$H|\varphi_i\rangle = E_i|\varphi_i\rangle$.

$$|\varphi_i\rangle = \sum_j U_{ji}|x_j\rangle.$$

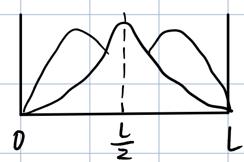
$\sum_j U_{ji} H|x_j\rangle = E_i \sum_j U_{ji}|x_j\rangle$. $\quad \langle x_k|x_j\rangle = \delta_{kj}$.

$\langle x_k|$ $\quad \langle x_k|$

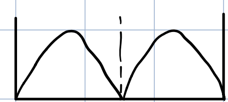
$\therefore \sum_j \underset{\sim}{H_{kj}} U_{ji} = E_i \sum_j \underset{\sim}{U_{ji}} \delta_{kj}$

$\langle x_k|H|x_j\rangle$. $\quad = E_i U_{kj}$. $\quad$ U_{ji}是个数值.

H是个矩阵.



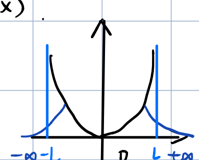
目的：怎么用程序求离散结果.

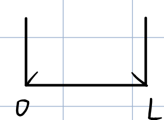


Harmonic Oscillator. 谐振子(模型)

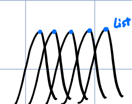
$H = \frac{p^2}{2m} + V(x)$.

$V(x) = \frac{1}{2}kx^2$.





$w = \sqrt{\frac{k}{m}}$. $\quad V(x) = \frac{1}{2}mw^2x^2$.



高斯函数 ⇒ 基.

$|\varphi_i\rangle = \sum_j U_{ji}|x_j\rangle$.

$H|\varphi_i\rangle = E_i|\varphi_j\rangle$.

$\sum_j H U_{ji}|x_j\rangle = \sum_j E_i U_{ji}|x_j\rangle$. $\quad \langle x_k|x_j\rangle = \delta_{kj}$.

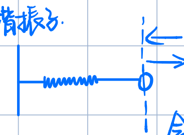
$\langle x_k|$

$\sum_j H_{kj} U_{ji} = \sum_j E_i U_{ji} \delta_{kj}$

广义本征值问题.

$HU = ESU$. $\quad$ Generalized Eigen Problem.

谐振子.



$\rightarrow F = -kx$.

会沿平衡点来回振动.

$F = -kx$.

$m\frac{d^2x}{dt^2} + kx = 0$.

$x(t) = A\sin wt + B\cos wt$. $\quad w = \sqrt{\frac{k}{m}}$.

$V(x) = \frac{1}{2}mw^2x^2$.

$H = \frac{p^2}{2m} + \frac{1}{2}mw^2x^2$.

因式分解. $v^2 + u^2 = (v + iu)(v - iu)$.

$\therefore H = \frac{mw}{2\hbar}\left(x - \frac{i}{mw}p\right)\left(x + \frac{i}{mw}p\right)\hbar w + \frac{1}{2}\hbar w$.

$a_+ = \sqrt{\frac{mw}{2\hbar}}\left(x - \frac{i}{mw}p\right)$. $\quad a_- = \sqrt{\frac{mw}{2\hbar}}\left(x + \frac{i}{mw}p\right)$

$H = a_+a_-\hbar w + \frac{1}{2}\hbar w = (\underbrace{a_+a_-}_{N} + \frac{1}{2})\hbar w$

能量单位.

$N=0$. 基态. $H = \frac{1}{2}\hbar w$.

$N=1$. 第一激发态. $H = (\frac{1}{2}+1)\hbar w$.

.....

$S^{\frac{1}{2}}:\ S^{\frac{1}{2}}S^{\frac{1}{2}}=S$

$S^{-\frac{1}{2}}:\ S^{-\frac{1}{2}}S^{\frac{1}{2}}=I.$

$$\Rightarrow \underbrace{S^{-\frac{1}{2}}HS^{\frac{1}{2}}}_{\tilde{H}}\ \underbrace{S^{\frac{1}{2}}u}_{A}=E\underbrace{S^{\frac{1}{2}}u}_{A}$$

$\tilde{H}A = EA \qquad A=S^{\frac{1}{2}}u.$

$u=S^{-\frac{1}{2}}A.$ U是一个矩阵.

性质
$$\begin{cases} a_+^{+}=a_-. \quad a_-^{+}=a_+. \\ [a_-,a_+]=1=a_-a_+-a_+a_-. \\ [N,a_-]=-a_-. \\ [N,a_+]=a_+. \end{cases}$$

哈密顿量

$H=(N+\frac{1}{2})\hbar w.$

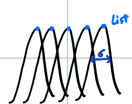
本征值. 代表在第n个能级.

