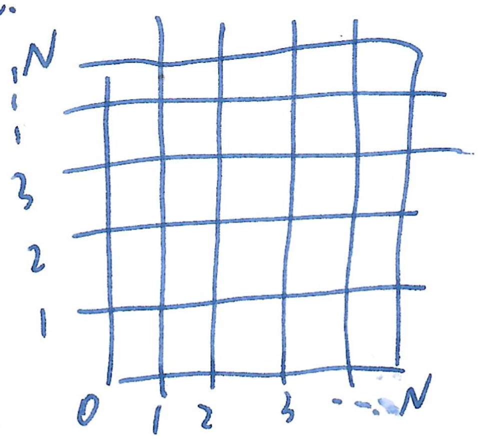
$\nabla^2\phi = q(x,y)$, $(x,y)\in D$, $D\to$ 正方形

$\phi|_G = g(s)$, $s\in\partial D$

(1) 格点化.



均匀分割.

边界正好在网格上...

待解量:

$$\begin{pmatrix}\phi_1\\ \phi_2\\ \vdots\\ \phi_{N-1}\end{pmatrix} \quad \phi_1 \to \begin{pmatrix}\phi_{11}\\ \phi_{12}\\ \vdots\\ \phi_{1N-1}\end{pmatrix}$$

共 $(N-1)\times(N-1)$ 个.

(2) 格点方程:

$$\nabla^2\phi_{ij} = \frac{\phi_{i+1j}+\phi_{i-1j}+\phi_{ij+1}+\phi_{ij-1}-4\phi_{ij}}{h^2} = q_{ij}$$

内 $\Rightarrow$ $\phi_{ij} - \frac{1}{4}(\phi_{i+1j}+\phi_{i-1j}+\phi_{ij+1}+\phi_{ij-1}) = -\frac{q_{ij}}{4}h^2$

边: $\phi_{ij} = g_{ij}$.

系数矩阵. K

不邻边: $k_{ij} = -\frac{I}{4}$, $i-j=\pm1$

$\uparrow$. $\downarrow$. $\rightarrow$ 每一行只与上、下行同位置耦合.

邻边: ~~k_{ij}~~ $k_{12} = -\frac{I}{4}$

~~$k_{NN-1} = k_{N-1N} = -\frac{I}{4}$~~ $k_{N-1\,N-2} = -\frac{I}{4}$

大致形式:

$$K = \begin{pmatrix} G & -\frac{I}{4} & & 0 \\ -\frac{I}{4} & G & -\frac{I}{4} & \\ & -\frac{I}{4} & G & \ddots \\ 0 & & & \ddots \end{pmatrix}$$ $(N-1)\times(N-1)$ 个块.

主、±1对角线. 非零.

$$G = \begin{pmatrix} 1 & -\frac{1}{4} & & \\ -\frac{1}{4} & 1 & -\frac{1}{4} & \\ & -\frac{1}{4} & 1 & \\ & & & \ddots \end{pmatrix} \rightarrow (N-1)\times(N-1)\text{个元.}$$

G是内部耦合.

~~?~~ 对 ϕ_{ij}, 在内部与 ϕ_{ij-1}、~~?~~ ϕ_{ij+1} 耦合, $-\frac{1}{4}$ 的系数.

在位能 1.

对而 ϕ_{i1} 只与 ϕ_{i2} 耦合. $\begin{pmatrix} 1 & -\frac{1}{4} \end{pmatrix}$

ϕ_{iN-1} 只与 ϕ_{iN-2} 耦合 $\begin{pmatrix} -\frac{1}{4} & 1 \end{pmatrix}$

形式解：

$$K\Phi = B.$$

$B = ?$ 内部$_{ij}$： $B = \begin{pmatrix} B_1 \\ B_2 \\ \vdots \\ B_{N-1} \end{pmatrix} \to \begin{pmatrix} B_{11} \\ B_{12} \\ \vdots \\ B_{1N-1} \end{pmatrix}$

$$B_{ij} = -\frac{h^2}{4} g_{ij}$$

与Φ的结构相似。

而第1行与第$N-1$行邻边，故

$$\phi_{1j} - \frac{1}{4}(\phi_{2j} + \underline{\underline{\phi_{0j}}} + \phi_{1j+1} + \phi_{1j-1}) = -\frac{h^2}{4} g_{1j}$$

