Schrödinger Equation.

$$i\hbar \frac{\partial}{\partial t} |\varphi\rangle = H|\varphi\rangle. \qquad H = \hat{T} + \hat{V}.$$

$$|\varphi\rangle = |x\rangle e^{-iEt/\hbar}.$$

$$E|x\rangle = \hat{H}|x\rangle$$ Eigen problem

Stationary solution

Free particle

$$\hat{H} = \hat{T} = \frac{p^2}{2m}. \qquad \langle x|p = -i\hbar \frac{\partial}{\partial x} \langle x|.$$

$$\langle x| \frac{p^2}{2m} |x\rangle = \langle x| E |x\rangle$$

$$-\frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \chi(x) = E\chi(x)$$

$$\chi(x) = Ce^{ikx} = \langle x|p\rangle = \frac{1}{\sqrt{2\pi\hbar}} \cdot e^{\frac{ipx}{\hbar}}$$

$$\frac{\hbar^2}{2m} k^2 = E. \qquad k = \pm\sqrt{\frac{2Em}{\hbar^2}} \qquad p = \hbar k.$$

$$\hat{p}|p\rangle = p|p\rangle.$$

$$\hat{H}|p\rangle = \frac{\hat{p}^2}{2m} |p\rangle = \frac{p^2}{2m} |p\rangle$$

orthogonal :

$$\langle p'|p\rangle = \int \langle p'|x\rangle\langle x|p\rangle dx$$

$$= \int dx \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{-ip'x}{\hbar}} \cdot \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}$$

记住.

$$= \frac{1}{2\pi\hbar} \int dx \cdot e^{\frac{-i(p'-p)x}{\hbar}} = \delta(p'-p) = \begin{cases} \infty. & p = p' \\ 0. & p \neq p' \end{cases}$$

completiness : 完整性.

$$\langle x|\alpha\rangle = \int dp \langle x|p\rangle\langle p|\alpha\rangle$$

$$\alpha(x) = \int dp \underbrace{\langle p|\alpha\rangle}_{\alpha(p)} \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{ipx}{\hbar}}$$

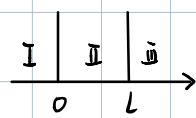
$$\alpha(p) = \int dx \langle p|x\rangle\langle x|\alpha\rangle$$

$$= \frac{1}{\sqrt{2\pi\hbar}} \int dx \, \alpha(x) e^{\frac{-ipx}{\hbar}}$$

一维势阱.

Particle in a box:

$$H = \frac{p^2}{2m} + V(x)$$



$$V(x) = \begin{cases} \infty & x \le 0 & \text{I} \\ 0 & 0 < x < L & \text{II} \\ \infty & x \ge L. & \text{III} \end{cases}$$

势能

$$\left(-\frac{\hbar^2}{2m} \cdot \frac{\partial^2}{\partial x^2} + V\right) \varphi(x) = E\varphi(x)$$

$$\varphi_{\text{I}} = \varphi_{\text{III}} = 0$$

$0 < x < L$. $$-\frac{\hbar^2}{2m} \cdot \frac{\partial^2}{\partial x^2} \varphi_{\text{II}}(x) = E\varphi_{\text{II}}(x)$$

$$\varphi_{\text{II}}(x) = C_1 e^{ikx} + C_2 e^{-ikx}$$ 表示平面波.

$$e^{ikx} = \cos(kx) + i\sin(kx).$$

$$= C_1[\cos(kx) + i\sin(kx)] + C_2[\cos(kx) - i\sin(kx)]$$

$$= \underbrace{(C_1 + C_2)}_{A} \cos kx + i\underbrace{(C_1 - C_2)}_{B} \sin kx$$

$\varphi(x=0) = 0$. $\varphi(x=L) = 0$.