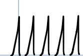
$N|n\rangle = n|n\rangle.$ 能级的状态/本征态.

$E_n=(n+\frac{1}{2})\hbar w.$

田老师的讲义

$E_0=\frac{1}{2}\hbar w.$	基态
$E_1=(\frac{1}{2}+1)\hbar w.$	第一激发态
$E_n=(\frac{1}{2}+n)\hbar w.$	第n激发态.

 高斯函数

若把$\sigma\to 0$. 则图象为  $|x_i\rangle.$

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

$[-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+\frac{1}{2}mw^2x^2]\varphi(x)=E\varphi(x).$

令 $\varphi_0(x)=e^{-cx^2}.$

$\varphi_0'(x)=-2cxe^{-cx^2}.$

$\varphi_0''(x)=(4c^2x^2-2c)e^{-cx^2}.$

$-\frac{\hbar^2}{2m}4c^2x^2+\frac{\hbar^2}{2m}\cdot 2c+\frac{1}{2}mw^2x^2=E.$

$-\frac{\hbar^2}{2m}4c^2+\frac{1}{2}mw^2=0. \Rightarrow c=\frac{1}{2}\cdot\frac{mw}{\hbar}$

$E_0=\frac{\hbar^2}{2m}\cdot 2c=\frac{\hbar^2}{2m}\cdot\frac{mw}{\hbar}=\frac{\hbar w}{2}.$

一维谐振子的通解:

$N_nH_n(\frac{x}{a})e^{-\frac{x^2}{2a^2}}$

$\varphi_1(x)=xe^{-cx^2}.$ 计算本征函数.

$\varphi_1'(x)=(1-2cx^2)e^{-cx^2}$

$\varphi_1''(x)=[-4cx-(1-2cx^2)2cx]e^{-cx^2}.$

$[-\frac{\hbar^2}{2m}[4cx^3-6cx]+\frac{1}{2}mw^2x^3=Ex.]\ e^{-cx^2}.$

$\frac{\hbar^2}{2m} \cdot 4c = \frac{1}{2} m\omega^2$. $C = \frac{1}{2} \cdot \frac{m\omega}{\hbar}$.

$\frac{\hbar^2}{2m} \cdot bc = E_1$

$E_1 = \frac{3}{2}\hbar\omega$.

$a_+ = \sqrt{\frac{m\omega}{2\hbar}}\left(x - \frac{i}{m\omega}p\right) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x - \frac{i}{\sqrt{m\omega\hbar}}p\right)$.

$a_- = \sqrt{\frac{m\omega}{2\hbar}}\left(x + \frac{i}{m\omega}p\right) = \frac{1}{\sqrt{2}}\left(\sqrt{\frac{m\omega}{\hbar}}x + \frac{i}{\sqrt{m\omega\hbar}}p\right)$.

取 $p = \frac{\hat{p}}{\sqrt{m\omega\hbar}}$. $x = \hat{x}\sqrt{\frac{m\omega}{\hbar}}$.

$\hat{H} = \frac{\hat{p}^2}{2m} + m\omega^2\frac{\hat{x}^2}{2}$. $p = \frac{\hat{p}}{\sqrt{m\hbar\omega}}$. $x = \hat{x}\sqrt{\frac{m\omega}{\hbar}}$.

$= \frac{1}{2}\hbar\omega\,(x^2+p^2)$ $[\hat{x},\hat{p}] = i\hbar$.

$\Downarrow$

$[x,p] = i$.

$a = \frac{1}{\sqrt{2}}(x+ip)$ $[a,a^+] = \frac{1}{2}[x+ip,\, x-ip]$

$a^+ = \frac{1}{\sqrt{2}}(x-ip)$. $= \frac{1}{2}[x,-ip] + [+ip,x]$

$= \frac{1}{2}(1+1)$

$x = \frac{1}{\sqrt{2}}(a+a^+)$. $= 1$.

$p = -\frac{i}{\sqrt{2}}(a-a^+)$.

$x^2+p^2 = \frac{1}{2}(a+a^+)^2 - \frac{1}{2}(a-a^+)^2$

$= aa^+ + a^+a$.

$= a^+a + [a,a^+] + a^+a$

$= 2a^+a + 1$.

$H = \frac{1}{2}\hbar\omega(2a^+a+1) = \hbar\omega\left(a^+a+\frac{1}{2}\right)$.

define $N = a^+a$. number operator. 全都是算符. $\hat{a}$, $\hat{a}^+$. $\hat{N}$.

要考.