$\frac{1}{4}\phi_{0j}$

或$\frac{1}{4} g_{0j}$

$$B_{1j} = -\frac{h^2}{4} g_{1j} + \frac{1}{4} g_{0j}$$

同理：

$$B_{N-1j} = -\frac{h^2}{4} g_{N-1j} + \frac{1}{4} g_{Nj}$$

而 每行第1个与第$N-1$个也邻边。

$$B_{i1} = -\frac{h^2}{4} g_{i1} + \frac{1}{4} g_{i0}$$

$$B_{iN-1} = -\frac{h^2}{4} g_{iN-1} + \frac{1}{4} g_{iN}$$

注 B_{11}，B_{1N-1}，B_{N-11}，B_{N-1N-1} 会有三项：体+横边+纵边.

解法：

(1) 直接法.

$$K\phi = B$$
$$\phi = K^{-1}B$$

(2) 随机游走：

$$K = I - P$$

$$(I-P)\phi = B$$
$$\phi = (I-P)^{-1}B$$
$$= (I+P+P^2+\cdots)B.$$

(3). 迭代法.

$$P = \begin{pmatrix} G_0 & \frac{I}{4} & & \\ \frac{I}{4} & G_0 & \frac{I}{4} & \\ & \frac{I}{4} & \ddots & \\ & & & \ddots \end{pmatrix}$$

$$G_0 = \begin{pmatrix} 0 & \frac{1}{4} & & \\ \frac{1}{4} & 0 & \frac{1}{4} & \\ & \frac{1}{4} & 0 & \ddots \\ & & & \ddots \end{pmatrix}$$

本征值问题：$P\phi = E\phi$

内部：$\phi_{i+1,j} + \phi_{i-1,j} + \phi_{i,j+1} + \phi_{i,j-1} = E\phi_{ij}$

P.S.

与二维晶格非常类似.

紧束缚近似.

实际上, 考虑二维正方晶格:

$$\hat{H} = \sum_{\langle ij \rangle} t\, c_i^\dagger c_j$$

$$=(c_1^\dagger \cdots c_N^\dagger)\begin{pmatrix} & & t & & \\ \text{列内} & t & 0 & t & \text{行内} \\ & & t & & \end{pmatrix}\begin{pmatrix} c_1 \\ \vdots \\ c_N \end{pmatrix} \quad N\text{个}$$

作Fourier Transformation.

$$\phi_{ij} = \sum_{ij} \phi_{k_1} e^{ik_1 i + ik_2 j}$$

内部, 本征方程:

$$\frac{1}{4}(\phi_{i+1j} + \phi_{i-1j} + \phi_{ij+1} + \phi_{ij-1}) = E\phi_{ij}$$

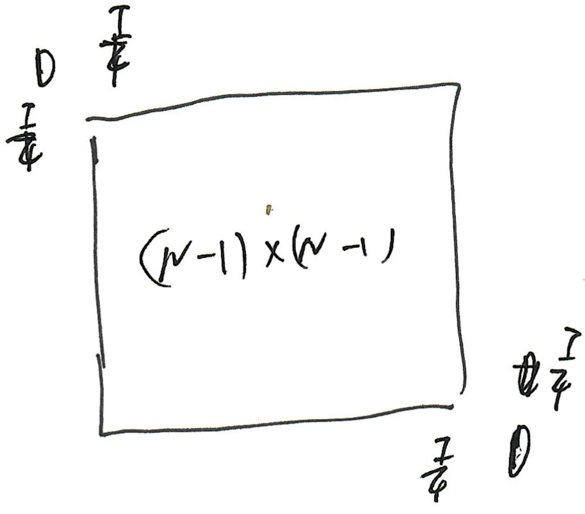
$$\Rightarrow \frac{1}{4}(e^{ik_1} + e^{-ik_1} + e^{ik_2} + e^{-ik_2}) = E$$

$$\Rightarrow E = \frac{1}{2}(\cos k_1 + \cos k_2).$$

边条件: 扩充. $(N-1)\times(N-1) \to N\times N$

$$\phi_{0j}=0,\ \phi_{Nj}=0,\ \phi_{i0}=0,\ \phi_{iN}=0.$$

解不变.



