2021.9.30.

目的：$\{-\frac{\hbar^2}{2m}\nabla^2+V(x)\}\psi(x)=E\psi(x)$

Method：有限差分方法.

要求 1D, 2D Schrödinger Equation

缺点：内存随维度增长而增长。

3D：$\underline{\underline{N^3}}$

双倍以指数.

步骤：① 无量纲化待求解的方程.

② 离散化无量纲后的方程.

$$\begin{cases}\frac{\partial}{\partial x}\psi(x)\simeq\frac{\psi(x+h)-\psi(x)}{h}+o(h)\\ \frac{\partial^2}{\partial x^2}\psi(x)\simeq\frac{\psi(x+h)-2\psi(x)+\psi(x-h)}{h^2}+o(h^2)\end{cases}$$

取一个有限的 h，而不是 $h\to 0$（有限差分）

Schrödinger 方程 $\left(-\frac{1}{2}\frac{\partial^2}{\partial x^2}+V(x)\right)\psi(x)=E\psi(x)$

$\Downarrow$

$$-\frac{1}{2}\frac{1}{h^2}(\psi_{i-1}+\psi_{i+1}-2\psi_i)+V_i\psi_i=E\psi_i$$

$H|\psi\rangle=E|\psi\rangle$

$$H=\begin{pmatrix}\frac{1}{h^2} & -\frac{1}{2h^2} & & \\ -\frac{1}{2h^2} & \frac{1}{h^2} & -\frac{1}{2h^2} & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots\end{pmatrix}+\begin{pmatrix}V_1 & & & \\ & V_2 & & \\ & & \ddots & \\ & & & V_N\end{pmatrix}$$

难点：(1d)

1> 稀疏矩阵，三对角矩阵。

2> $h \to 0$ 时，动能似乎发散，如何理解？

作业：

① $V(x) = \frac{1}{2} m\omega^2 x^2$

比较数值结果与精确结果的误差。(分离散长度 h？量子数 n？)

误差 10^{-7}. $h \sim 10^{-3} \sim 10^{-4}$

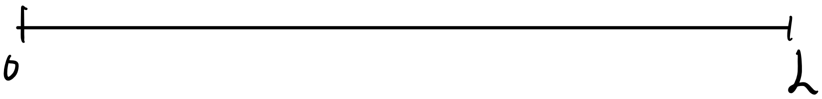
② $V(x) = \frac{1}{2} m\omega^2 x^2 + A\cos(kx+\theta)$

① 数值

② 微扰解 (A 小时)

低能的态，精确至二阶

考虑



$$\begin{cases} \psi(0) = \psi(L) = 0. \\ \psi'(0) = \psi'(L) = 0 \\ -\frac{1}{2}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \end{cases}$$

解是 $\psi \sim \sin\left(\frac{2\pi n x}{L}\right)$，$E = \frac{n^2\pi^2}{2L^2}$

离散化

$$H = -\frac{1}{2h^2}\begin{pmatrix} -2 & 1 & & & \\ 1 & -2 & 1 & & \\ & \ddots & \ddots & \ddots & \\ & & \ddots & \ddots & \ddots \\ & & & \ddots & \ddots \end{pmatrix}$$

对角化后得到 $E(h)$. 而

$$E = \lim_{h\to 0} E(h) = \frac{n^2\pi^2}{2L^2}$$

方程形式为

$$-\frac{1}{2h^2}(\psi_{i+1} + \psi_{i-1} - 2\psi_i) = E\psi_i$$

☆ 解是什么样子的.

$$\begin{cases} a_{n+1} = x a_n + y a_{n-1} \\ \text{令 } a_n = q^n. \end{cases}$$

令 $\psi_n = e^{iknh}$

$$\Rightarrow -\frac{1}{2h^2}(e^{ikh} + e^{-ikh} - 2) = E$$

$$\Rightarrow E(h) = \frac{1}{h^2}(1 - \cos(kh))$$

$$\simeq \frac{1}{h^2}\left(1 - 1 + \frac{1}{2}k^2h^2 + o(h^2)\right)$$

$$\overset{\lim h\to 0}{=} \frac{1}{2}k^2$$

边界条件：

$$\psi_n = A e^{iknh} + B e^{-iknh}$$

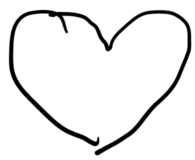
$$\begin{cases} -2\psi_1 + \psi_2 = E\psi_1 \\ \psi_{N-1} - 2\psi_N = E\psi_N \end{cases}$$

⇒ 代入求解出 k

⇒ $E_n = \frac{n^2\pi^2}{2L^2}$.

