- 自由粒子波函数

高斯波包与经典粒子，相速度和群速度

- 位置和动量算符

位置算符和动量算符的引入，算符的对易关系

- 算符方法的应用：一维谐振子的代数解法

升算符和降算符及其性质， 占据数算符，波函数，空间反演

- 自由粒子

一维问题：粒子在自由空间运动，$V=0$

定态薛定谔方程 $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}=E\psi$

定义 $k\equiv\frac{\sqrt{2mE}}{\hbar}$

$$\frac{d^2\psi}{dx^2}=-k^2\psi$$

通解为 $\psi(x)=Ae^{ikx}+Be^{-ikx}$

代入时间部分 $\Psi(x,t)=\left(Ae^{ikx}+Be^{-ikx}\right)e^{-iEt/\hbar}$

利用 $\frac{E}{\hbar}=\frac{\hbar k^2}{2m}$

$$\Psi(x,t)=Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)}+Be^{-ik\left(x+\frac{\hbar k}{2m}t\right)}$$

分别代表向左或向右传播的波

$$\Psi(x,t)=Ae^{ik\left(x-\frac{\hbar k}{2m}t\right)}+Be^{-ik\left(x+\frac{\hbar k}{2m}t\right)}$$ 可统一写成 $$\boxed{\Psi_k(x,t)=Ae^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}}$$

k的取值可正可负 $k=\pm\frac{\sqrt{2mE}}{\hbar}$

讨论：**1**、该解满足初始条件：$\Psi(x,0)=Ae^{ikx}$

即在给定该初始条件的情况下，解为 $\Psi(x,t)=Ae^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}$

从而确定***k***

2、该解对应的相速度大小 $kx-\frac{\hbar k^2}{2m}t=\text{const}\ \Rightarrow\ v_k=\frac{\hbar|k|}{2m}=\sqrt{\frac{E}{2m}}$

经典自由运动粒子速度 $E=\frac{1}{2}mv^2\rightarrow v_{\text{classical}}=\sqrt{\frac{2E}{m}}=2v_k$

3、归一化 $\int_{-\infty}^{+\infty}\Psi_k^*\Psi_k dx=|A|^2\cdot\infty$ 不满足波函数的条件，即给定***k***的解无法作为波函数

$\boxed{\text{自由空间中运动的粒子无确定能量}}$

回顾：一般定态问题

通过定态薛定谔方程 $\hat{H}\psi(\vec{r}) = E\psi(\vec{r})$ 确定系列的本征值 $\{E_1, E_2, E_3 \ldots\}$

和本征函数 $\{\psi_1(\vec{r}), \psi_2(\vec{r}), \psi_3(\vec{r}) \ldots\}$ 设这些本征函数构成正交归一函数集

含时薛定谔方程的解可写成 $\Psi(\vec{r},t) = \sum_{n=1}^{\infty} c_n e^{\frac{iE_n t}{\hbar}} \psi_n(\vec{r})$

一维自由粒子定态薛定谔方程 $-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2} = E\psi$

本征值***E***可取**0**到∞的连续变化的数值

本征函数 $\psi_k(x) = e^{i\frac{\sqrt{2mE}}{\hbar}x} = e^{ikx}$

含时薛定谔方程的一般解可写成

$$\Psi(x,t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{+\infty} \phi(k) e^{i\left(kx - \frac{\hbar k^2}{2m}t\right)} dk$$

连续谱到离散谱：求和化为积分

回顾：一般定态问题

利用初始条件：粒子最初处于波函数为 $\Psi(\vec{r},t=0)$ 的状态

$$\Psi(\vec{r},0)=\sum_{n=1}^{\infty}c_n\psi_n\left(\vec{r}\right) \qquad c_m=\int\psi_m^*(\vec{r})\Psi(\vec{r},0)d\vec{r}$$

一维自由运动含时薛定谔方程的一般解可写成

$$\boxed{\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}dk}$$

$\phi(k)$可利用初始条件确定：

$$\Psi(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{ikx}dk$$

$\phi(k)$即为$\Psi(x,0)$的傅里叶变换后函数，所以

$$\boxed{\phi(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(x,0)e^{-ikx}dx}$$

波包的群速度和相速度：

$$\boxed{\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{i\left(kx-\frac{\hbar k^2}{2m}t\right)}dk=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{i(kx-\omega t)}dk}\qquad \omega=\frac{\hbar k^2}{2m}$$

相速度： $kx-\omega t=\mathrm{const}\Rightarrow v_k=\frac{\omega}{k}=\frac{\hbar k}{2m}$

群速度：设$\phi(k)$在k_0点有最大值

$$\omega(k)\simeq\omega(k_0)+\left.\frac{d\omega(k)}{dk}\right|_{k=k_0}(k-k_0)=\omega_0+\omega_0'(k-k_0)$$

$$\Psi(x,t)\simeq\frac{1}{\sqrt{2\pi}}\int\phi(k)e^{i\left[kx-\omega_0 t-\omega_0'(k-k_0)t\right]}dk\qquad=\frac{1}{\sqrt{2\pi}}e^{-i\omega_0 t+ik_0\omega_0' t}\int\phi(k)e^{ik\left(x-\omega_0' t\right)}dk$$

与t=0时波函数比较

$$\Psi(x,t=0)=\frac{1}{\sqrt{2\pi}}\int\phi(k)e^{ikx}dk$$

t增加， $x\to x-\omega_0' t=x-v_g t$

群速度：$\boxed{v_g=\omega_0'=\left.\frac{d\omega(k)}{dk}\right|_{k=k_0}=\frac{\hbar k_0}{m}}$

与相速度比较：$\boxed{v_k=\left.\frac{\hbar k}{2m}\right|_{k=k_0}=\frac{\hbar k_0}{2m}=\frac{1}{2}v_g}$

$$\Psi(x,t)\simeq\frac{1}{\sqrt{2\pi}}\int\phi(k)e^{i\left[kx-\omega_0 t-\omega_0'(k-k_0)t\right]}dk \quad =\frac{1}{\sqrt{2\pi}}e^{-i\omega_0 t+ik_0\omega_0' t}\int\phi(k)e^{ik\left(x-\omega_0' t\right)}dk$$