$[A,BC] = [A,B]C + B[A,C]$

$[a,N] = [a,a^+a] = a^+[a,a] + [a,a^+]a = a$

$[a^+,N] = -a^+$.

#1 Lemma. 引理

The eigenvalues υ of the operator N are positive or zero. N的本征值≥0.

$N = a^+ a$. $\quad N|\upsilon\rangle = \upsilon|\upsilon\rangle$.

证明：$a^+ a|\upsilon\rangle = \upsilon|\upsilon\rangle$.

$\underbrace{\langle\upsilon|a^+ a|\upsilon\rangle}_{\langle x|x\rangle} = \langle\upsilon|\upsilon|\upsilon\rangle = \upsilon \geq 0$.

$\begin{cases} |x\rangle = a|\upsilon\rangle \\ \langle x| = \langle\upsilon|a^+ \end{cases}$.

a|υ>是N的一个非零本征态. 它的本征值是υ-1. a是降算符.

#2 if $\upsilon > 0$, $a|\upsilon\rangle$ is a non-zero eigenvector of N with the eigenvalue $\upsilon - 1$.

$$\hat{N}(a|\upsilon\rangle) = (\upsilon-1)a|\upsilon\rangle.$$

证明：

$$a^+ a(a|\upsilon\rangle) = (aa^+ - 1)a|\upsilon\rangle$$

$$= a(a^+ a - 1)|\upsilon\rangle \qquad N|\upsilon\rangle = \upsilon|\upsilon\rangle.$$

$$= (\upsilon-1)a|\upsilon\rangle$$

$\upsilon = 1$. $a|\upsilon\rangle = |0\rangle$ $\quad N a|\upsilon\rangle = |0\rangle$

$\langle x|N|x\rangle \geq 0$. $\quad |x\rangle = a|\upsilon\rangle$.

$a|x\rangle = |\varphi\rangle$.

$\langle\varphi|\varphi\rangle \geq 0$.

$a^n = \overbrace{a \cdots\cdots a}^{n}$. $\quad N a^n|\upsilon\rangle = a^+ a(a^n|\upsilon\rangle)$ $\qquad$ if $N a^{n-1}|\upsilon\rangle = (\upsilon-n+1)a^{n-1}|\upsilon\rangle$.

数学归纳法.

$$= (aa^+ - 1)a^n|\upsilon\rangle$$

方法一.

$$= (aa^+ a^n - a^n)|\upsilon\rangle$$

$$= a(N-1)a^{n-1}|\upsilon\rangle.$$

$$= a[(\upsilon-n+1)a^{n-1}|\upsilon\rangle - a^{n-1}|\upsilon\rangle]$$

$$= a(\upsilon-n)a^{n-1}|\upsilon\rangle$$

$$= (\upsilon-n)a^n|\upsilon\rangle.$$

方法二： $[N, a^n] = [a^+a, a^n]$

$$= [a^+, \underbrace{a^n}_{a\cdot a^{n-1}}]a = -na^{n-1}a = -na^n.$$

$$Na^n|\nu\rangle = ([N, a^n] + a^n N)|\nu\rangle$$

$$= (-na^n + \nu a^n)|\nu\rangle$$

$$= (\nu - n)a^n|\nu\rangle$$

考题 $[a^+, a^n] = -na^{n-1} = -\frac{\partial}{\partial a}a^n$

$[a^+, f(a)] = -\frac{\partial}{\partial a}f(a).$

作业 1.

$a^n|\nu\rangle$ is the eigenvector of N with eigenvalues $\nu - n$.

a lowering Operator

a^+, a are Ladder operator. 阶梯算符.

a^+ Raising Operator

$(a^+)^n|\nu\rangle$ is the eigenvector of N with eigenvalues $\nu + n$.

$$N(a^+)^n|\nu\rangle = (\nu + n)(a^+)^n|\nu\rangle.$$

$$N(a^n)|\nu\rangle = (\nu - n)(a^n)|\nu\rangle \qquad \nu - n \geq 0.$$

$$\nu - n < 1.$$

$$\nu - (n+1) < 0.$$

ν must be an positive interger (整数.) or 0.

$$N|n\rangle = n|n\rangle.$$

$$|0\rangle, |1\rangle, |2\rangle, \cdots, |n\rangle.$$

$$H = \hbar\omega(N + \tfrac{1}{2}). \qquad N|n\rangle = n|n\rangle.$$

$$H|n\rangle = \hbar\omega(n + \tfrac{1}{2})|n\rangle$$

基态. $\frac{1}{2}\hbar\omega$.

$\langle x|0\rangle =$ $\quad a|0\rangle = 0.$

n=0的态在X表象上的表示.