作业. 2D下推广

1)  操场

2)  心型.

内部势能为零，波函数在边界上等于0

$$V(x) = \begin{cases} 0, & \text{区域内} \\ \text{Infinite}, & \text{区域外} \end{cases}$$

1000~10000，足够

二维下的偏微分方程.

$$-\frac{1}{2}\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right)\psi(x,y) + V(x,y)\psi(x,y) = E\psi(x,y)$$

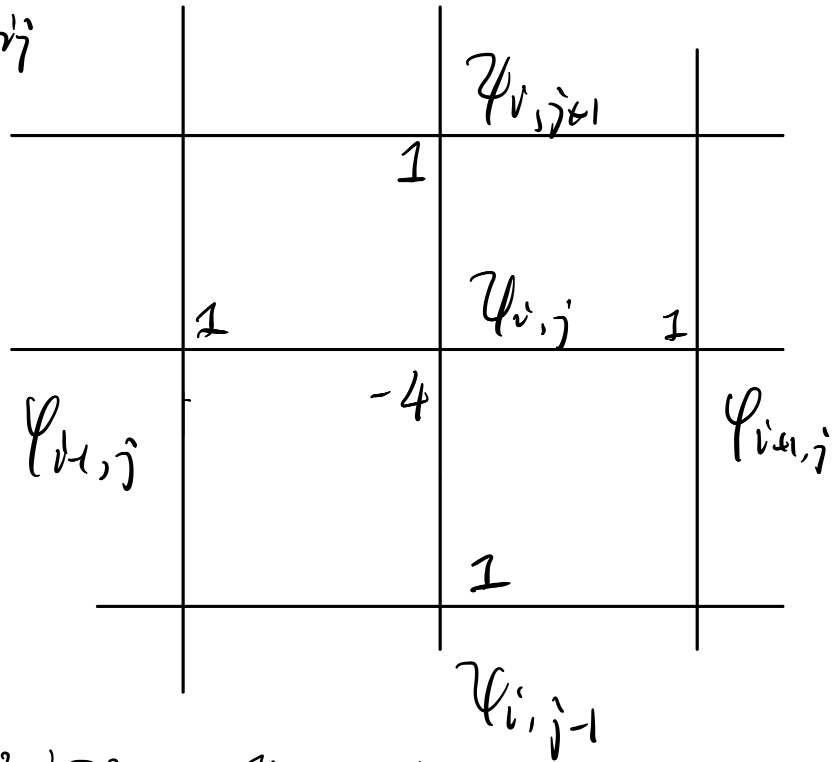
⇒ 离散化

$$-\frac{1}{2h^2}\left(\psi_{i+1,j} + \psi_{i-1,j} - 2\psi_{i,j} + \psi_{i,j+1} + \psi_{i,j-1} - 2\psi_{i,j}\right)$$