高斯波包与经典粒子

$$\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int\phi(k)e^{i(kx-\omega t)}dk=\frac{1}{\sqrt{2\pi\hbar}}\int\phi(p)\exp\left[\frac{i}{\hbar}\left(px-\frac{p^2}{2m}t\right)\right]dp$$

这里：$p=\hbar k$

设一维高斯波包：

$$\phi(p)=Ae^{-(p-p_0)^2d^2/\hbar^2}$$

代入$\Psi(x,t)$，积分并归一化，得 $|\Psi(x,t)|^2=\frac{1}{d\sqrt{2\pi\left(1+\Delta^2\right)}}\exp\left[-\frac{(x-vt)^2}{2d^2\left(1+\Delta^2\right)}\right]$

这里： $v=\frac{p_0}{m}$ $\quad\Delta=\frac{\hbar}{2md^2}t$

$$|\Psi(x,t)|^2=\frac{1}{d\sqrt{2\pi\left(1+\Delta^2\right)}}\exp\left[-\frac{(x-vt)^2}{2d^2\left(1+\Delta^2\right)}\right] \qquad v=\frac{p_0}{m} \qquad \Delta=\frac{\hbar}{2md^2}t$$

讨论：**1**、波包的最大值已群速度移动 $v=\dfrac{p_0}{m}=\left.\dfrac{\partial E}{\partial p}\right|_{p_0}$

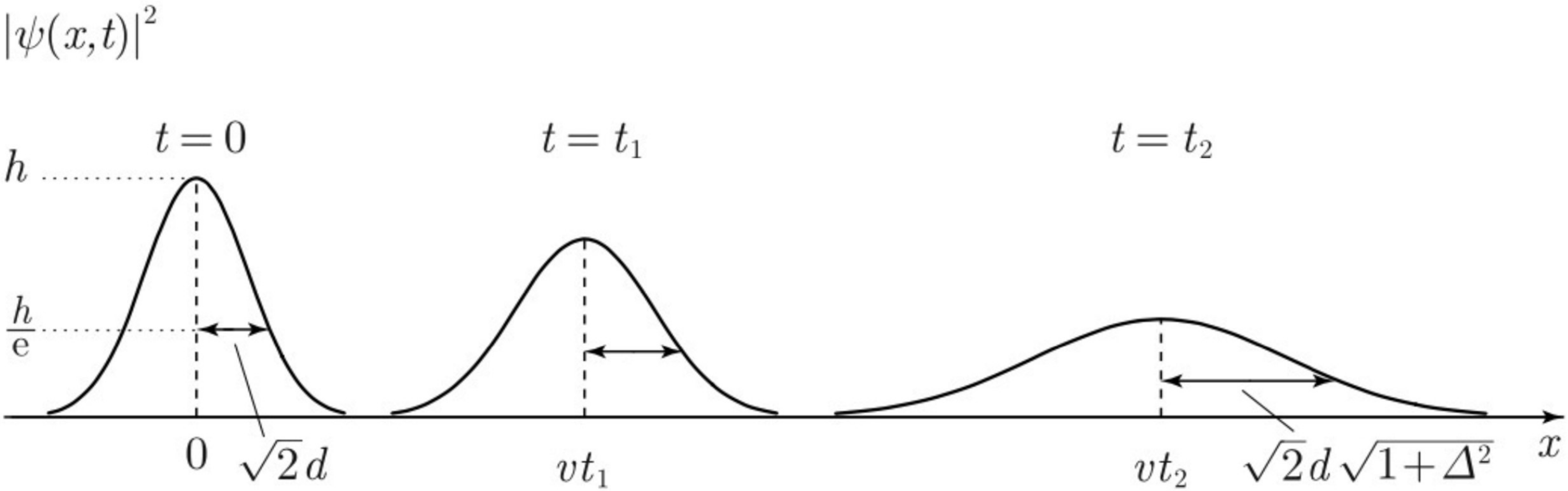
2、宽度Δ随着时间增大而增大

3、波包的平均坐标

$$\langle x\rangle=\int|\Psi(x,t)|^2\,xdx=\int dx\,|\Psi(x,t)|^2\,(x-vt)+\int dx\,|\Psi(x,t)|^2\,vt=vt$$

4、位置坐标的方差

$$\sigma_x^2=\int dx\,|\Psi(x,t)|^2\,(x-vt)^2=d^2\left(1+\Delta^2\right)$$



随着t增大，波包越来越宽

波包在t->∞时　　质量为m的自由粒子，初始波函数为 $\Psi(x,0)$

$$\Psi(x,0)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\phi(k)e^{ikx}dk$$

$$\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int\phi(k)e^{i\left(kx-\frac{hk^2}{2m}t\right)}dk=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{\infty}\phi(k)e^{-i\frac{\hbar t}{2m}\left(k-\frac{mx}{\hbar t}\right)^2+i\frac{mx^2}{2\hbar t}}dk$$

$$=\frac{1}{\sqrt{2\pi}}e^{i\frac{mx^2}{2\hbar t}}\int_{-\infty}^{\infty}e^{-i\frac{\hbar t}{2m}k^2}\phi\left(k+\frac{mx}{\hbar t}\right)dk$$

$$\lim_{t\to\infty}\Psi(x,t)=\lim_{t\to\infty}\frac{1}{\sqrt{2\pi}}e^{i\frac{mx^2}{2\hbar t}}\int_{-\infty}^{\infty}e^{-i\frac{\hbar t}{2m}k^2}\phi\left(k+\frac{mx}{\hbar t}\right)dk=\sqrt{\frac{m}{\hbar t}}e^{i\frac{mx^2}{2\hbar t}}\int\delta(k)e^{-i\frac{\pi}{4}}\phi\left(k+\frac{mx}{\hbar t}\right)dk$$

利用　$\lim_{\alpha\to\infty}\sqrt{\frac{\alpha}{\pi}}e^{i\frac{\pi}{4}}e^{-i\alpha x^2}=\delta(x)$

$$=\sqrt{\frac{m}{\hbar t}}e^{-i\pi/4}e^{i\frac{mx^2}{2\hbar t}}\phi\left(\frac{mx}{\hbar t}\right)$$

t->∞时，$\left|\Psi(x,t)\right|^2\to 0$，波扩展到全空间

- **位置和动量算符**　　一维情况：质量为m的自由粒子，波函数表示为

$$\Psi(x,t)=\frac{1}{\sqrt{2\pi}}\int\phi(k)e^{i(kx-\omega t)}dk=\frac{1}{\sqrt{2\pi\hbar}}\int\phi(p)\exp\left[\frac{i}{\hbar}\left(px-\frac{p^2}{2m}t\right)\right]dp$$