$$\therefore A\cos(k \cdot 0) + B\sin(k \cdot 0) = 0 \Rightarrow A = 0$$

$$A\cos(kL) + B\sin(kL) = 0$$

$$\Downarrow$$

$$B\sin(kL) = 0.$$

$$kL = \pm n\pi.$$

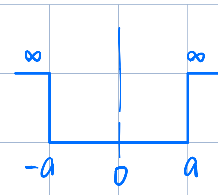
$$k = \pm\frac{n\pi}{L}. \quad n = 1, 2, 3, \cdots$$

$$\varphi_{\text{II}}(x) = B\sin\left(\pm\frac{n\pi}{L}x\right) = \underbrace{\pm B}_{C} \sin\left(\frac{n\pi}{L}x\right).$$

$$\varphi_{\text{II}}'(x) = C \cdot \frac{n\pi}{L} \cos\left(\frac{n\pi}{L}x\right).$$

$$\varphi_{\text{II}}''(x) = -C \cdot \left(\frac{n\pi}{L}\right)^2 \sin\left(\frac{n\pi}{L}x\right).$$

$$-\frac{\hbar^2}{2m}(-C)\left(\frac{n\pi}{L}\right)^2 \sin\left(\frac{n\pi}{L}x\right) = EC\sin\left(\frac{n\pi}{L}x\right).$$



$$V(x) = \begin{cases} 0. & |x| < a \\ \infty & |x| > a \end{cases}$$

$$\hat{H} = \frac{p^2}{2m} + V(x).$$

$|x| < a$. $H = \frac{p^2}{2m}$. 代入 $H\varphi = E\varphi$.

(定态薛定谔方程. 即不随时间变化)

$$-\frac{\hbar^2}{2m} \cdot \frac{d^2}{dx^2}\varphi = E\varphi.$$

$$\frac{d^2}{dx^2}\varphi + \frac{2mE}{\hbar^2}\varphi = 0.$$ 即 $\varphi'' - k^2\varphi = 0$.

二维微分方程有通解.

通解形式

① $\varphi = A\sin kx + B\cos kx$

② $\varphi = Ae^{ikx} + Be^{-ikx}$

③ $\varphi = A\sin(kx + \delta)$

选择①计算.

$\because \varphi(x=-a) = 0$. $\varphi(x=a) = 0$

$$\therefore \begin{cases} A\sin ka + B\cos ka = 0 \\ -A\sin ka + B\cos ka = 0. \end{cases}$$

$$\Rightarrow \begin{cases} B\cos ka = 0 \\ A\sin ka = 0 \end{cases}$$

$\Rightarrow \begin{cases} A = 0. \\ \cos ka = 0 \end{cases}$ 即 $ka = \frac{\pi}{2}n$. n为奇

或 $\begin{cases} B = 0 \\ \sin ka = 0 \end{cases}$ 即 $ka = \frac{\pi}{2}n$. n为偶.

$$\because k^2 = \frac{2mE}{\hbar^2} = \left(\frac{\pi n}{2a}\right)^2$$

$$\therefore E = \frac{\pi^2 n^2}{4a^2} \cdot \frac{\hbar^2}{2m} = \frac{\pi^2 n^2 \hbar^2}{8ma^2}.$$

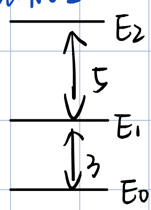
n为奇. $$\varphi_n = \begin{cases} B\cos\frac{n\pi}{2a}x. & |x| < a \\ 0. & |x| > a \end{cases}$$

n为偶. $$\varphi_n = \begin{cases} A\sin\frac{n\pi}{2a}x. & |x| < a \end{cases}$$

$0. \quad |x|>a$

E是 $\hat{H}|\psi\rangle = E|\psi\rangle$ 的本征值.

哈密顿量的本征值代表能量.



$$E = \frac{\hbar^2}{2m}\cdot\left(\frac{n\pi}{L}\right)^2. \quad n=1,2,3,\cdots$$

$$E_0 = \frac{\hbar^2}{2m}\frac{\pi^2}{L^2}. \quad n=1$$

$$E_1 = \frac{\hbar^2}{2m}\cdot\frac{4\pi^2}{L^2} = 4E_0. \quad n=2.$$

$$E_2 = 9E_0. \quad n=3.$$

$$E_n = n^2 E_0$$

$\Downarrow$

$$\varphi_n = \begin{cases} D\sin\frac{n\pi}{2a}(x+a). & |x|<a \\ 0. & |x|>a. \end{cases}$$

$$\varphi_n(x) = C_n\sin\left(\frac{n\pi}{L}x\right)$$

求波函数需进行归一化.