$$\phi = E\phi$$

简并: $\pm k_1$, $\pm k_2$ 共4种组合, 能量相同.

$$\phi_{ij} = \sum_{k_1 k_2} C(k_1, k_2)\, e^{ik_1 i + ik_2 j}$$

$$\phi_{ij} = A_1 e^{ik_1 i + ik_2 j} + A_2 e^{-ik_1 i + ik_2 j} + A_3 e^{-ik_1 i - ik_2 j} + A_4 e^{ik_1 i - ik_2 j}$$

$\Rightarrow$ $\cancel{A_1 + A_2 + A_3 + A_4 = 0}$

$\left.\begin{aligned} &A_1 + A_2 = 0 \\ &A_3 + A_4 = 0. \end{aligned}\right\} i = 0$

$\left.\begin{aligned} &A_1 e^{ik_1 N} + A_2 e^{-ik_1 N} = 0 \\ &A_3 e^{-ik_1 N} + A_4 e^{ik_1 N} = 0 \end{aligned}\right\} i = N \Rightarrow \sin k_1 N = 0$

$k_1 = \frac{\pi}{N} \cdot p$, $p = 1, \cdots, N-1$

$k_1 = 0$ 不是解

$\left.\begin{aligned} &A_1 + A_4 = 0 \\ &A_2 + A_3 = 0 \end{aligned}\right\} j = 0$

$\left.\begin{aligned} &A_1 e^{ik_2 N} + A_4 e^{-ik_2 N} = 0 \\ &A_2 e^{ik_2 N} + A_3 e^{-ik_2 N} = 0 \end{aligned}\right\} j = N$

$\Rightarrow \sin k_2 N = 0$ $k_2 = \frac{\pi}{N} \cdot q$, $q = 1, \cdots, N-1$

$k_2 = 0$ 不是解.

迭代.

$$\Phi_\infty = P\,\Phi_\infty + B.$$

$$\Phi^{(k)} = P\,\Phi^{(k-1)} + B.$$

$$\Delta\Phi_0 = \sum_{\vec{k}} \delta\psi(\vec{k})\, e^{i\vec{k}\cdot(i,j)}$$

$\Phi^{(0)}$

结合P的特征值, 收敛很慢.

$\cancel{P\Phi_0 + B}$

$\Delta\Phi^{(k)} = \Phi^{(k)} - \Phi_\infty$

$$\Rightarrow \Delta\Phi^{(k)} = P\,\Delta\Phi^{(k-1)}$$

$$P\,\Delta\Phi_0 = \sum_k E(k)\,\delta\psi(k)\, e^{i\vec{k}\cdot(i,j)}$$

$$P^{(k)}\Delta\Phi_0 = \sum_k E^k\,\delta\psi(k)\, e^{i\vec{k}\cdot(i,j)}$$

$$|E| < 1 \Rightarrow P^{(k)}\Delta\Phi_0 \to 0$$

收敛性:

$$\Delta \Phi^{(k)} = P \, \Delta \Phi^{(k-1)}$$

范数(长度) vector: $\|x\|_2 = (\sum x_i^2)^{\frac{1}{2}}$ (欧式范数)

矩阵范数: P $(n \times n)$

1 范数: $\max\limits_{j} \sum\limits_{i} |P_{ij}|$ (列和)

