平均场方法数值计算

Hilbert space ⇒ 经典力学：自由度，x_i，p_i，eq of motion

$L\to\infty$ or $L=40$

每个格子 $\sigma=0,1$. 2^L $L=40$

量子力学：指数级 $|\psi\rangle=\sum_{i=1}^{k} c_i|\varphi_i\rangle$, $k\sim d^L$

$2^{40}=(1000)^4=10^{12}$

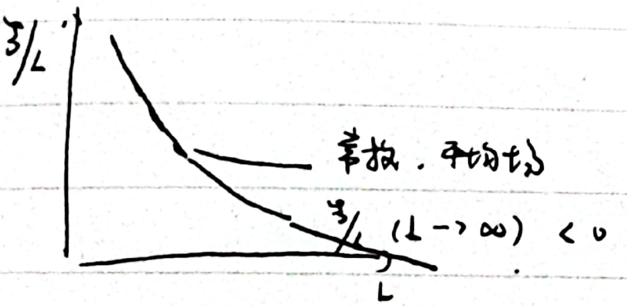
⇒ 怎么办.

1) 平均场 { 空间 $d^L - d$.
多体 ⇒ 单体 + 自洽.

2) 严格/精确对角化. ⇒ 有限计算 + 外推.

☆ Lanczos 方法

☆ MC 计算.



$L=11, 12, \dots, 16, 17, \dots \to\infty$

但可能不对物理图像.
已知解的结果，对严格可解 Model.

方法：从简单到复杂，一项一项处理.

上节课

$x^3=2x^2+5$. $x=m$ $\Rightarrow$ $m^2x=2x^2+5$ 且 $x=m=f(m)$ 自洽.

0-0 2 spin $H=h(\sigma_1+\sigma_2)+J\sigma_1\sigma_2$

$=h(\sigma_1+\sigma_2)+Jm(\sigma_1+\sigma_2)-Jm^2$.

$AB=\bar{A}B+\bar{B}A-\bar{A}\bar{B}+$ correlation

平均场：忽略涨落与关联，将其变为经典问题。

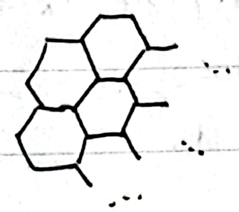
$$H = h(\sigma_1+\sigma_2+\sigma_3) + J(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_1\sigma_3)$$

$$= h(\sigma_1+\sigma_2+\sigma_3) + \underbrace{2}_{\text{配位数}}Jm(\sigma_1+\sigma_2+\sigma_3) - \underbrace{3}_{\text{bond 数}}Jm^2$$

$$K\sigma_1\sigma_2\sigma_3 = Km^2(\sigma_1+\sigma_2+\sigma_3) - 2Km^3.$$

if $\sigma_1=\sigma_2=\sigma_3$ $\quad Km^3 = 3Km^3 - 2Km^3 = Km^3.$

$$H = h(\sigma_1+\sigma_2+\sigma_3+\sigma_4) + J(\sigma_1\sigma_2+\sigma_2\sigma_3+\sigma_3\sigma_4+\sigma_4\sigma_1) + K\sigma_1\sigma_2\sigma_3\sigma_4.$$



Bose-Hubbard 平均场，相变。

晶格中

$$H = \underbrace{\frac{p^2}{2m} + U(\vec{x})}_{\text{周期性晶格}} + g\delta(\vec{x}-\vec{y}).$$

二次量子化。 周期 $\begin{cases} \text{Bloch} \Rightarrow \text{浅晶格} \\ \text{Wannier} \Rightarrow \text{深。} \end{cases}$

$\psi = \sum_i c_i \varphi_i \quad \varphi_i(x) = W(\vec{x} - \vec{R}_i)$ 中心。

$$H_0 = \int \psi^+ H_0 \psi \, dx$$

$$= \sum_{ij} c_i^+ c_j \int \varphi_i^* \left[-\frac{\nabla^2}{2m} + U(x) \right] \varphi_j \, dx .$$

① $i=j$ $\quad -\mu c_i^+ c_i$ $\quad$ ↑ 可以计算.