这里：$p=\hbar k$

$$\phi(p)=\phi(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(x,0)e^{-ikx}dx=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\Psi(x,0)e^{-i\frac{px}{\hbar}}dx$$

重新定义

$$C(p,t)=\frac{1}{\sqrt{\hbar}}\phi(p)e^{-i\frac{Et}{\hbar}}$$

$$\boxed{\Psi(x,t)=\frac{1}{\sqrt{2\pi\hbar}}\int C(p,t)\exp\left(\frac{i}{\hbar}px\right)dp}$$

$$C(p,t)=\frac{1}{\sqrt{\hbar}}\phi(p)e^{-i\frac{Et}{\hbar}}$$

$$=\frac{1}{\sqrt{2\pi\hbar}}e^{-i\frac{Et}{\hbar}}\int\Psi(x,t=0)e^{-i\frac{px}{\hbar}}dx$$

$$\boxed{C(p,t)=\frac{1}{\sqrt{2\pi\hbar}}\int\Psi(x,t)\exp\left(-i\frac{px}{\hbar}\right)dx}$$

$$\Psi(x,t)=\frac{1}{\sqrt{2\pi\hbar}}\int C(p,t)\exp\left(\frac{i}{\hbar}px\right)dp$$

$$C(p,t)=\frac{1}{\sqrt{2\pi\hbar}}\int \Psi(x,t)\exp\left(-i\frac{px}{\hbar}\right)dx$$

二式为Fourer变换式，针对非自由粒子也成立。

二式互为Fourer变换式，所以$\Psi(x,t)$ 与$C(p,t)$ 一一对应，是同一量子态的两种不同描述方式。

$\Psi(x,t)$	$C(p,t)$
以坐标x为自变量的波函数，坐标空间（坐标表象）波函数	以动量p为自变量的波函数，动量空间（动量表象）波函数
$\lvert\Psi(x,t)\rvert^2$ 给出t 时刻粒子处在位置$\bar{r}$处的几率	$\lvert C(p,t)\rvert^2$给出t 时刻粒子动量为p 的几率
二者描写同一量子状态	

推广到三维空间

$$\boxed{\Psi(\vec{r},t)=\frac{1}{\left(2\pi\hbar\right)^{3/2}}\int C(\vec{p},t)\exp\left(\frac{i}{\hbar}\vec{p}\cdot\vec{r}\right)d^3\vec{p}}$$

$$\boxed{C(\vec{p},t)=\frac{1}{\left(2\pi\hbar\right)^{3/2}}\int \Psi(\vec{r},t)\exp\left(-\frac{i}{\hbar}\vec{p}\cdot\vec{r}\right)d^3\vec{r}}$$

$\Psi(\vec{r},t)$ 与 $C(\vec{p},t)$ 一一对应, 是同一量子态的两种不同描述方式。

一、位置算符

根据波函数的统计解释：$\langle x\rangle = \iiint_{-\infty}^{\infty} \Psi^*(\vec{r},t) x \Psi(\vec{r},t) dxdydz$

量子力学中将物理量用算符来表示，在位置表象中算符 $\hat{O}$ 的平均值定义为

$$\langle\hat{O}\rangle = \iiint_{-\infty}^{\infty} \Psi^*(\vec{r},t)\left[\hat{O}\Psi(\vec{r},t)\right] dxdydz$$

所以，位置坐标算符 $\hat{x}$ 可定义为 $\hat{x}\Psi(\vec{r},t) = x\Psi(\vec{r},t)$

同理，可定义位置坐标算符 $\hat{y}$ 和 $\hat{z}$：$\hat{y}\Psi(\vec{r},t) = y\Psi(\vec{r},t)$ $\hat{z}\Psi(\vec{r},t) = z\Psi(\vec{r},t)$

可定义位置算符 $\boxed{\hat{\vec{r}}\Psi(\vec{r},t) = \vec{r}\Psi(\vec{r},t)}$

可见，$\Psi(\vec{r},t)$ 为位置算符 $\hat{\vec{r}}$ 本征值为 $\vec{r}$ 的本征函数。

位置算符函数：

$$F(\hat{x},\hat{y},\hat{z})\Psi(\vec{r},t)=F(x,y,z)\Psi(\vec{r},t)$$

证明：位置算符是厄米算符 $\left(\hat{\vec{r}}\right)^{\dagger}=\hat{\vec{r}}$

回顾：共轭算符的定义

$$\left\langle\Phi,\ \hat{\vec{r}}\Psi\right\rangle=\left\langle\left(\hat{\vec{r}}\right)^{\dagger}\Phi,\ \Psi\right\rangle$$

$$\left\langle\Phi,\ \hat{\vec{r}}\Psi\right\rangle=\int_{-\infty}^{\infty}\Phi^{*}(\vec{r},t)\hat{\vec{r}}\Psi(\vec{r},t)dx=$$

$$=\int_{-\infty}^{\infty}\Phi^{*}(x,t)\vec{r}\Psi(x,t)dx$$

$$=\int_{-\infty}^{\infty}\left[\vec{r}\Phi(x,t)\right]^{*}\Psi(x,t)dx$$

$$=\left\langle\hat{\vec{r}}\Phi,\ \Psi\right\rangle$$

二、动量算符

粒子动量几率密度： $|C(\vec{p},t)|^2$

根据波函数的统计解释，粒子动量平均值：

$$\langle \vec{p} \rangle = \iiint_{-\infty}^{\infty} |C(\vec{p},t)|^2 \ \vec{p} dp_x dp_y dp_z$$

$$= \iiint_{-\infty}^{\infty} C(\vec{p},t) \vec{p} C^*(\vec{p},t) dp_x dp_y dp_z$$

