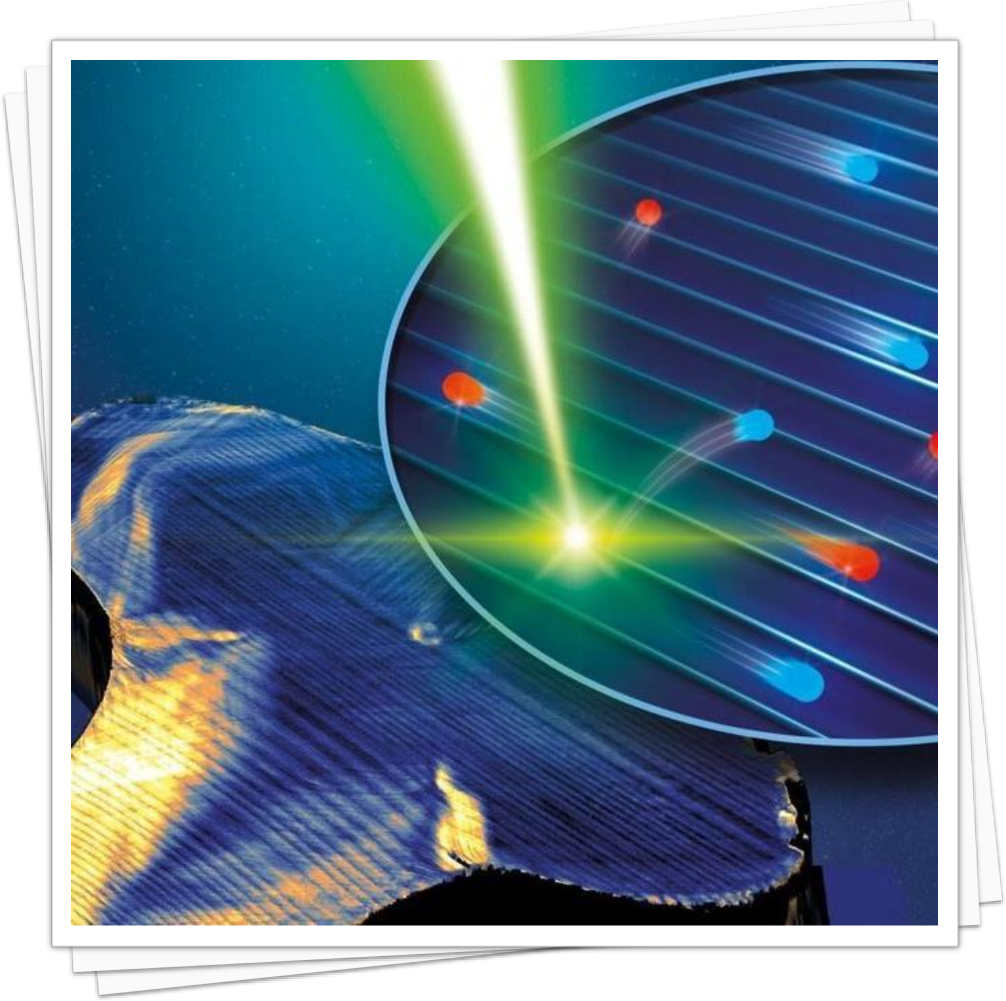

量子力学中的物理量

物理量的算符

对易关系

不确定关系

力学量的演化

量子力学的基本假设

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坐标和势能

- 理论（波函数）怎样和实验量比较？
- 几率

粒子出现在$\vec{r}$处的体积元$dv = dxdydz$中的概率为

$$\rho dv = \psi^*(\vec{r},t)\psi(\vec{r},t)dxdydz$$

- 位置

$$\langle\vec{r}\rangle \equiv \iiint \vec{r}\rho dv = \iiint \psi^*(\vec{r},t)\vec{r}\psi(\vec{r},t)dxdydz$$

