\hat{\varphi}_i) + \frac{1}{2M}(\hat{P}_\varphi^{(i)}-\tfrac{1}{2})^2\right]} \quad (1)$$

耦合，有磁通 $\frac{1}{2}$，二维 Rotors chain.

- 考虑 $M\to 0$，$\frac{1}{2M}(\hat{P}_\varphi-\frac{1}{2})^2$ 重要，GS：$m=0$ 与 1，简并.

总简并度 2^{N_S}

把 t 项看成微扰：$t \ll \frac{1}{2M}$.

利用 $\cos(\hat{\varphi}) = \frac{1}{2}(e^{i\hat{\varphi}} + e^{-i\hat{\varphi}})$

$$e^{i\hat{\varphi}}|m\rangle = |m+1\rangle, \qquad (\hat{P}_\varphi|m\rangle = m|m\rangle)$$

证：$\langle\varphi|e^{i\hat{\varphi}}|m\rangle = e^{i\varphi}\langle\varphi|m\rangle = e^{i(m+1)\varphi} = \langle\varphi|m+1\rangle$ ← 坐标表象波函数

$\langle\varphi|m\rangle = \frac{1}{\sqrt{2\pi}}e^{im\varphi}$

同理：$e^{-i\hat{\varphi}}|m\rangle = |m-1\rangle$

$$\cos(\hat{\varphi}_i-\hat{\varphi}_{i+1}) = \frac{1}{2}(e^{i\hat{\varphi}_i}e^{-i\hat{\varphi}_{i+1}} + e^{i\hat{\varphi}_{i+1}}e^{-i\hat{\varphi}_i})$$

记 $|m=1\rangle \to |\uparrow\rangle$，$|m=0\rangle\to|\downarrow\rangle$. 那么 $e^{i\hat{\varphi}} = \sigma^+$，$e^{-i\hat{\varphi}} = \sigma^-$

$$\langle i|\sum_i[-t\cos(\hat{\varphi}_{i+1}-\hat{\varphi}_i)]|j\rangle \equiv \langle i|\hat{H}_{eff}|j\rangle, \quad |i\rangle,|j\rangle \in 2^{N_S}\ GS$$

$$H_{eff} = -\frac{t}{2}\sum_i[\sigma_i^+\sigma_{i+1}^- + \sigma_{i+1}^+\sigma_i^-] = -\frac{t}{4}\sum_i(\sigma_i^x\sigma_{i+1}^x + \sigma_i^y\sigma_{i+1}^y)$$

因为：$\sigma_i^+ = \frac{\sigma_i^x + i\sigma_i^y}{2}$，$\sigma_i^- = \frac{\sigma_i^x - i\sigma_i^y}{2}$

这正是 $S=\frac{1}{2}$ XY chain！

① 的路径积分是单个 rotor 的简单推广： $Z = \int \mathcal{D}\varphi(\tau) e^{-S(\tau)}$

$$S = \sum_j \left\{ -i\pi Q_j + \int_0^\beta d\tau \left[\frac{M\dot{\varphi}_j^2}{2} - t\cos(\varphi_{j+1}^{(\tau)} - \varphi_j^{(\tau)}) \right] \right\}$$

$$Q_j = (\varphi_j(\beta) - \varphi_j(0))/2\pi$$

- 忽略 θ-term， 余下为经典 2D XY model.

$$\frac{\Delta\tau\dot{\varphi}_j^2}{2} = \frac{(\varphi_j(\tau+1) - \varphi_j(\tau))^2}{2\Delta\tau} = \frac{1}{\Delta\tau}[1 - \cos(\varphi_j(\tau+1) - \varphi_j(\tau))]$$

$$\therefore H_C = -J_x \sum_{j,\tau} \cos(\varphi_{j,\tau} - \varphi_{j+1,\tau}) - J_\tau \sum_{j\tau} \cos(\varphi_{j\tau+1} - \varphi_{j\tau})$$

$J_x = t\Delta\tau = t\frac{\beta}{N}$， 把 β 离散成 N 份， $\Delta\tau = \beta/N$

$$J_\tau = \frac{M}{\Delta\tau} = \frac{MN}{\beta} = \frac{MN}{\beta t} \times t = \frac{k\beta}{N} \cdot t$$