$\langle x|a|0\rangle = 0.$

$$\cancel{\frac{1}{\sqrt{2}}}\langle x|\sqrt{\frac{m\omega}{\hbar}}x + i\frac{p}{\sqrt{m\hbar\omega}}|0\rangle = 0$$

$$x\sqrt{\frac{m\omega}{\hbar}}\langle x|0\rangle + \hbar\cdot\frac{1}{\sqrt{m\hbar\omega}}\frac{\partial}{\partial x}\langle x|0\rangle = 0$$

$$x\sqrt{\frac{m\omega}{\hbar}}\varphi_0(x) + \hbar\cdot\frac{1}{\sqrt{m\hbar\omega}}\frac{\partial}{\partial x}\varphi_0(x) = 0$$

$$\frac{\partial}{\partial x}\varphi_0(x) = -\frac{m\omega}{\hbar}x\varphi_0(x)$$

$$\langle x|0\rangle = \varphi_0(x) = Ce^{-\frac{m\omega}{\hbar}\cdot\frac{x^2}{2}}.$$

$$\int_{-\infty}^{+\infty}\langle 0|x\rangle\langle x|0\rangle dx = |C|^2\int_{-\infty}^{+\infty}e^{-\frac{m\omega}{\hbar}x^2}dx$$

$$= |C|^2\sqrt{\frac{\pi\hbar}{m\omega}} - 1$$

$$C = \sqrt[4]{\frac{m\omega}{\pi\hbar}}.$$

$$\therefore \langle x|0\rangle = \varphi_0(x) = \cdots\cdots = \sqrt[4]{\frac{m\omega}{\pi\hbar}}e^{-\frac{m\omega}{\hbar}\cdot\frac{x^2}{2}}.$$

基态波函数.

$a^+|n\rangle = \sqrt{n+1}|n+1\rangle.$

$Na^+|n\rangle = (n+1)a^+|n\rangle.$

$a^+|n\rangle = C_n|n+1\rangle$

$N|n+1\rangle = (n+1)|n+1\rangle.$

$\therefore \langle n|aa^+|n\rangle = |C_n|^2\langle n+1|n+1\rangle$

$\langle n|(N+1)|n\rangle = |C_n|^2$

$n+1 = |C_n|^2$

$C_n = \sqrt{n+1}.$

$a|n\rangle = \sqrt{n}|n-1\rangle.$

$a|n\rangle = \sqrt{n}|n-1\rangle$

$Na|n\rangle = (n-1)a|n\rangle$

$a|n\rangle = C_n|n-1\rangle$

$\langle n|a^+a|n\rangle = \langle n-1||C_n|^2|n-1\rangle$

$\langle n|N|n\rangle = |C_n|^2$

$C_n = \sqrt{n}.$

$\varphi_1(x)$

$\langle x|1\rangle = \langle x|a^+|0\rangle$

$$= \frac{1}{\sqrt{2}}\langle x|\sqrt{\frac{m\omega}{\hbar}}x - i\frac{p}{\sqrt{m\omega\hbar}}|0\rangle$$

偏导 $\quad p = \frac{\hbar}{i}\frac{\partial}{\partial x}.$

$$= \frac{1}{\sqrt{2}}\Big(\sqrt{\frac{m\omega}{\hbar}}x\langle x|0\rangle - \frac{\hbar}{\sqrt{m\omega\hbar}}\frac{\partial}{\partial x}\langle x|0\rangle\Big)$$

$$= \frac{1}{\sqrt{2}} \sqrt[4]{\frac{m\omega}{\hbar}} \left(\sqrt{\frac{m\omega}{\hbar}}\, x + \frac{\cancel{\hbar}}{\sqrt{m\omega\hbar}} \cdot \frac{m\omega}{\cancel{\hbar}} x \right) e^{-\frac{m\omega}{\hbar}\cdot\frac{x^2}{2}}$$

$$= \sqrt{2} \sqrt[4]{\frac{m\omega}{\pi\hbar}} \sqrt{\frac{m\omega}{\hbar}}\, x e^{-\frac{m\omega}{\hbar}\cdot\frac{x^2}{2}}.$$

$\langle x|n\rangle =$ ______ .

$(a^+)^n|0\rangle = \sqrt{n!}\,|n\rangle.$

$$\langle x|n\rangle = \langle x|\frac{1}{\sqrt{n!}}(a^+)^n|0\rangle = \frac{1}{\sqrt{n!}}\left(\sqrt{\frac{m\omega}{2\hbar}}\, x - \frac{\hbar}{\sqrt{2m\omega\hbar}}\frac{\partial}{\partial x}\right)^n \varphi_0(x).$$