- 势能

$$\langle V\rangle \equiv \iiint V(\vec{r},t)\rho(\vec{r},t)dv = \iiint \psi^*(\vec{r},t)V(\vec{r},t)\psi(\vec{r},t)dxdydz$$

动量表象和动量的平均值

傅里叶变换对

$$\begin{cases} u(\vec{r}) = \dfrac{1}{(2\pi\hbar)^{3/2}} \iiint \varphi(\vec{p}) e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}} dp_x dp_y dp_z \\ \varphi(\vec{p}) = \dfrac{1}{(2\pi\hbar)^{3/2}} \iiint u(\vec{r}) e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}} dx dy dz \end{cases}$$

动量为$\vec{p}$的平面波

$$\frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$$

- 空间波函数$u(\vec{r})$是平面波

$$\frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}$$

的线性叠加，叠加系数为$\varphi(\vec{p})$

- 傅里叶变换可逆：给定$u(\vec{r})$能够推出$\varphi(\vec{p})$，反之亦然
- $\varphi(\vec{p})$提供的系统信息与$u(\vec{r})$一样多
- 可以用$\varphi(\vec{p})$表示系统的状态

动量表象：$\varphi(\vec{p})$称为动量表象的波函数

按统计解释，动量的期望值是

$$\langle\vec{p}\rangle \equiv \iiint \varphi^*(\vec{p})\vec{p}\varphi(\vec{p}) dp_x dp_y dp_z$$

- 同一个量子态，既可以用坐标表象的波函数表示，也可以用动量表象的波函数表示
- 两者可以通过傅立叶变换互相转换，称为表象变换
- 一般我们使用坐标表象的波函数和算符
- 有时为了方便，也会使用其它的表象
- 表象变换，类似于线性空间的坐标变换

动量算符-1D

- 动量的期望值

$$\langle\vec{p}\rangle \equiv \iiint \varphi^*(\vec{p})\vec{p}\varphi(\vec{p})dp_x dp_y dp_z$$

- 希望把表达式变换到坐标表象

- 傅立叶变换公式，单频信号：

$$\int_{\mathbb{R}} \delta(k-k_0)\frac{1}{\sqrt{2\pi}}e^{ikx}dk = \frac{1}{\sqrt{2\pi}}e^{ik_0x}$$

$$\int_{\mathbb{R}} \frac{1}{\sqrt{2\pi}}e^{ik_0x}\frac{1}{\sqrt{2\pi}}e^{-ikx}dx = \delta(k-k_0)$$

- 把波矢替换成动量，

$$p = \hbar k$$

$$\delta(p-p_0) = \frac{1}{\hbar}\delta(k-k_0)$$

$$\frac{1}{\sqrt{2\pi\hbar}}\int_{\mathbb{R}} \delta(p-p_0)e^{ipx/\hbar}dp = \frac{1}{\sqrt{2\pi\hbar}}e^{ip_0x/\hbar}$$

$$\int_{\mathbb{R}} \frac{1}{\sqrt{2\pi\hbar}}e^{ip_0x/\hbar}\frac{1}{\sqrt{2\pi\hbar}}e^{-ipx/\hbar}dx = \delta(p-p_0)$$

- 动量算符

$$\langle p\rangle = \frac{1}{2\pi\hbar}\int_{\mathbb{R}} u^*(x)\left(-i\hbar\frac{\partial}{\partial x}\right)u(x)dx$$

- 一维问题

$$\langle p\rangle = \int_{\mathbb{R}} p\varphi^*(p)\varphi(p)dp$$

$$\varphi(p) = \frac{1}{(2\pi\hbar)^{1/2}}\int_{\mathbb{R}} u(x_1)e^{-\frac{i}{\hbar}px_1}dx_1$$

$$\varphi^*(p) = \frac{1}{(2\pi\hbar)^{1/2}}\int_{\mathbb{R}} u^*(x_2)e^{+\frac{i}{\hbar}px_2}dx_2$$

$$\langle p\rangle = \frac{1}{2\pi\hbar}\iiint u(x_1)e^{-\frac{i}{\hbar}px_1}pu^*(x_2)e^{+\frac{i}{\hbar}px_2}dpdx_1dx_2$$

$$= \frac{1}{2\pi\hbar}\iiint \left(i\hbar\frac{\partial}{\partial x_1}e^{-\frac{i}{\hbar}px_1}\right)u(x_1)u^*(x_2)e^{+\frac{i}{\hbar}px_2}dpdx_1dx_2$$

