Review

矩阵复习，矩阵 → 本征值

$\begin{cases} Ax=b \\ \text{本征值问题} \end{cases}$ — 方阵 / 非方阵 $\begin{cases} LU\text{分解} \\ QR\text{分解} \\ SVD\text{分解} \end{cases}$

$\frac{\partial}{\partial t}P = D\frac{\partial^2}{\partial x^2}P$ $\begin{cases} \text{① 降阶} \\ \text{② 差分} \\ \text{③ } x\text{差分，}t\text{龙格库塔} \end{cases}$

概率问题

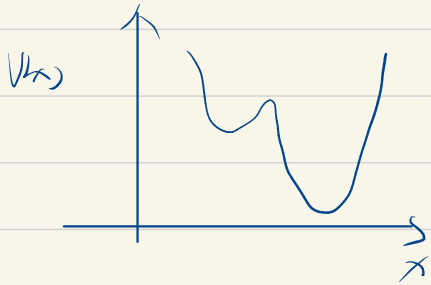
$X = \frac{1}{n}(x_1 + x_2 + \cdots x_n)$

$P(X) \sim N(\mu, \frac{\sigma^2}{n})$

求本征值

$$H = -\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + V(x)$$

$\underline{H\varphi(x) = E\varphi(x)}$，边界条件



① 无量纲化

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\varphi(x) + V(x)\varphi(x) = E\varphi(x)$$

令 $x = ay$，则 ⇓

$$-\frac{\hbar^2}{2ma^2}\frac{d^2}{dy^2}\varphi(y) + V(y)\varphi(y) = E\varphi(y)$$

$$\Rightarrow \frac{\hbar^2}{ma^2}\left(-\frac{1}{2}\frac{d^2}{dy^2} + u(y)\right)\varphi(y) = E\varphi(y)$$

估计 $\frac{\hbar^2}{ma^2}$ 的量级

$$\Rightarrow \boxed{\left(-\frac{1}{2}\frac{d^2}{dy^2}+u(y)\right)\varphi(y)=\frac{E}{\frac{\hbar^2}{ma^2}}\cdot\varphi(y)}$$

$\Uparrow$

无量纲的微分方程

差分

$$-\frac{1}{2}\cdot\frac{\varphi_{n+1}+\varphi_{n-1}-2\varphi_n}{(\Delta x)^2}+u_n\varphi_n=\tilde{E}\varphi_n$$

$\Downarrow$

$$\left\{-\frac{1}{2(\Delta x)^2}\begin{pmatrix}-2 & 1 & & \\ 1 & -2 & 1 & \\ & \ddots & \ddots & \ddots \\ & & \ddots & \ddots\end{pmatrix}+\begin{pmatrix}u_1 & & & \\ & u_2 & & \\ & & \ddots & \\ & & & u_N\end{pmatrix}\right\}\begin{pmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \varphi_N\end{pmatrix}=E\begin{pmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \varphi_N\end{pmatrix}$$

作业.

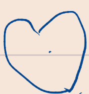
① $H=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2+A\sin(bx)$

求解 $H\varphi(x)=E\varphi(x)$

能级是否是等间距的？

② 求解如下形状的势阱中的

$H\varphi=E\varphi$.



心形势

开边界

$\varphi_0=\varphi_{N+1}=0$

$$\Rightarrow H\begin{pmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \varphi_N\end{pmatrix}=E\begin{pmatrix}\varphi_1\\ \varphi_2\\ \vdots\\ \varphi_N\end{pmatrix}$$ 转化为矩阵求本征值问题.

$$H = -\frac{1}{2(\Delta y)^2}\cdot\begin{pmatrix} -2 & 1 & & & 0 \\ 1 & -2 & 1 & & \\ & 1 & -2 & 1 & \\ & & \ddots & \ddots & \ddots \\ 0 & & & \ddots & \ddots \end{pmatrix} + \begin{pmatrix} u_1 & & & \\ & u_2 & & \\ & & \ddots & \\ & & & u_N \end{pmatrix}$$

更高精度的差分方法

$$\frac{d^2}{dy^2}\psi(y) = a_1[\psi(y+2dy)+\psi(y-2dy)] + a_2[\psi(y+dy)+\psi(y-dy)] + a_3\psi(y)$$

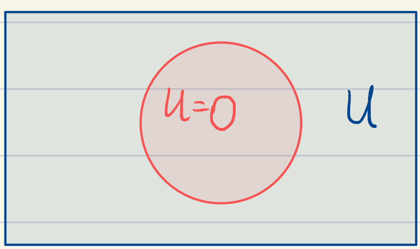
泰勒展开

$$= (2a_1+2a_2+a_3)\psi(y) + \left[\frac{2}{2!}a_1(2dy)^2 + \frac{2}{2!}a_2(dy)^2\right]\psi''(y) + (\ldots\ldots)\psi^{(4)}(y) + O(dy^4)$$

令四阶导数为0，我们可以得到更高阶的运动方程。

2维下的方程

$$-\frac{1}{2}\left(\frac{d^2}{dx^2}+\frac{d^2}{dy^2}\right)\psi(x,y) + U(x,y)\psi(x,y) = E\psi(x,y)$$



在区域外使用一个有限的势能

在区域内使用等于零的势能。

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

$$-\frac{1}{2}\frac{1}{dy^2}\left(\psi_{i,j+1} + \psi_{i,j-1} - 2\psi_{i,j}\right) + U_{ij}\psi_{ij} = E\psi_{ij}$$

$$\Rightarrow \quad \Psi = \begin{pmatrix} \psi_{11} \\ \psi_{12} \\ \psi_{13} \\ \vdots \\ \psi_{21} \\ \psi_{22} \\ \vdots \end{pmatrix} \Leftarrow \text{将二维的波函数写成一个一维的矢量.}$$

$\vdots$