$$\int_0^L |\varphi_n(x)|^2 = 1.$$

$$|C_n|^2\int_0^L \sin^2\left(\frac{n\pi}{L}x\right)dx = 1.$$

$$\int_0^L \frac{1-\cos\left(\frac{2n\pi}{L}x\right)}{2}dx$$

$$|C_n|^2\cdot\frac{L}{2} = 1. \quad C_n = \sqrt{\frac{2}{L}}.$$

$$\varphi_n(x) = \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi}{L}x\right).$$

$$\int_{-a}^{a}\psi^*\psi\,dx = 1.$$

$$1 = \int_{-a}^{a}|D|^2\sin^2\frac{n\pi}{2a}(x+a)\,dx$$

$$|D| = \frac{1}{\sqrt{a}}.$$

$$\varphi_n = \begin{cases} \frac{1}{\sqrt{a}}\sin\frac{n\pi}{2a}(x+a). & |x|<a \\ 0. & |x|>a. \end{cases}$$

Fourier Series. 傅立叶级数

$f(0)=0. \quad f(L)=0.$

$$f(x) = \sum_n a_n\varphi_n(x).$$

$f(x)$是包含所有情况的总波函数.

以 $\sin nx$ 和 $\cos nx$ 为基，所有函数都可以展开.

Complete. 完备.

$$f(x) = \sum_n a_n\varphi_n(x)$$

For any smooth function with $\begin{cases} f(x=0)=0. \\ f(x=L)=0. \end{cases}$ $\Rightarrow$ 正弦函数.

$$g(x) = \sum_n a_n\varphi_n(x).$$

$$\varphi_n(x) = \sqrt{\frac{2}{L}}\cos\left(\frac{n\pi}{L}x\right).$$

$\begin{cases} g(x=-\frac{L}{2})=0 \\ g(x=\frac{L}{2})=0 \end{cases}$ $\Rightarrow$ 余弦函数.

Orthogonal 为了证明该组傅立叶级数可以做为一组基.

$$\langle \varphi_n | \varphi_m \rangle = \delta_{nm} = \begin{cases} 1 & n=m. \\ 0 & n\neq m. \end{cases}$$ (任意两者都正交)

$$\int \langle \varphi_n | x \rangle \langle x | \varphi_m \rangle \, dx = \int_0^L \varphi_n^*(x)\, \varphi_m(x) \, dx$$

$$= \int_0^L \frac{2}{L} \sin\left(\frac{n\pi}{L} x\right) \sin\left(\frac{m\pi}{L} x\right) dx$$ 积化和差.

$$= \int_0^L \frac{1}{2}\left[\cos \frac{(n-m)\pi}{L} x - \cos \frac{(n+m)\pi}{L} x \right] dx. \quad n,m = 1,2,3,\ldots$$

$$= \delta_{nm}$$

画图.

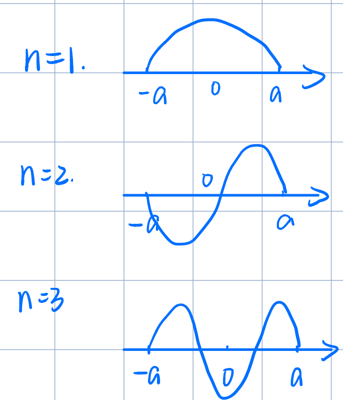
$\varphi(x_n) = 0. \quad 0 < x < L.$

x_n is nth node.

$\varphi_{m=2}, \; x_1 = \frac{L}{2}.$

$\varphi_{m=3}.$ 2 nodes

$\varphi_m(x)$, I have $m-1$ nodes. 节点



数学物理方法.

Sturm - Liouville eigen problems

$$a_2(x)\frac{\partial^2}{\partial x^2} y + a_1(x)\frac{\partial}{\partial x} y + a_0(x) y = f(x).$$

$$L = a_2(x)\frac{\partial^2}{\partial x^2} + a_1(x)\frac{\partial}{\partial x} + a_0(x)$$ is my operator.

$Ly = f(x) \; = 0$ homogeneous 均匀的

$\neq 0$ In homogeneous. 不均匀的

$Ly = \lambda y.$ y is a function x.