对分部积分，

$$\langle p\rangle = \frac{1}{2\pi\hbar}\iiint \left(-i\hbar\frac{\partial}{\partial x_1}u(x_1)\right)u^*(x_2)e^{-\frac{i}{\hbar}px_1}e^{+\frac{i}{\hbar}px_2}dpdx_1dx_2$$

$$= \iint dx_1dx_2\left\{u^*(x_2)\left(-i\hbar\frac{\partial}{\partial x_1}u(x_1)\right)\right\}\frac{1}{2\pi\hbar}\int e^{-\frac{i}{\hbar}p(x_1-x_2)}dp$$

$$= \iint dx_1dx_2\left\{u^*(x_2)\left(-i\hbar\frac{\partial}{\partial x_1}u(x_1)\right)\right\}\delta(x_1-x_2)$$

$$= \int_{\mathbb{R}} u^*(x_1)\left(-i\hbar\frac{\partial}{\partial x_1}u(x_1)\right)dx_1$$

动量算符

定义动量算符

$$\hat{\vec{p}} \stackrel{\text{def}}{=} -i\hbar\nabla$$

$$\begin{cases} \hat{p}_x = -i\hbar\dfrac{\partial}{\partial x} \\ \hat{p}_y = -i\hbar\dfrac{\partial}{\partial y} \\ \hat{p}_z = -i\hbar\dfrac{\partial}{\partial z} \end{cases}$$

$$\langle\vec{p}\rangle \equiv \iiint \varphi^*(\vec{p})\vec{p}\varphi(\vec{p})dp_x dp_y dp_z$$

$$= \iiint \psi^*(\vec{r},t)(-i\hbar\nabla)\psi(\vec{r},t)dxdydz$$

$$\boxed{\langle\vec{p}\rangle = \iiint \psi^*(\vec{r},t)\hat{\vec{p}}\psi(\vec{r},t)dxdydz = \left(\psi,\hat{\vec{p}}\psi\right) = \langle\psi|\hat{\vec{\boldsymbol{p}}}|\psi\rangle}$$

动能和能量平均值

动能

$$T=\frac{\vec{p}^2}{2m},\qquad \hat{T}=-\frac{\hbar^2}{2m}\nabla^2$$

期望值

$$\langle T\rangle=\iiint\psi^*(\vec{r},t)\left(-\frac{\hbar^2}{2m}\nabla^2\right)\psi(\vec{r},t)dxdydz$$

机械能的期望值

$$E=T+V,\qquad \hat{H}=-\frac{\hbar^2}{2m}\nabla^2+V(\vec{r},t)\Rightarrow\langle E\rangle=\iiint\psi^*(\vec{r},t)\,\hat{H}\psi(\vec{r},t)dxdydz$$

利用薛定谔方程

$$i\hbar\frac{\partial}{\partial t}\psi=\hat{H}\psi$$

也可以写成

$$\langle E\rangle=\iiint\psi^*(\vec{r},t)\left(i\hbar\frac{\partial}{\partial t}\right)\psi(\vec{r},t)dxdydz$$