随着 t 的增大，rotors 倾向于指向同一方向. $J_\tau = \frac{MN}{t\beta} \cdot t$，固定 $\frac{k\beta}{N} = \frac{MN}{t\beta}$

那 t 可视为经典 model 的倒温度：t 小 = 高温， t 大 = 低温

- 把转子转动一圈： $\varphi(\beta) - \varphi(0) = 2\pi$， 视为自旋期望值转动一圈，而

自旋波函数获得位相 π： $\chi(\beta) = -\chi(0) = e^{i\pi Q}\chi(0)$

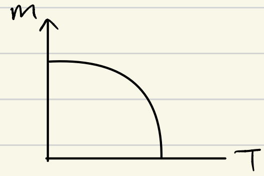
磁场中自旋 $H = -B \cdot S_z = -\frac{\omega}{2}\sigma_z$

进动： $\langle\alpha| e^{iHt} \vec{S} e^{-iHt} |\alpha\rangle = \langle\vec{S}\rangle(t)$ 一周后，波函数出一负号.

§ 相与相变: 热力学量不光滑，不连续或发散

• 连续相变又称临界现象: 对称性发生变化，自发破缺

§ 临界现象的刻画: 以 FM 临界点为例.

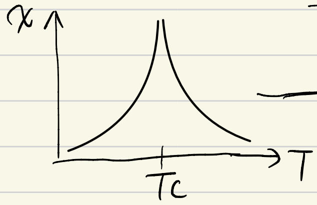


• 序参量 $m \propto (T_c - T)^{\beta}$ β critical exponent

• $T = T_c$. $m \propto h^{\frac{1}{\delta}}$

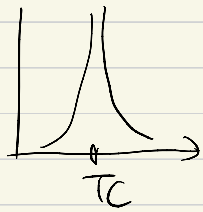
• $h=0$, 磁化率

$\chi \propto |T - T_c|^{-\gamma}$



• 比热:

$C \propto |T - T_c|^{-\alpha}$



§ Landau 平均场:

在Tc附近，序参量很小.

$$f(T, m) = f(T, 0) + \frac{1}{2} s(T) m^2 + \frac{1}{4} u(T) m^4 + \cdots$$

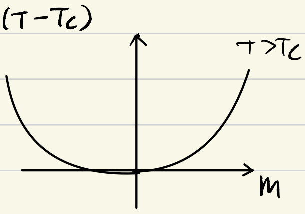
由于对称性，没有奇次项: (m 与 $-m$ 对应相同 f)

热平衡要求: $\frac{\partial f}{\partial m} = 0 \Rightarrow sm + um^3 = 0$ ①

稳定条件: $\frac{\partial^2 f}{\partial m^2} > 0 \Rightarrow s + 3um^2 > 0 \Rightarrow u > 0$.

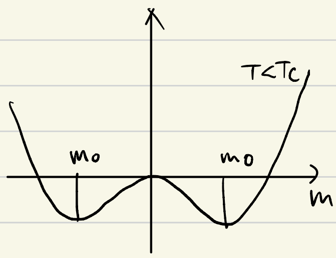
Landau 假设: $s(T) = s_0 \cdot (T - T_c)$

① $T > T_c$, $s(T) > 0$



① $\Rightarrow m_0 = 0$ 另一解 $m^2 = -\frac{s}{u}$ 舍

② $T < T_c$, $s(T) < 0$



① $m_0^2 = -\frac{s(T)}{u}$, $m_0 = \pm\sqrt{\frac{s_0(T_c - T)}{u}}$

$m_0 = 0$, 不稳定

临界指数计算：进一步假设 $u(T)\approx u(T_c)=u_0$ 基本不变

$T<T_c$：$m_0\propto (T_c-T)^{\frac{1}{2}}$ 即 $\beta=\frac{1}{2}$

$$C=-T\frac{\partial f}{\partial T^2} \qquad (F=-SdT-pdV,\ dQ=TdS)$$

引入 $t=\frac{T-T_c}{T_c}$，$\qquad m^2=\frac{s_0}{u_0}(T_c-T)$，$u_0 m^4=\frac{s_0^2}{u_0^2}(T_c-T)^2$

$T<T_c$，$\quad f=f_0-\frac{1}{2}\frac{s_0^2(T-T_c)^2}{u_0}+\frac{u_0}{4}\frac{s_0^2}{u_0^2}(T-T_c)^2=f_0-\frac{T_c^2 s_0^2}{4u_0}t^2$

$T>T_c$，$\quad f=f_0$

$\Rightarrow\ C(t\to 0^-)=\frac{T_c s_0^2}{2u_0}$，$\ C(t\to 0^+)=0$。跳跃，但 $\alpha=0$.