② i,j 近邻. $-t \, c_i^+ c_j$.

$$H = -t \sum_{\langle ij \rangle} c_i^+ c_j \underbrace{\left(-t' \sum_{\langle\langle i,j \rangle\rangle} c_i^+ c_j \right)}_{\text{次近邻项, 一般不考虑}} - \mu \sum_i c_i^+ c_i$$

$$+ U c_i^+ c_i^+ c_i c_i + h.c.$$

$$\int \psi^+(x) \psi^+(y) \, g \delta(x-y) \, \psi(x) \psi(y) \, dx dy$$

$$= \cancel{g \, c_i^+ c_j^+ c_k c_l \, g \int \varphi_i^*(x) \varphi_j^*(y) \delta(x-y) \varphi_k(y) \varphi_l(x) \, dx dy}$$

$i=j=k=l$. $\quad U.$

$$c_i^+ c_i^+ c_i c_i = c_i^+ (c_i c_i^+ - 1) c_i \quad (c_i c_i^+ - c_i^+ c_i = 1)$$

$$= n_i^2 - n_i = n_i (n_i - 1) .$$

$$\therefore H = -t \sum_{\langle ij \rangle} c_i^+ c_j - \mu \sum_i n_i + U \sum_i n_i (n_i - 1) .$$

理解其相图.

图像平均场.

微扰: ① $t=0$ 时. $\quad |n_1, n_2, n_3, \cdots n_L \rangle$ 本征态.

$$E = -\mu \sum_i n_i + U \sum_i n_i (n_i - 1) .$$

$$\frac{E}{L} = -\mu n \quad + U n (n - 1) \quad \ldots$$

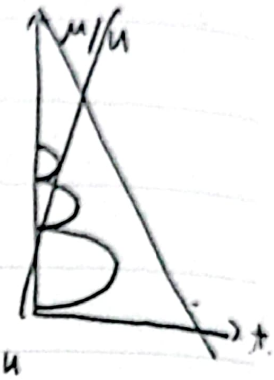
$\cancel{un^2 - un}$ $\quad n^2 + an$. $\quad 2un \geq \mu$. $\quad n \leq \frac{\mu}{2u} + 1$

$$-\mu n + u n(n-1) \leq -\mu(n+1) + u(n+1)n$$

$$-\mu n + u n(n-1) \leq -\mu(n-1) + u(n-1)(n-2)$$

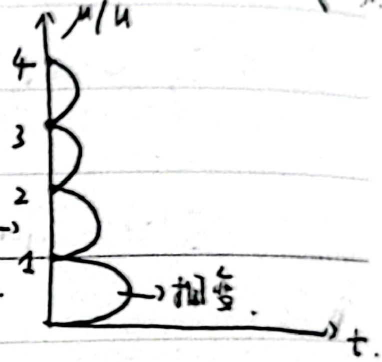
$$\cancel{\frac{\mu}{2u} \geq n \geq \frac{\mu}{2u}} \Rightarrow \frac{\mu}{2u}.$$

$$1 + \frac{\mu}{2u} \geq n \geq \frac{\mu}{2u}.$$



Mott insulator.

$$\Rightarrow n \in \left[\frac{\mu}{2u}, \frac{\mu}{2u}+1\right].$$



② $t \to \infty$. $H = -t \sum_{\langle ij \rangle} c_i^+ c_j$.

自由扩散，超流。

$J\sigma_1\sigma_2 = Jm(\sigma_1 + \sigma_2) - Jm^2 \Rightarrow \langle \sigma \rangle = m$.

$-t\, c_i^+ c_j \Rightarrow -t(\Delta^* c_i + c_j^+ \Delta - |\Delta|^2)$ 令 $\langle a_i \rangle = \langle a_j \rangle = \Delta$.

i —— j. $\quad z$：配位数. 1D $z=2$ 2D $z=4$ 3D: $z=6$

第 i 个格子

$$H_i = -\mu\, \underbrace{\cancel{c_i^+ c_i}}_{n_i} + u n_i(n_i - 1) - t\left[z(\Delta^* c_i + \Delta c_i^+) - z|\Delta|^2\right]$$

perturbation: $-tz(\Delta^* c_i + \Delta c_i^+)$

$$H = -\mu n + u n(n-1) - tz(\Delta^* c + \Delta c^+) + tz|\Delta|^2$$

基态 $|n\rangle \triangleq |n\, n \cdots n\rangle$.