L is a functional.

$$\langle x | H | \varphi \rangle \stackrel{\langle x|}{=} E |\varphi\rangle.$$

$$\left(-\frac{\hbar^2}{} \frac{\partial^2}{} + V(x) \right) \varphi(x) = E\varphi(x)$$

$(\ \ 2m\ \partial x^2 \ \ldots$

$Ly = -\lambda \sigma(x) y.$

$L = \frac{d}{dx}\left(p(x)\frac{d}{dx}\right) + q(x)$

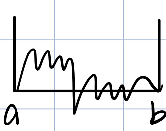
$\frac{d}{dx}\left(p(x)\frac{d}{dx}\right)y + q(x)y + \lambda\sigma(x)y = 0. \qquad x \in (a,b)$

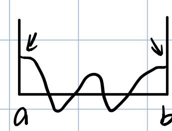
$p(x).\ p'(x).\ q(x).\ \sigma(x)$ to be continuous on (a,b).

$p(x) > 0.\ \ \sigma(x) > 0$ on $[a,b]$.

$y(x=a) = 0$
$y(x=b) = 0$ fixed boundry condition

$y'(x=a) = 0$
$y'(x=b) = 0$





open boundry condition

1. The eigenvalues are real, comtable (可数的), ordered (可排序的) and there is a smallest eigenvalue.

   Thus, we can write down them as $\lambda_0 < \lambda_1 < \lambda_2 < \lambda_3 < \cdots < \lambda_n$.

   However, there is no largest eigenvalues, $n \to \infty$.
   $\lambda_n \to \infty$.

2. For each eigenvalue λ_n, there exists an eigenfunction ϕ_n with $n-1$ zeros on (a,b).

3. Eigenfunctions corresponding to different eigenvalues are orthogonal with respect to the weight function.

   Define the inner product of f and g:

   $\langle f|g\rangle = \int_a^b f(x)g(x)\sigma(x)dx.$

   $\langle f|f\rangle = \int_a^b f^2(x)\sigma(x)\,dx > 0.$

   $\langle \phi_n|\phi_m\rangle = \int_a^b \phi_n(x)\phi_m(x)\sigma x\, dx = \delta_{nm}.$

4. The set of eigenfunction is complete, i.e. any smooth function can be presented by a generalized series expansion of the eigenfunctions.

$$f(x) = \sum_n C_n \phi_n. \quad L\phi_n = \lambda \sigma \phi_n.$$

$$C_n = \langle \phi_n | f \rangle = \int_a^b \phi_n(x) f(x) \sigma(x)\, dx.$$

$$L = \frac{\partial}{\partial x}\left(p \frac{\partial}{\partial x}\right) + q(x).$$

$$\varphi_n(x) = \sqrt{\frac{2}{L}} \sin\left(\frac{n\pi}{L} x\right).$$

$$H|\varphi_n\rangle = E_n |\varphi_n\rangle.$$

$$H'|X_m\rangle = \lambda_m |X_m\rangle.$$

$$|X_m\rangle = \sum_n C_{mn} |\varphi_n\rangle$$

$$\sum_n H' C_{mn} |\varphi_n\rangle = \sum_n \lambda_m C_{mn} |\varphi_n\rangle$$

$$\langle \varphi_k |$$

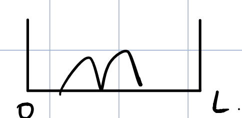
$$\sum_n \langle \varphi_k | H' | C_{mn} | \varphi_n \rangle = \sum_n \lambda_m C_{mn} \underbrace{\langle \varphi_k | \varphi_n \rangle}_{\delta_{kn}}$$

$$\sum_n H'_{kn} C_{mn} = \lambda_m C_{mk}$$

$$(H'_{kn} = \langle \varphi_k | H' | \varphi_n \rangle)$$

$$H' C = \lambda C.$$

$$H' = T + V'(x)$$



$$\langle \varphi_k | H' | \varphi_n \rangle = H'_{kn}.$$

$$H'C = \lambda C. \quad H' = \frac{p^2}{2m} + V(x)$$

$$T_{kn} = \langle \varphi_k | \frac{p^2}{2m} | \varphi_n \rangle.$$

$$V_{kn} = \langle \varphi_k | V | \varphi_n \rangle.$$

$$T_{kn} = \int \langle \varphi_k | x \rangle - \frac{\hbar^2}{2m} \frac{\partial^2}{\partial x^2} \langle x | \varphi_n \rangle\, dx$$

$\varphi_k^*(x)$ $\varphi_n(x)$

$$V_{kn} = \int \varphi_k^*(x)\, V(x)\, \varphi_n(x)\, dx$$

python.

$$|\chi_m\rangle = \sum_n C_{mn} |\varphi_{mn}\rangle .$$