2 范数: $\max\limits_{i} |\lambda_i|$

∞ 范数: $\max\limits_{i} \sum\limits_{j} |P_{ij}|$ 行和

谱半径: $\rho(P) = \max\limits_{i} \{|\lambda_i|\}$

$$\rho(P) \le \|P\|$$

$$\|\Delta \Phi^{(k)}\|_2 = \| P \, \Delta \Phi^{(k-1)} \|_2$$
$$= \| S D S^{-1} \Delta \Phi^{(k-1)} \|_2$$
$$= \| D S^{-1} \Delta \Phi^{(k-1)} \|_2$$
$$\le \rho(P) \| S^{-1} \Delta \Phi^{(k-1)} \|_2$$
$$= \rho(P) \| \Delta \Phi^{(k-1)} \|_2$$

$\rho(P) < 1$ 则收敛.

判断 $\rho(P) \le \|P\|$

改善: Gauss-Seidel.

原理: 混合一部分旧的, 一部分新的, 方法:

$$\Phi^{(k)} = R \, \Phi^{(k-1)} + B$$

$$R = L + U \quad (R \text{对角元为} 0)$$

Φ例 L下消 $\begin{pmatrix} 0 & & \\ & 0 & 0 \\ 非0 & 0 & 0 \end{pmatrix}$，U上消 $\begin{pmatrix} 0 & & 非0 \\ & 0 & \\ 0 & 0 & 0 \end{pmatrix}$

改进：

$$\Phi_G^{(k)} = \overset{L}{\cancel{D}}\Phi^{(k)} + U\Phi^{(k-1)} + B$$

$$\Phi_{G,1}^{(k)} = \underset{\downarrow\ 0}{L_{1i}}\Phi_i^{(k)} + U_{1i}\Phi_i^{(k-1)} + B_1$$

$$\Phi_{G,i}^{(k)} = L_{ij}\Phi_j^{(k)} + U_{ij}\Phi_j^{(k-1)} + B_i$$

$i<j$ 非0　前已求出

$i\geq j = 0$

(收敛快些)

格式：

$$\phi_{ij}^{(k)} = \frac{1}{4}\left(\Phi_{i,j+1}^{(k-1)} + \Phi_{i+1,j}^{(k-1)} + \Phi_{i-1,j}^{(k)} + \Phi_{i,j-1}^{(k)} - h^2 q_{ij}\right)$$

$K = I - L - U$，(1) K 对称正定

(2) K 对角占优：$\begin{cases} |K_{ii}| \geq \sum_{j\neq i}|K_{ij}|, \forall i \\ \exists i, |K_{ii}| > \sum_{j\neq i}|K_{ij}| \end{cases}$

SOR (超松弛).

(1) 作为 Gauss-Seidel　当前　上一步

$$\Phi_{G\omega}^{(k)} = L\Phi_{\omega}^{(k)} + U\Phi_{\omega}^{(k-1)} + B$$

(2) 组合：
$$\Phi_\omega^{(k)} = \Phi_\omega^{(k-1)} + \omega\left(\Phi_G^{(k)} - \Phi_\omega^{(k-1)}\right)$$

$$= \omega\Phi_{G\omega}^{(k)} + (1-\omega)\Phi_{\omega}^{(k-1)}$$

$$= R_\omega \Phi_\omega^{(k-1)} + TB$$

$$R_\omega = \cancel{\omega(1-L)^{-1}U + (1-\omega)I}\ (I-\omega L)^{-1}(\omega L + (1-\omega)I)$$

$$T = \omega(I-\omega L)^{-1}B.$$

$$\omega \Phi_{GS}^{(k)} + (1-\omega)\Phi_{\omega}^{(k-1)}$$

格式：$\phi_{ij}^{(k)} = (1-\omega)\phi_{ij}^{(k-1)} + \frac{\omega}{4}\left(\phi_{i,j+1}^{(k-1)} + \phi_{i+1,j}^{(k-1)} + \phi_{i,j-1}^{(k)} + \phi_{i-1,j}^{(k)} - h^2 g_{ij}\right)$

收敛性：若 $K = I - L - U$ 对称正定，且 $0 < \omega < 2$，

则 $\rho(R_\omega) < 1$

如何选 ω？

$K = D - L - U$

若 $J = I - D^{-1}K$.