$+ V_{ij}\psi_{ij} = E\psi_{ij}$

或者

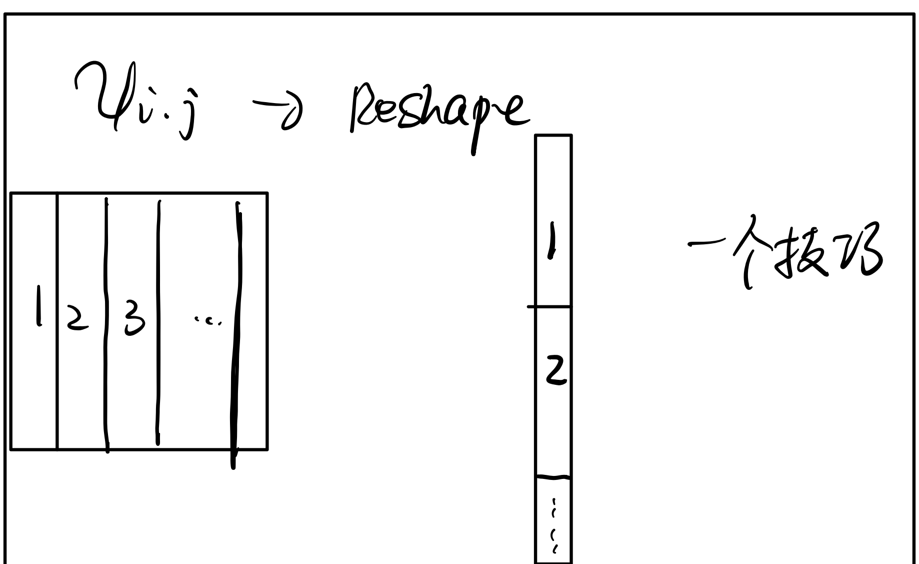
$$-\frac{1}{2h^2}(\psi_{i+1,j}+\psi_{i-1,j}+\psi_{i,j+1}+\psi_{i,j-1}-4\psi_{i,j}) + V_{ij}\psi_{ij} = E\psi_{ij}$$



特点、①稀疏矩阵，非三对角阵.

② 矩阵维度 正比于离散点、N^2, ($N=\frac{x}{h}$)