量子力学中将物理量用算符来表示，位置表象中算符 $\hat{\vec{p}}$ （即为动量的平均值）的平均值定义为

$$\langle \hat{\vec{p}} \rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Psi^*(x,y,z,t) \hat{\vec{p}} \Psi(x,y,z,t) dxdydz$$

$$\hat{\vec{p}} = ?$$

***x*分量:(以一维情况为例)**

$$\langle p_x \rangle = \int_{-\infty}^{\infty} C(p_x,t)\, p_x C^*(p_x,t)\, dp_x$$

$$= \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}p_x x}\Psi(x,t)\, p_x e^{\frac{i}{\hbar}p_x x'}\Psi^*(x',t)\, dx\, dx'\, dp_x$$

$$p_x e^{-\frac{i}{\hbar}p_x x} = -\frac{\hbar}{i}\frac{d}{dx} e^{-\frac{i}{\hbar}p_x x}$$

$$\langle p_x \rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}p_x x'}\Psi^*(x',t)\left[\int_{-\infty}^{\infty} -\frac{\hbar}{i}\frac{d}{dx} e^{-\frac{i}{\hbar}p_x x}\Psi(x,t)\, dx\right] dx'\, dp_x$$

$$\int_{-\infty}^{\infty} -\frac{\hbar}{i}\left(\frac{d}{dx} e^{-\frac{i}{\hbar}p_x x}\right)\Psi(x,t)\, dx = -\frac{\hbar}{i} e^{-\frac{i}{\hbar}p_x x}\Psi(x,t)\Big|_{-\infty}^{\infty} + \frac{\hbar}{i}\int_{-\infty}^{\infty} e^{-\frac{i}{\hbar}p_x x}\frac{d\Psi(x,t)}{dx}\, dx$$

$$\Psi(x,t)|_{-\infty}^{\infty}=0$$

$$\langle p_x \rangle = \frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}p_x(x'-x)}\Psi^*(x',t)\left[\frac{\hbar}{i}\frac{d\psi(x,t)}{dx}\right]dp_x dx' dx$$

$$\frac{1}{2\pi\hbar}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} e^{\frac{i}{\hbar}p_x(x'-x)}\Psi^*(x',t)dp_x dx' = \frac{1}{(2\pi\hbar)^{1/2}}\int_{-\infty}^{\infty} C^*(p_x,t)e^{\frac{i}{\hbar}(-p_x x)}dp_x = \Psi^*(x,t)$$

$$\boxed{\langle p_x \rangle = \int_{-\infty}^{\infty}\Psi^*(x,t)\frac{\hbar}{i}\frac{d}{dx}\Psi(x,t)dx}$$

推广到三维情况

$$\boxed{\langle p_x \rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\Psi^*(x,y,z,t)\frac{\hbar}{i}\frac{d}{dx}\Psi(x,y,z,t)dxdydz}$$

$$\hat{p}_x \to \frac{\hbar}{i}\frac{\partial}{\partial x}, \hat{p}_y \to \frac{\hbar}{i}\frac{\partial}{\partial y}, \hat{p}_z \to \frac{\hbar}{i}\frac{\partial}{\partial z}$$

$$\hat{\vec{p}} \to \frac{\hbar}{i}\nabla$$

$$\boxed{\left\langle \vec{p} \right\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \Psi^*(x,y,z,t)\hat{\vec{p}}\Psi(x,y,z,t)dxdydz}$$

推广

$$\boxed{\left\langle p_x^n \right\rangle = \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \psi^*(x,y,z,t)\hat{p}_x^n\psi(x,y,z,t)dxdydz}$$

证明：动量算符是厄米算符

回顾：共轭算符的定义

$$\left\langle \Phi, \hat{p}_x \Psi \right\rangle = \left\langle \left(\hat{p}_x\right)^\dagger \Phi, \Psi \right\rangle$$

***x*分量:(以一维情况为例)**

要证 $\left(\hat{p}_x\right)^\dagger = \hat{p}_x$

$$\left\langle \Phi, \hat{p}_x \Psi \right\rangle = \int_{-\infty}^{\infty} \Phi^*(x,t) \frac{\hbar}{i} \frac{d}{dx} \Psi(x,t) dx =$$

$$= \frac{\hbar}{i} \Phi^*(x,t) \Psi(x,t) \Big|_{x=-\infty}^{\infty} - \int_{-\infty}^{\infty} \frac{\hbar}{i} \frac{d}{dx} \Phi^*(x,t) \Psi(x,t) dx$$

$$= \int_{-\infty}^{\infty} \left[\frac{\hbar}{i} \frac{d}{dx} \Phi(x,t) \right]^* \Psi(x,t) dx$$

$$= \left\langle \hat{p}_x \Phi, \Psi \right\rangle$$

三、位置算符与动量算符的对易关系

数学上，将算符$\hat{A}$ 和$\hat{B}$的乘积定义为 $\left[\hat{A}\hat{B}\right]\Psi=\hat{A}\left[\hat{B}\Psi\right]$

即先作用算符 $\hat{B}$，再作用算符$\hat{A}$

量子力学中，将$\hat{A}\hat{B}-\hat{B}\hat{A}$ 称为算符 $\hat{A}$ 和 $\hat{B}$ 的对易关系（或称为对易子），并记为 $\left[\hat{A},\hat{B}\right]$

$$\left[\hat{A},\hat{B}\right]=\hat{A}\hat{B}-\hat{B}\hat{A}$$

若 $[\hat{A},\hat{B}]=0$ ，则 $\hat{A}$与 $\hat{B}$对易

若 $[\hat{A},\hat{B}]\neq 0$ ，则 $\hat{A}$与 $\hat{B}$不对易

$$\left.\begin{aligned}[\hat{x},\hat{y}]&=0\\ [\hat{y},\hat{z}]&=0\\ [\hat{z},\hat{x}]&=0\end{aligned}\right\} \Rightarrow [x_\alpha, x_\beta]=0 \quad \alpha,\beta=1,\ 2,\ 3$$

$$(x_1=x,\ x_2=y,\ x_3=z)$$

$$\left.\begin{aligned}[\hat{p}_x,\ \hat{p}_y]&=0\\ [\hat{p}_y,\ \hat{p}_z]&=0\\ [\hat{p}_z,\ \hat{p}_x]&=0\end{aligned}\right\} \Rightarrow \left[\hat{p}_\alpha,\ \hat{p}_\beta\right]=0 \quad \alpha,\beta=1,\ 2,\ 3$$