J只有实本征值，且 $\mu = \rho(J) < 1$

$K = D - L - U$ 满足：$\det(\lambda D - zL - \frac{1}{z}U) = \det(\lambda D - L - U)$ for complex z.

$$\rho(R_\omega) = \begin{cases} \frac{1}{4}\left[\omega\mu + \sqrt{\omega^2\mu^2 - 4(\omega-1)}\right]^2, & 0 < \omega < \omega_0 \\ \omega - 1 \nearrow, & \omega_0 < \omega < 2 \end{cases}$$

$$\omega_0 = 1 + \left(\frac{\mu}{1+\sqrt{1-\mu^2}}\right)^2 = \frac{2}{1+\sqrt{1-\mu^2}} > 1$$

$\omega\mu + \sqrt{\omega^2\mu^2 - 4(\omega-1)}$ 递减：

$$\frac{d}{d\omega}: \mu + \frac{\omega\mu^2 - 2\omega}{\sqrt{}} < 0$$

$$\Leftrightarrow \sqrt{} < \frac{2}{\mu} + \omega\mu$$

$$\Leftrightarrow 4 < \frac{4}{\mu^2}$$

ω_0 是最优选，$\rho(R_{\omega_0})$ 最小。

特解：$\omega=1$

$$\rho(R_G)=\frac{1}{4}(\mu+\sqrt{\mu^2-0})^2=\mu^2=\rho^2(J)$$

正方区域：$J=I-D^{-1}K$，$D=I$

$$\Rightarrow J=I-K=P.$$

$$\rho(R_G)=\rho^2(P)$$

$$Eig(P)=\frac{1}{2}\left(\cos\frac{i}{n}\pi+\cos\frac{j}{n}\pi\right),\quad i,j=1,\cdots n-1$$

最优解：$\rho(J)=\cos\frac{n-1}{n}\pi=\mu$

$$\omega=\frac{2}{1+\sqrt{1-\mu^2}}=\frac{2}{1+\sin\frac{\pi}{n}}$$

$$\rho(R_{\omega_0})=\omega_0-1=\frac{1-\sin\frac{\pi}{n}}{1+\sin\frac{\pi}{n}}$$

若，横 n 份，纵 m 份，则

$$\rho(P)\ Eig(P)=\frac{1}{2}\left(\cos\frac{n-1}{n}\pi+\cos\frac{m-1}{m}\pi\right)$$

$$\omega_0=\frac{2}{1+\sqrt{1-\frac{1}{4}(\cos\frac{\pi}{n}+\cos\frac{\pi}{m})^2}}$$

$$\approx\frac{2}{1+\sqrt{1-\frac{1}{4}(1-\frac{\pi^2}{2n^2}+1-\frac{\pi^2}{2m^2})^2}},\quad \rho(R_\omega)=\omega_0-1$$

$$=\frac{2}{1+\sqrt{\frac{\pi^2}{2}(\frac{1}{n^2}+\frac{1}{m^2})}}$$

$$\approx 2\left(1-\sqrt{\frac{\pi^2}{2}\left(\frac{1}{n^2}+\frac{1}{m^2}\right)}\right)$$

$$=2-\pi\sqrt{2\left(\frac{1}{n^2}+\frac{1}{m^2}\right)}$$

一般情况，若不知

$\rho(J)=\mu$，怎么办!

(i) 选 ω_t，进行多次迭代 $(n\gg 1)$

(ii) 误差: $\Delta\Phi^{(k)} = \lambda\, \Delta\Phi^{(k-1)}$

$$\lambda \approx \rho(R_{\omega_t})$$

(iii) $$\lambda = \frac{1}{4}\left(\omega_t\mu + \sqrt{\omega_t^2\mu^2 - 4(\omega_t-1)}\right)^2$$

$$\Rightarrow \mu = \left|\frac{1-\omega_t-\lambda}{\omega_t\sqrt{\lambda}}\right|$$

(iv) 代入 $\omega_0 = \dfrac{2}{1+\sqrt{1-\mu^2}}$ 算 ω_0

(v) 判断 $\omega \le \omega_0$，否则继续重选 ω_t，直到满足此不等式.