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任意的力学量的平均值

每个力学量都可以用一个厄密算符表示

厄密算符的定义：$(\phi, \hat{A}\psi) = (\hat{A}\phi, \psi)$

$$\iiint \phi^*(\vec{r},t)\hat{A}\psi(\vec{r},t)dxdydz = \iiint \left(\hat{A}\phi(\vec{r},t)\right)^* \psi(\vec{r},t)dxdydz$$

$$\bar{A} \equiv \langle A\rangle \stackrel{\text{def}}{=} \iiint \psi^*(\vec{r},t)\hat{A}\psi(\vec{r},t)dxdydz$$

$$\equiv (\psi, \hat{A}\psi) \equiv \langle\psi|\hat{A}|\psi\rangle$$

函数空间的内积

$$(f,\quad g) \equiv \int f^*(x)g(x)dx$$

$$(f,\quad g) \equiv \iiint f^*(\vec{r})g(\vec{r})dxdydz$$

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角动量算符

- 轨道角动量

$$\vec{L} = \vec{r} \times \vec{p} \rightarrow \hat{\vec{L}} = \hat{\vec{r}} \times \hat{\vec{p}}$$

$$\hat{L}_x = \hat{y}\hat{p}_z - \hat{z}\hat{p}_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$\hat{L}_y = \hat{z}\hat{p}_x - \hat{x}\hat{p}_z = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

$$\hat{L}_z = \hat{x}\hat{p}_y - \hat{y}\hat{p}_x = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

力学量的算符表示

- 在坐标表象(coordinate representation)中波函数

$$\psi(\vec{r},t) = \frac{1}{(2\pi\hbar)^{3/2}}\iiint \phi(\vec{p})e^{\frac{i}{\hbar}\vec{p}\cdot\vec{r}}dp_x dp_y dp_z$$

- 力学量算符

$$\hat{x} = x, \qquad \hat{\vec{r}} = \vec{r},$$

$$\hat{V} = V(\vec{r},t)$$

$$\hat{\vec{p}} = -i\hbar\nabla, \qquad \hat{T} = -\frac{\hbar^2}{2m}\nabla^2,$$

$$\hat{H} = -\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r},t)$$

通常使用坐标表象

- 在动量表象中的波函数

$$\phi(\vec{p},t) = \frac{1}{(2\pi\hbar)^{3/2}}\iiint \psi(\vec{r},t)e^{-\frac{i}{\hbar}\vec{p}\cdot\vec{r}}dxdydz$$

- 力学量算符

$$\hat{x} = i\hbar\frac{\partial}{\partial p_x}, \qquad \hat{\vec{r}} = i\hbar\nabla_{\vec{p}},$$

$$\hat{V} = V(i\hbar\nabla_{\vec{p}},t)$$

$$\hat{\vec{p}} = \vec{p}, \qquad \hat{T} = \frac{\vec{p}^2}{2m},$$

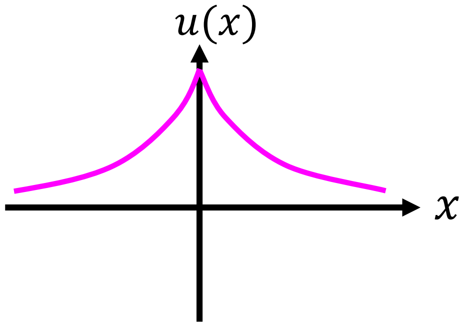
$$\hat{H} = \frac{\vec{p}^2}{2m} + V\left(i\hbar\nabla_{\vec{p}},t\right)$$

例 δ势阱

- 束缚态坐标表象波函数

$$u(x) = \frac{\sqrt{m\alpha}}{\hbar} e^{-\frac{m\alpha}{\hbar^2}|x|}$$

$$E = -\frac{m\alpha^2}{2\hbar^2}$$



- 坐标期望值

$$\bar{x} = \langle x \rangle = \int_{\mathbb{R}} u^*(x) x u(x) dx = 0$$

- 方差

$$\Delta x^2 = \langle (x-\bar{x})^2 \rangle = \int_{\mathbb{R}} u^*(x) x^2 u(x) dx = \frac{\hbar^4}{2m^2\alpha^2}$$

- 势能期望值

$$\langle V \rangle = \int_{\mathbb{R}} u^*(x)\big(-\alpha\delta(x)\big)u(x)dx = -\alpha u(0)^2 = -\frac{m\alpha^2}{\hbar^2}$$