e.g. x方向100个点、矩阵维度 $N = 10000$

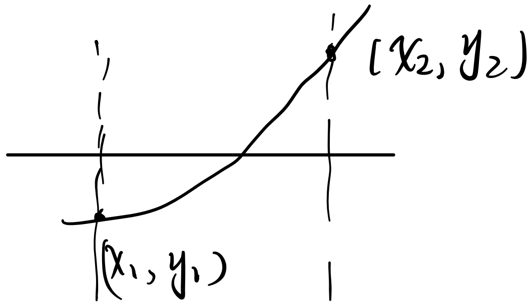


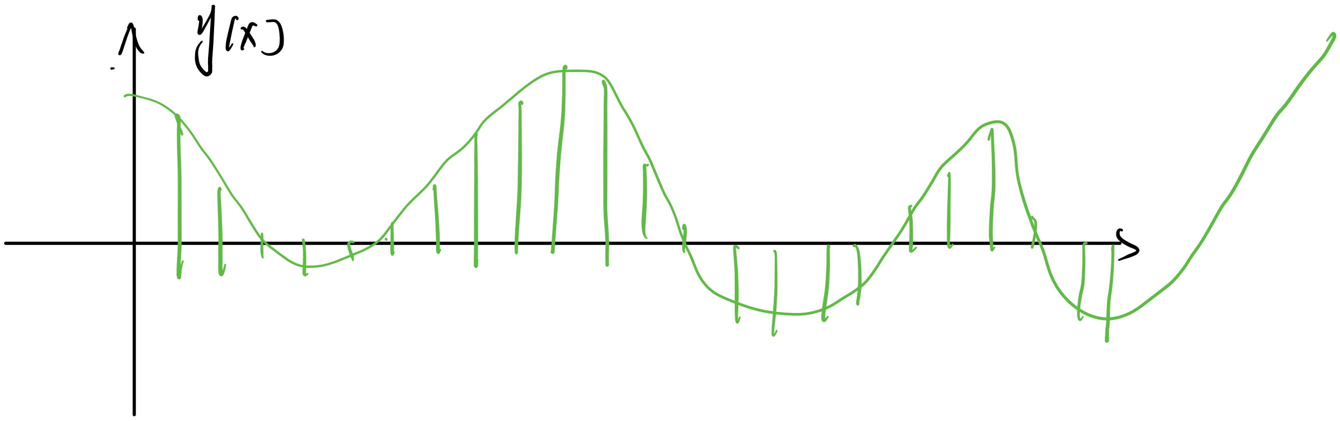
一个技巧

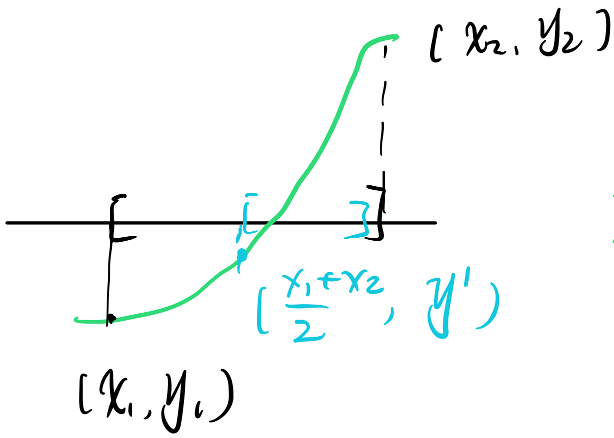
求根（二分法）

$x_1x_2<0$，

系统至少存在两个解.





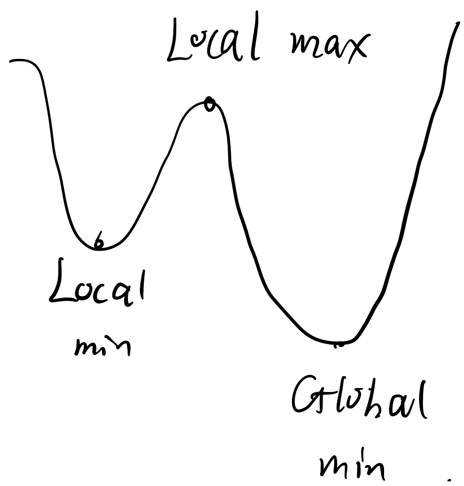


二分法.

不停找.　还会讲牛顿法.

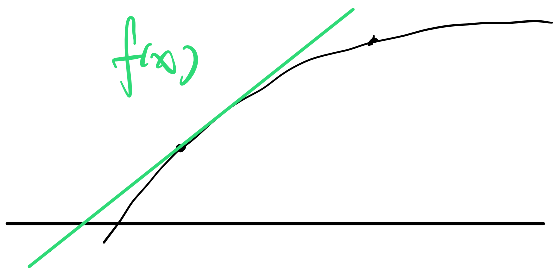
思想 | 求根 / 极值

$$\begin{cases} F(x)\ \text{极小值}. \\ \frac{\partial F(x)}{\partial x} = 0 \end{cases}$$



牛顿法

$$f(x) = f(x_0) + f'(x_0)(x - x_0)$$



$$f(x) = 0$$
$$\Downarrow$$
$$f(x_0) + f'(x_0)(x - x_0) = 0$$
$$\Downarrow$$
$$x = x_0 - \frac{f(x_0)}{f'(x_0)}$$

$$\lim_{n\to\infty} x_n = x^* \Leftrightarrow x^* = x^* - p\frac{f(x^*)}{f'(x^*)}$$
$$\Leftrightarrow f(x^*) = 0$$

推广高维

$$f(\vec{x}) = f(\vec{x}_0) + \frac{\partial f}{\partial x^i}(x^i - x_0^i) = 0$$

$$\vec{x} = \vec{x}_0 + (\qquad)$$

求解 $\begin{cases} y' = f(x, y) \\ \frac{\partial^2}{\partial t^2} u(\vec{x}, t) = a^2 \nabla^2 u(\vec{x}, t) \end{cases}$

龙格-库塔方法

mma 中 $\begin{cases} \text{DSolve} \\ \text{NDSolve} \end{cases}$

一个程序

matlab ode

ode45

$$y' = f(x, y)$$

$$y(x_{n+1}) = y(x_n) + f(x_n, y_n)h$$

(x_1, y_1)

$\downarrow$

(x_2, y_2)

$\downarrow$

$\vdots$

$$x_{n+1} = x_n + h$$

向后，隐式的方法

$$y_{n+1} = y_n + \frac{h}{2} f(x_n, y_n) + \frac{h}{2} f(x_{n+1}, y_n + h f(x_n, y_n))$$