谱分解:

$$\hat{L}\phi = Q, \quad \vec{r} \in D$$

$\hat{T}\phi|_{\partial D}=0$ [如 $\phi|_{\partial D}=0$ 或 $\frac{\partial\phi}{\partial n}|_{\partial D}=0$]

且边界较规则，如正方形，长方形，圆形.

方法: 正傅: 延拓成周期函数.

$\phi = \sum_n c_n \phi_n$

$\langle \psi_m | L\phi - a \rangle = 0$

取 $\psi_m = \phi_m$

$\langle \phi_m | L\phi - a \rangle = 0$ → 要算二维积分.

书中问题：沿一个方向分离变量

$\phi(x,y) = \sum B_j(x) \sin\frac{\pi j y}{L}$

↑ y方向的基函数.

具体做法：x, y 方向都划分为 2^N 个 $= n$.

$\sin\frac{\pi}{n} j i = \pm \sin\frac{\pi}{n}(n-j) i$

对于 y 方向：$y_i = \frac{L}{n} \cdot i$

$\sin\frac{\pi j}{L}\cdot\frac{L}{n} i = \sin\frac{\pi}{n} j i$, $j = 1, 2, \cdots, n-1$

故 j 只能取 $1, 2, \cdots, \frac{n}{2}$.

α $\quad$ $n-\alpha$

$\sin\frac{\pi}{n}\alpha i$ $\quad$ $\sin\frac{\pi}{n}(n-\alpha) i = \pm \sin\frac{\pi}{n}\alpha i$

不独立.

将 $a(x,y)$ 作离散傅里叶变换:

$a(x,y) = \sum_j C_j(x) \sin\frac{\pi j y}{L}$

对于 x 方向有: $B_j''(x) - \left(\frac{\pi j}{L}\right)^2 B_j(x) = C_j(x)$

$B_j(0) = B_j(L) = 0$

$$\frac{B_j^{i-1}+B_j^{(i+1)}-2B_j^{(i)}}{h^2}-\left(\frac{\pi j}{L}\right)^2 B_j^i=C_j^i$$

$$\Rightarrow B_j^{(i-1)}-\lambda_j B_j^{(i)}+B_j^{(i+1)}=h^2C_j^i$$

$$\lambda_j=\left(\frac{\pi j}{L}h\right)^2+2$$

$$i\to x=\frac{L}{n}i$$

$$B_j^{(i-1)}-\lambda_j B_j^{(i)}+B_j^{(i+1)}=h^2C_j^i \quad \times\lambda_j$$

$$B_j^{(i-2)}-\lambda_j B_j^{(i-1)}+B_j^{(i)}=h^2C_j^{i-1}$$

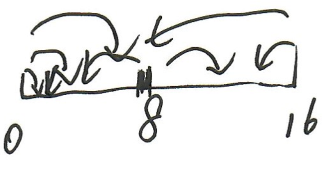
$$B_j^{i}-\lambda_j B_j^{(i+1)}+B_j^{(i+2)}=h^2C_j^{i+1}$$

$$B_j^{(i-2)}-\lambda_j^2 B_j^{(i)}+B_j^{(i)}+\lambda_j B_j^{(i+1)}=h^2(\lambda C_j^i+C_j^{i-1})$$

$$B_j^{(i-2)}-\lambda_j^2 B_j^i+2B_j^{(i)}+B_j^{(i+2)}=h^2(\lambda C_j^i+C_j^{i-1}+C_j^{i+1})$$

$$\Rightarrow B_j^{(i-2)}-\lambda_j' B_j^i+B_j^{(i+2)}=h^2 - -$$

$$\lambda_j'=\lambda_j^2-2$$



2分求解.