$$(\hat{p}_1=\hat{p}_x,\ \hat{p}_2=\hat{p}_y,\ \hat{p}_3=\hat{p}_z)$$

$$\begin{aligned}&[x,\hat{p}_x]=i\hbar \qquad [x,\hat{p}_y]=[x,\hat{p}_z]=0\\ &[y,\hat{p}_y]=i\hbar \qquad [y,\hat{p}_x]=[y,\hat{p}_z]=0\\ &[z,\hat{p}_z]=i\hbar \qquad [z,\hat{p}_x]=[z,\hat{p}_y]=0\end{aligned} \Rightarrow \begin{aligned}&[x_\alpha,\ \hat{p}_\beta]=i\hbar\delta_{\alpha\beta}\\ &(\alpha,\beta=1,\ 2,\ 3)\end{aligned}$$

对易关系的一些恒等式

$$[\hat{A},\ \hat{A}] = 0$$

$$[\hat{A},\ \hat{B}] = -[\hat{B},\ \hat{A}]$$

$$[\hat{A}, \hat{B} + \hat{C}] = [\hat{A}, \hat{B}] + [\hat{A}, \hat{C}]$$

$$[\hat{A} + \hat{B}, \hat{C}] = [\hat{A}, \hat{C}] + [\hat{B}, \hat{C}]$$

$$[\hat{A}, \hat{B}\hat{C}] = [\hat{A}, \hat{B}]\hat{C} + \hat{B}[\hat{A}, \hat{C}]$$

$$[\hat{A}\hat{B}, \hat{C}] = [\hat{A}, \hat{C}]\hat{B} + \hat{A}[\hat{B}, \hat{C}]$$

$$[\hat{A},\ [\hat{B}, \hat{C}]] + [\hat{B},\ [\hat{C}, \hat{A}]] + [\hat{C},\ [\hat{A}, \hat{B}]] = 0$$

- **算符方法的应用：一维谐振子的代数解法**

一维谐振子定态薛定谔方程 $$-\frac{\hbar^2}{2m}\frac{d^2\psi}{dx^2}+\frac{1}{2}m\omega^2x^2\psi=E\psi$$

哈密顿算符 $$\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2\hat{x}^2=\frac{1}{2m}\left[\hat{p}^2+(m\omega\hat{x})^2\right]$$ $$\hat{p}=\frac{\hbar}{i}\frac{d}{dx}$$

引入升降算符 $$\hat{a}_+\equiv\frac{1}{\sqrt{2\hbar m\omega}}(-i\hat{p}+m\omega\hat{x}) \qquad \hat{a}_-\equiv\frac{1}{\sqrt{2\hbar m\omega}}(i\hat{p}+m\omega\hat{x})$$

$$a_+a_-\psi(x)=\frac{(-i\hat{p}+m\omega\hat{x})(i\hat{p}+m\omega\hat{x})}{2\hbar m\omega}\psi(x)=\frac{\hat{p}^2-im\omega\hat{p}\hat{x}+im\omega\hat{x}\hat{p}+(m\omega\hat{x})^2}{2\hbar m\omega}\psi(x)$$

$$=\frac{\hat{p}^2-im\omega[\hat{p},\hat{x}]+(m\omega\hat{x})^2}{2\hbar m\omega}\psi(x)=\frac{1}{\hbar\omega}\left[\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega\hat{x}^2\right]\psi(x)-\frac{1}{2}\psi(x)$$

$$\Longrightarrow \qquad \hat{H}=\hbar\omega\left(\hat{a}_+\hat{a}_-+\frac{1}{2}\right)$$

性质1：$$(\hat{a}_+)^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(-i\hat{p}+m\omega\hat{x})^\dagger = \frac{1}{\sqrt{2\hbar m\omega}}(+i\hat{p}+m\omega\hat{x}) = \hat{a}_-$$ $$\boxed{(\hat{a}_-)^\dagger = \hat{a}_+}$$

$$\langle\psi(x),\hat{a}_+\hat{a}_-\psi(x)\rangle = \langle\psi(x),\hat{a}_+[\hat{a}_-\psi(x)]\rangle = \langle(\hat{a}_+)^\dagger\psi(x),[\hat{a}_-\psi(x)]\rangle$$

$$= \langle(\hat{a}_-)\psi(x),\hat{a}_-\psi(x)\rangle \geq 0$$ $$\boxed{\langle\psi(x),\hat{a}_+\hat{a}_-\psi(x)\rangle \geq 0}$$

性质2：$$[\hat{a}_+,\hat{a}_-] = \frac{1}{2\hbar m\omega}[-i\hat{p}+m\omega\hat{x}, i\hat{p}+m\omega\hat{x}]$$

$$= \frac{1}{2\hbar m\omega}\{[-i\hat{p},i\hat{p}]+[-i\hat{p},m\omega\hat{x}]+[m\omega\hat{x},i\hat{p}]+[m\omega\hat{x},\hat{x}]\}$$ $$\boxed{[\hat{a}_+,\hat{a}_-] = -1}$$

$$= \frac{1}{2\hbar m\omega}\{0+(-im\omega)(-i\hbar)+(im\omega)(i\hbar)+0\} = -1$$

性质3：$$[\hat{a}_+,\hat{a}_+\hat{a}_-] = [\hat{a}_+,\hat{a}_+]\hat{a}_- + \hat{a}_+[\hat{a}_+,\hat{a}_-] = 0-\hat{a}_+$$ $$\boxed{[\hat{a}_+,\hat{a}_+\hat{a}_-] = -\hat{a}_+}$$

$$[\hat{a}_-,\hat{a}_+\hat{a}_-] = [\hat{a}_-,\hat{a}_+]\hat{a}_+ + \hat{a}_+[\hat{a}_-,\hat{a}_-] = \hat{a}_- + 0$$ $$\boxed{[\hat{a}_-,\hat{a}_+\hat{a}_-] = \hat{a}_-}$$