- 考虑外场：$\qquad df=-SdT+\mu_0 H dm$

$$f(T,m)=f_0+\frac{1}{2}S(T)m^2+\frac{1}{4}u_0m^4-hm$$

在 T_c：$\left.\begin{array}{l} m\approx 0, \\ S(T_c)=0, \end{array}\right\}\ \frac{\partial f}{\partial m}=0 \Rightarrow m\propto h^3 \Rightarrow \delta=3$

磁化率：$\chi=\left.\frac{\partial m}{\partial h}\right|_{h=0}$ 在 T_c 附近.

1. 首先：$T>T_c$. $\quad m_0=0$, $\quad m=m_0+\Delta m$

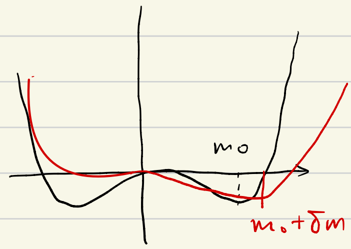
$$f(m_0+\delta m)=-h\,\delta m+\frac{1}{2}s_0(T-T_c)(m_0+\delta m)^2+\frac{1}{4}u_0(m_0+\delta m)^4$$
$$=-h\,\delta m+\frac{1}{2}s_0(T-T_c)\delta m^2$$

$\frac{\partial f}{\partial m}=0 \Rightarrow \delta m\propto\frac{h}{T-T_c} \Rightarrow \chi\propto\frac{1}{T-T_c}$ 即 $\gamma=1$

2. $T<T_c$：

$m_0=\sqrt{\frac{s_0(T_c-T)}{u_0}}$ 使 $s\,m_0+u_0m_0^3=0$.

$$f = f_0 - h(m_0+\delta m) + \frac{1}{2} S(T)(m_0+\delta m)^2 + \frac{1}{4} u_0 (m_0+\delta m)^4$$



$$\frac{\partial f}{\partial m} = -h + S(T)(m_0+\delta m) + u_0 (m_0+\delta m)^3 = 0$$

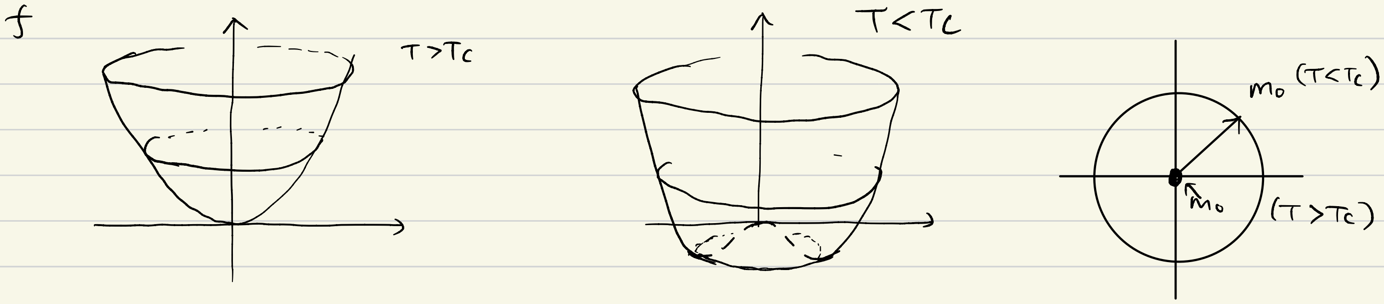
保留 δm 的一次，　$\delta m = \dfrac{h}{3u_0 m_0^2 - S} = \dfrac{h}{2S_0(T_c-T)}$

$\chi \sim \dfrac{1}{T_c - T}$　　同样 $\gamma = 1$.