激发态：$|n+1\rangle \quad - \quad c^+|n\rangle$

$|n-1\rangle$

→ 一阶 最小能量 → 排序.

$$\bar{E}_g = \bar{E}_g^{0} + \bar{E}_g^{(1)} + \left(\bar{E}_g^{(2)}\right)$$

$$\bar{E}_g^{0} = -\mu n + U n(n-1) + t z |\Delta|^2 \qquad (t>0)$$

$$V' = -t z (\Delta^* c + \Delta c^+)$$

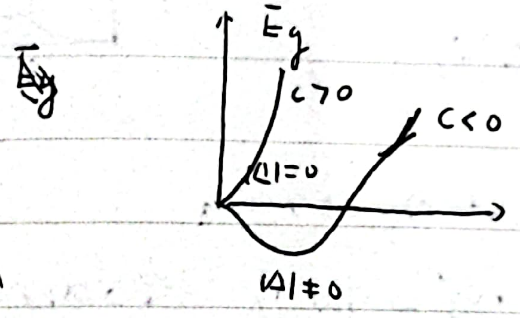
$$\bar{E}_g^{(1)} \Rightarrow \langle n | V' | n \rangle = 0$$

$$\bar{E}_g^{(2)} \sim -t^2 z^2 |\Delta|^2 \cancel{f(n)}\, f(n, \mu, U)$$

$$\Rightarrow -\frac{\langle n | V' | n+1 \rangle \langle n+1 | V' | n \rangle}{\varepsilon_{n+1}^{0} - \varepsilon_n^{0}}$$

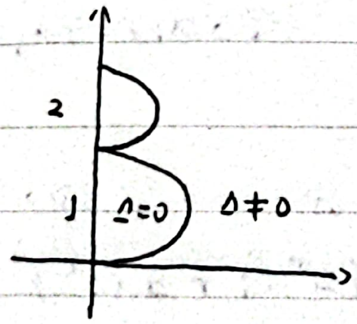
$$\Rightarrow \bar{E}_g \sim (\underbrace{t z - t^2 z^2 f}_{\Downarrow\, C}) |\Delta|^2$$

$$\bar{E}_g^{(4)} = A^{(4)} |\Delta|^4$$



$$\bar{E}_g = \bar{E}_g^{0} + a|\Delta|^2 + b|\Delta|^4$$

$\Rightarrow$ Landau 二级相变理论.



$1 - t z f(\mu, n, U) = 0$ 相边界.

$$\varepsilon_n = -\mu n + U n(n+1)$$

$$f = \frac{|\langle n | c^+ | n-1 \rangle|^2}{\varepsilon_{n-1} - \varepsilon_n} + \frac{|\langle n | c | n+1 \rangle|^2}{\varepsilon_{n+1} - \varepsilon_n} \cdots$$

b: Ref

讨论各种平均场近似.

① $J\sigma_1\sigma_2 = Jm(\sigma_1+\sigma_2) - Jm^2$

② $c_i^+ c_j \to \Delta^* c_j + \Delta c_i^+ - |\Delta|^2$

③ $H = \vec{h}\cdot(\vec{\sigma}_1+\vec{\sigma}_2) + J\vec{\sigma}_1\cdot\vec{\sigma}_2$

$= \vec{h}\cdot(\vec{\sigma}_1+\vec{\sigma}_2) + J\vec{m}\cdot(\vec{\sigma}_1+\vec{\sigma}_2) - J|\vec{m}|^2$

$\vec{m}$ is a vector $\quad \vec{m} = (m_x, m_y, m_z)$

$h\sigma_i + \underline{f(i-j)\sigma_i\sigma_j} \Rightarrow$ 长程相互作用.

$f(i-j)\,m(\sigma_i+\sigma_j) - f(i-j)\,m^2$