性质4：　　定义算符 $\hat{N} \equiv \hat{a}_{+}\hat{a}_{-}$ 设 ψ_n 为其本征值为 **n** 的归一化本征函数，即

$$\hat{N}\psi_n = n\psi_n$$

考察函数 $\phi = \hat{a}_{-}\psi_n(x)$

利用性质3 $\left[\hat{a}_{-}, \hat{a}_{+}\hat{a}_{-}\right] = \hat{a}_{-} \Rightarrow \hat{a}_{-}\hat{N} - \hat{N}\hat{a}_{-} = \hat{a}_{-} \Rightarrow \hat{N}\hat{a}_{-} = \hat{a}_{-}\hat{N} - \hat{a}_{-}$

$$\hat{N}\phi = \hat{N}\hat{a}_{-}\psi_n = \hat{a}_{-}\hat{N}\psi_n - \hat{a}_{-}\psi_n = n\hat{a}_{-}\psi_n - \hat{a}_{-}\psi_n$$

$$= (n-1)(\hat{a}_{-}\psi_n) = (n-1)\phi$$

函数 $\phi = \hat{a}_{-}\psi_n(x)$ 为算符 $\hat{N}$ 本征值为 **n-1** 的本征函数

算符 $\hat{a}_{-}$ 作用到算符 $\hat{N}$ 的本征函数上，得到的函数的本征值减少**1**

算符 $\hat{a}_{-}$ 称为降算符

利用性质3 $\left[\hat{a}_{+}, \hat{a}_{+}\hat{a}_{-}\right] = -\hat{a}_{+}$ 可得

算符 $\hat{a}_{+}$ 作用到算符 $\hat{N}$ 的本征函数上，得到的函数的本征值增加**1**

算符 $\hat{a}_{+}$ 称为升算符

占据数算符　　考察算符$\hat{N} \equiv \hat{a}_+ \hat{a}_-$

设ψ_n为其本征值为n的归一化本征函数，即　$\hat{N}\psi_n = n\psi_n$

➢ **结论：n为大于等于零的整数**

证明：　利用性质1 $\langle \psi(x), \hat{a}_+ \hat{a}_- \psi(x) \rangle \geq 0$　　可得

$$\left\langle \psi_n(x), \hat{N}\psi_n(x) \right\rangle = n\left\langle \psi_n(x), \psi_n(x) \right\rangle = n \geq 0$$

用反证法证明n为整数，设存在本征函数ψ_{n+a}：$\hat{N}\psi_{n+\alpha} = (n+\alpha)\psi_{n+\alpha}$

$$0 < \alpha < 1$$

显然 $\hat{N}\left[(\hat{a}_-)^n \psi_{n+\alpha}(x)\right] = \alpha\left[(\hat{a}_-)^n \psi_{n+\alpha}(x)\right]$

$$\hat{N}\left[(\hat{a}_-)^{n+1} \psi_{n+\alpha}(x)\right] = (\alpha - 1)\left[(\hat{a}_-)^n \psi_{n+\alpha}(x)\right]$$

与算符$\hat{N}$ 的本征值总大于等于零矛盾。

算符$\hat{N}$ 的本征值为非负整数。

算符 $\hat{N}=\hat{a}_{+}\hat{a}_{-}$的本征值为非负整数。

一维谐振子的哈密顿算符 $\hat{H}=-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}+\frac{1}{2}m\omega^2\hat{x}^2=\hbar\omega\left(\hat{a}_{+}\hat{a}_{-}+\frac{1}{2}\right)$

所以哈密顿算符的本征值为

$$E=\hbar\omega\left(n+\frac{1}{2}\right),\qquad n=0,1,2,\ldots$$

波函数

占据数算符 $\hat{N}=\hat{a}_+\hat{a}_-$ 的本征值为零的本征函数记为 ψ_0

$$\hat{a}_-\psi_0=0 \qquad \frac{1}{\sqrt{2\hbar m\omega}}(i\hat{p}+m\omega\hat{x})\psi_0=0$$

即为微分方程

$$\left(\hbar\frac{d}{dx}+m\omega x\right)\psi_0=0 \qquad \frac{d\psi_0}{\psi_0}=-\frac{m\omega}{\hbar}xdx \qquad \ln\psi_0(x)=-\frac{m\omega}{2\hbar}x^2+\ \text{const}$$

$$\Rightarrow \quad \psi_0(x)=A_0e^{-m\omega x^2/(2\hbar)}$$

系数A_0由归一化条件决定

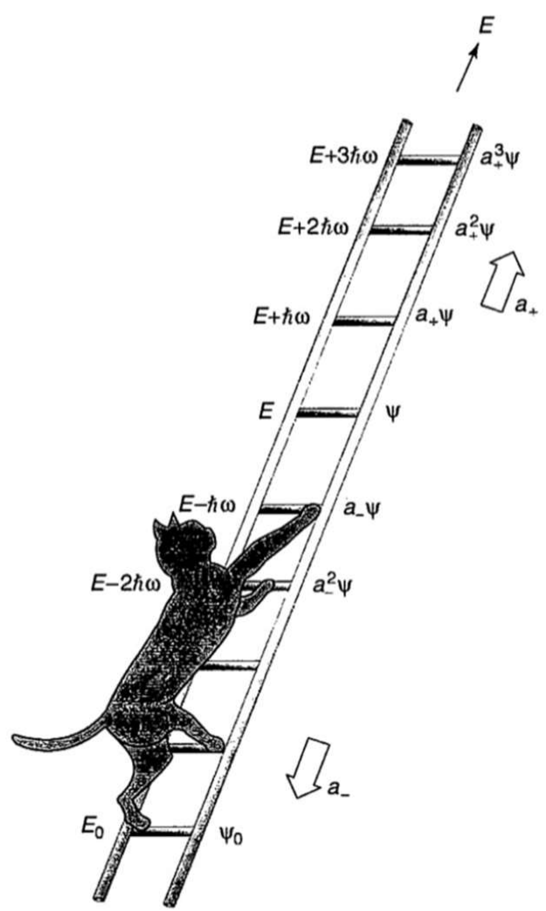
$$\int\psi_0^*\psi_0dx=|A_0|^2\int e^{-m\omega x^2/\hbar}dx=|A_0|^2\int\sqrt{\frac{\hbar}{m\omega}}e^{-u^2}du=1$$