· 序参量为多分量：　$\vec{m} = (m_1, m_2, \cdots, m_n)$　　$O(n)$ 旋转不变系统.

$$f(T, \vec{m}) = f(T, 0) + \frac{1}{2} S(T) m^2 + \frac{1}{4} u(T) m^4 + \cdots$$

其中　$m^2 = \vec{m}\cdot\vec{m} = \sum_{i=1}^{n} m_i^2$，　$m^4 = (\vec{m}\cdot\vec{m})^2 = \sum_{ij} m_i^2 m_j^2$



以 $n=2$ 为例

$T > T_c$.　$S(T) > 0$,　f 只跟 $|m| = \sqrt{m^2}$ 有关　$(m^2 = |m|^2)$

∴ 自由能极小要求 $\dfrac{\partial f}{\partial |m|} = 0$

$$\Rightarrow S(T)|m| + u_0 |m|^3 = 0. \Rightarrow m_0 = 0.$$

$T < T_c$.　$S(T) < 0$.　$\dfrac{\partial f}{\partial |m|} = 0 \Rightarrow m_0 = \sqrt{\dfrac{S_0(T_c-T)}{u_0}}$

对称性自发破缺要求：从 $(0, 2\pi)$ 中选一个方向确定

考虑 加上外磁场 $\vec{h}$.

$$f(T,m) = f_0 + \frac{1}{2} S(T) m^2 + \frac{1}{4} u_0 m^4 - \vec{h}\cdot\vec{m}$$

1. $T>T_c$. $|m|=0$. 外场诱导磁化：

设 $\vec{h} = (h, 0)$ 那么 $\delta\vec{m} = (\delta m, 0) = \vec{m}$

$$\delta m = \frac{h}{S(T)}, \quad \delta\vec{m} \propto \frac{\vec{h}}{T-T_c}, \quad \chi \propto \frac{1}{T-T_c} \qquad \gamma = 1.$$

2. $T<T_c$. 假设磁化方向为 x 方向: $\vec{m} = (m_0, 0)$

• 磁场加在 x 方向: $\vec{h} = (h, 0)$, $\vec{m} = (m_0+\delta m, 0)$

$$f = f_0 - h(m_0+\delta m) + \frac{1}{2} S(T)(m_0+\delta m)^2 + \frac{1}{4} u_0 (m_0+\delta m)^4$$

$$\frac{\partial f}{\partial m} = -h + S(T)(m_0+\delta m) + u_0 (m_0+\delta m)^3 = 0$$

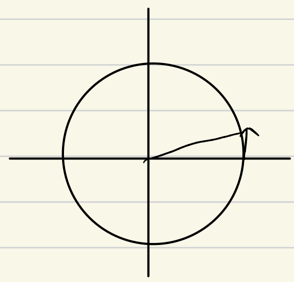
保留 δm 的一次, $\delta m = \dfrac{h}{3u_0 m_0^2 - S} = \dfrac{h}{2S_0(T_c-T)}$

$$\chi \sim \frac{1}{T_c - T} \qquad \text{同样} \quad \gamma = 1.$$

• 磁场加在 y 方向: $\vec{h} = (0, h)$, $\vec{m} = (m_0, \delta m)$

$$f = f_0 - h\,\delta m + \frac{1}{2} S(T)(m_0^2 + \delta m^2) + \frac{1}{4} u_0 (m_0^4 + 2 m_0^2 \delta m^2)$$

$\dfrac{\partial f}{\partial m_0} = 0$ 满足 $m_0^2 = \dfrac{S_0(T_c-T)}{u_0}$



$$\frac{\partial f}{\partial \delta m} = 0 \Rightarrow \delta m = \frac{h}{u_0 m_0^2 + S(T)} \propto \frac{h}{T_c - T}$$

$$\Rightarrow \chi_\perp \propto \frac{1}{T_c - T} \qquad \gamma = 1$$

平均场理论有效性:

- $d=1$, (量子 $d=0$) 完全失败 没有相变
- $d=2,3$ (量子 $d=1,2$) 基本图像是正确的. 指数错, 过"简单"
- $d\geq 4$, 完全正确.

下临界维数 (lower critical dimension) d_l:

$d\leq d_l$ MF 完全失效. $d_l=1$, for Ising; $d_l=2$. for $O(n\geq 2)$

上临界维数 (upper critical dimension) d_c

$d\geq d_c$ MF 有效.