$$A_0=\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} \qquad \psi_0(x)=\left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}}e^{-\frac{m\omega}{2\hbar}x^2},E_0=\hbar\omega/2$$

$$\psi_0(x) = \left(\frac{m\omega}{\hbar\pi}\right)^{\frac{1}{4}} e^{-\frac{m\omega}{2\hbar}x^2}, \qquad E_0 = \hbar\omega / 2$$

$$\psi_n(x) = A_n \left(\hat{a}_+\right)^n \psi_0(x), \qquad E_n = \hbar\omega\left(\frac{1}{2} + n\right)$$

$$A_n = ?$$



由于一维束缚态是非简并的，所以

$$\hat{a}_+\psi_n = C_n\psi_{n+1}, \qquad \hat{a}_-\psi_n = D_n\psi_{n-1}$$

已知 $\hat{a}_+\hat{a}_-\psi_n = n\psi_n \Rightarrow \left\langle \psi_n, \hat{a}_+\left(\hat{a}_-\psi_n\right)\right\rangle = n$　　即 $\left\langle \left(\hat{a}_+\right)^\dagger\psi_n, \hat{a}_-\psi_n \right\rangle = n$

因为 $\left(\hat{a}_+\right)^\dagger = \hat{a}_-$ $\left\langle \left(\hat{a}_+\right)^\dagger\psi_n, \hat{a}_-\psi_n \right\rangle = \left\langle \hat{a}_-\psi_n, \hat{a}_-\psi_n \right\rangle = n = \int \left[\hat{a}_-\psi_n(x)\right]^* \left[\hat{a}_-\psi_n(x)\right] dx = \left|D_n\right|^2$

取 $D_n = \sqrt{n}$　　所以有 $\boxed{\hat{a}_-\psi_n = \sqrt{n}\psi_{n-1}}$

已知 $\hat{a}_-\hat{a}_+\psi_n = \left(\hat{a}_+\hat{a}_- + 1\right)\psi_n = (n+1)\psi_n$　　即 $\left\langle \psi_n, \hat{a}_-\left(\hat{a}_+\psi_n\right)\right\rangle = n+1$

$$\left\langle \left(\hat{a}_-\right)^\dagger\psi_n, \left(\hat{a}_+\psi_n\right)\right\rangle = n+1 \Rightarrow \left\langle \hat{a}_+\psi_n, \hat{a}_+\psi_n \right\rangle = n+1 = \left|C_n\right|^2$$

取 $C_n = \sqrt{n+1}$　　$\boxed{\hat{a}_+\psi_n = \sqrt{n+1}\psi_{n+1}}$

$$\boxed{\hat{a}_+\psi_n = \sqrt{n+1}\,\psi_{n+1}}$$

$$\psi_{n+1} = \frac{1}{\sqrt{n+1}}\hat{a}_+\psi_n$$

$$\psi_1 = \frac{1}{\sqrt{1}}\hat{a}_+\psi_0$$

$$\psi_2 = \frac{1}{\sqrt{2}}\hat{a}_+\psi_1 = \frac{1}{\sqrt{2\cdot 1}}\left(\hat{a}_+\right)^2\psi_0$$

$$\psi_3 = \frac{1}{\sqrt{3}}\hat{a}_+\psi_2 = \frac{1}{\sqrt{3\cdot 2\cdot 1}}\left(\hat{a}_+\right)^3\psi_0$$

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\left(\hat{a}_+\right)^n\psi_0(x), \qquad E_n = \hbar\omega\left(\frac{1}{2}+n\right)$$

波函数的空间反演对称

定义:空间反演算符 $\hat{P}\psi(x)=\psi(-x)$

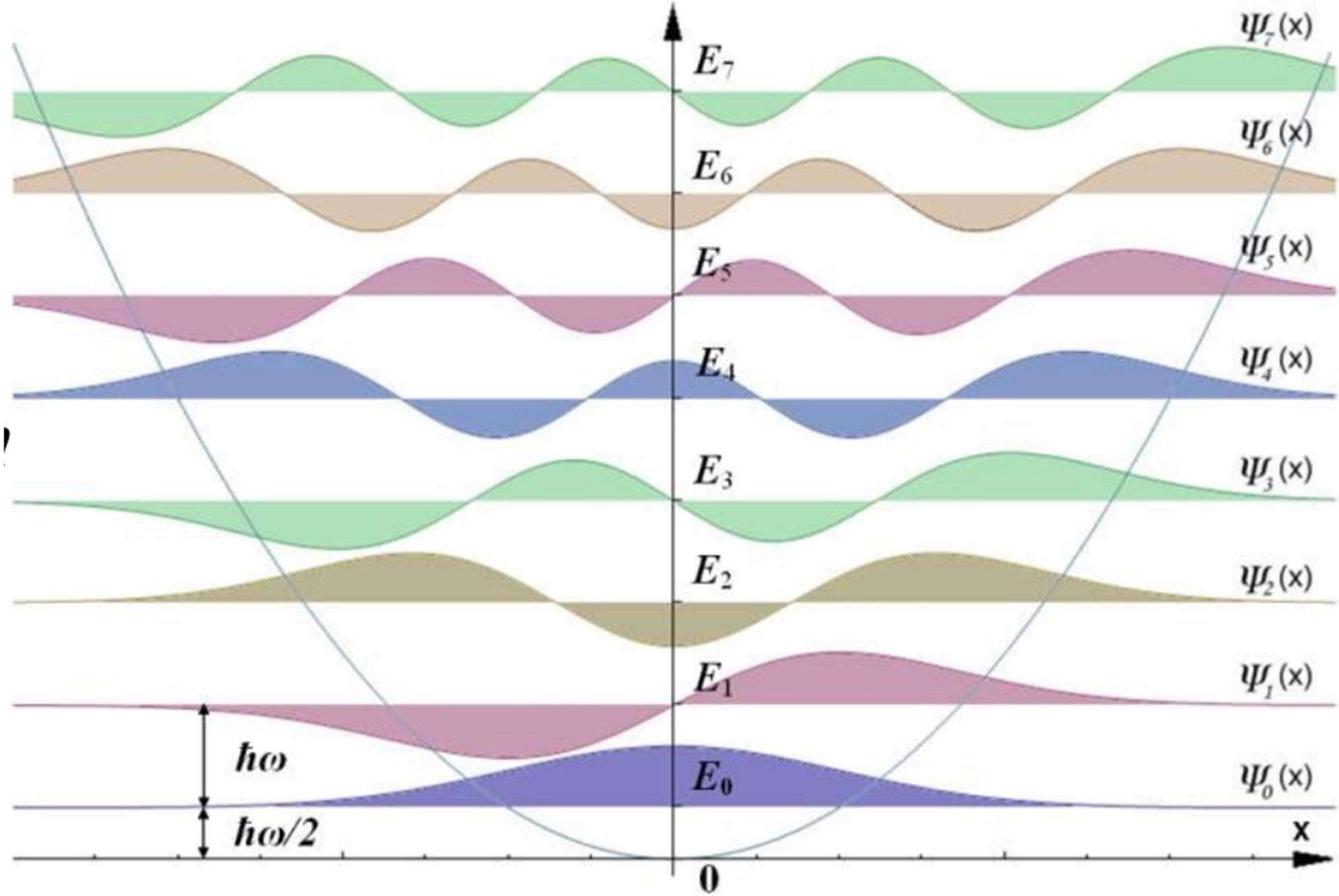
一维谐振子哈密顿算符基态本征波函数 $\hat{P}\psi_0(x)=\psi_0(-x)=\psi_0(x)$ 偶宇称

$$\hat{P}\psi_1(x)=A_1\hat{P}\left[\hat{a}_+\psi_0(x)\right]=A_1\hat{P}\left[\frac{1}{\sqrt{2m\omega\hbar}}\left(-\hbar\frac{d}{dx}+m\omega x\right)\psi_0(x)\right]$$

$$=A_1\left[\frac{1}{\sqrt{2m\omega\hbar}}\left(-\hbar\frac{d}{d(-x)}+m\omega(-x)\right)\psi_0(-x)\right]$$

$$=-A_1\left[\hat{a}_+\psi_0(x)\right]=-\psi_1(x)$$ 奇宇称

$$\boxed{\hat{P}\psi_n(x)=(-1)^n\psi_n(x)}$$



$\psi_7(x)$
E_7
$\psi_6(x)$
E_6
$\psi_5(x)$
E_5
$\psi_4(x)$
E_4
$\psi_3(x)$
E_3
$\psi_2(x)$
E_2
$\psi_1(x)$
E_1
$\hbar\omega$
$\psi_0(x)$
E_0
$\hbar\omega/2$
x
0

补充1：傅里叶变换

平方可积**L_2[-*l*,*l*]**函数空间中，选取基 $\left\{ e^{i\frac{n\pi}{l}x} \middle| n=0,\pm1,\pm2,\ldots \right\}$

$$f(x)=\sum_{n=-\infty}^{\infty} c_n \mathrm{e}^{i\frac{n\pi}{l}x} \qquad c_n=\frac{1}{2l}\int_{-l}^{l}\mathrm{e}^{-i\frac{n\pi}{l}x}f(x)dx$$

级数具有周期性

$l\to\infty$

$$\frac{lc_n}{\pi}=\frac{1}{2\pi}\int_{-l}^{l}\mathrm{e}^{-i\frac{n\pi}{l}x}f(x)dx \xrightarrow[\frac{lc_n}{\pi}\to\frac{F(k)}{\sqrt{2\pi}}]{n\to k;k=\frac{n\pi}{l}} F(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\mathrm{e}^{-ikx}f(x)dx$$

$$f(x)=\sum_{n=-\infty}^{\infty}c_n\mathrm{e}^{i\frac{n\pi}{l}x}\Delta n \xrightarrow[\frac{l}{\pi}c_n\to\frac{F(k)}{\sqrt{2\pi}}]{k=\frac{n\pi}{l},\Delta n=\frac{l\Delta k}{\pi}} \sum\frac{F(k)}{\sqrt{2\pi}}\mathrm{e}^{ikx}\Delta k \to \frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}F(k)\mathrm{e}^{ikx}dk$$

$$\boxed{f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}F(k)\mathrm{e}^{ikx}dk \qquad F(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\mathrm{e}^{-ikx}f(x)dx}$$

补充2：狄拉克δ函数

定义函数 $$\delta_\varepsilon(x)=\begin{cases}\dfrac{1}{\varepsilon}, & -\dfrac{\varepsilon}{2}<x<\dfrac{\varepsilon}{2}\\ 0, & |x|>\dfrac{\varepsilon}{2}\end{cases}$$

任一在**x=0**点有定义的函数**$f(x)$** $$\lim_{\varepsilon\to 0}\int_{-\infty}^{+\infty}\delta_\varepsilon(x)f(x)dx=f\left(0\right)\lim_{\varepsilon\to 0}\int_{-\varepsilon/2}^{+\varepsilon/2}\delta_\varepsilon(x)dx=f(0)$$

定义δ函数： $$\int_{-\infty}^{+\infty}\delta(x)f(x)dx=f\left(0\right)$$

性质：

（**1**） $$\int_{-\infty}^{+\infty}\delta(x-x_0)f(x)dx=f(x_0)$$

（**2**） $$\int_{-\infty}^{+\infty}\delta(x)dx=1$$

（**3**） $$\delta(-x)=\delta(x)$$

（**4**） $$\delta(ax)=\frac{1}{|a|}\delta(x)$$

（**5**） $$x\delta(x-x_0)=x_0\delta(x-x_0)$$

（**6**） $$\int_{-\infty}^{+\infty}\delta(x-y)\delta\left(y-z\right)dx=\delta\left(x-z\right)$$

$$F(k)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\delta(x-y)e^{-ikx}dx=\frac{e^{-iky}}{\sqrt{2\pi}}$$

$$\delta\left(x-y\right)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}F(k)e^{ikx}dx=\frac{1}{2\pi}\int_{-\infty}^{+\infty}e^{ik(x-y)}dx$$

$$f(x)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}F(k)\mathrm{e}^{ikx}dk \qquad F\left(k\right)=\frac{1}{\sqrt{2\pi}}\int_{-\infty}^{+\infty}\mathrm{e}^{-ikx}f(x)dx$$