- 动量期望值

$$\langle p \rangle = \int_{\mathbb{R}} u^*(x)(-i\hbar)\frac{d}{dx}u(x)dx = 0$$

- 动量的方差

$$\Delta p^2 = \langle (p-\bar{p})^2 \rangle = -\hbar^2 \int_{\mathbb{R}} u^*(x)\frac{d^2}{dx^2}u(x)dx$$

$$= \hbar^2 \int_{\mathbb{R}} \big(u'(x)\big)^2 dx = \frac{m^2\alpha^2}{\hbar^2}$$

- 不确定关系

$$\Delta x \Delta p = \frac{1}{\sqrt{2}}\hbar > \frac{1}{2}\hbar$$

- 动能期望值

$$\langle T \rangle = -\frac{\hbar^2}{2m}\int_{\mathbb{R}} u^*(x)\frac{d^2}{dx^2}u(x)dx = \frac{m\alpha^2}{2\hbar^2}$$

- 能量期望值

$$\langle E \rangle = \int_{\mathbb{R}} u^*(x)\hat{H}u(x)dx = \langle T \rangle + \langle V \rangle = -\frac{m\alpha^2}{2\hbar^2}$$

能量叠加态中，能量守恒吗？

能量期望值

$$\bar{E}(t)=\langle\hat{H}\rangle=\langle\psi|\hat{H}|\psi\rangle$$
$$=\int_{-\infty}^{+\infty}\psi^*(x,t)\hat{H}\psi(x,t)dx$$

$$\frac{d}{dt}\bar{E}(t)=\frac{d}{dt}\left\{\int_{-\infty}^{+\infty}\psi^*(x,t)\hat{H}\psi(x,t)dx\right\}$$
$$=\int_{-\infty}^{+\infty}\left(\frac{\partial}{\partial t}\psi^*(x,t)\right)\hat{H}\psi(x,t)dx$$
$$+\int_{-\infty}^{+\infty}\psi^*(x,t)\left(\frac{\partial}{\partial t}\hat{H}\right)\psi(x,t)dx$$
$$+\int_{-\infty}^{+\infty}\psi^*(x,t)\hat{H}\left(\frac{\partial}{\partial t}\psi(x,t)\right)dx$$

利用薛定谔方程

$$i\hbar\frac{\partial}{\partial t}\psi(x,t)=\hat{H}\psi(x,t)$$

$$\frac{d}{dt}\bar{E}(t)=\int_{-\infty}^{+\infty}\left(\frac{1}{-i\hbar}\hat{H}\psi^*(x,t)\right)\hat{H}\psi(x,t)dx$$
$$+\int_{-\infty}^{+\infty}\psi^*(x,t)\left(\frac{\partial}{\partial t}\hat{H}\right)\psi(x,t)dx$$
$$+\int_{-\infty}^{+\infty}\psi^*(x,t)\hat{H}\left(\frac{1}{i\hbar}\hat{H}\psi(x,t)\right)dx$$

$$\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x,\cancel{t})$$

是厄密算符，且$\frac{\partial\hat{H}}{\partial t}=0$

$$\frac{d\bar{E}(t)}{dt}$$
$$=\int_{-\infty}^{+\infty}\psi^*(x,t)\left\{\frac{1}{-i\hbar}\hat{H}\hat{H}+0+\frac{1}{i\hbar}\hat{H}\hat{H}\right\}\psi(x,t)dx$$
$$=0$$

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算符的对易关系

力学量是算符，
因而具有和矩阵类似的性质，
乘法不满足交换律

对易子（commutator）

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

在信号系统中，统计量同样不对易

$$s(t)=\frac{1}{\sqrt{2\pi}}\int \varphi(\omega)e^{-i\omega t}d\omega$$

$$\varphi(\omega)=\frac{1}{\sqrt{2\pi}}\int s(t)e^{i\omega t}dt$$

信号	$s(t)$	$\varphi(\omega)$
时间	t	$-i\frac{\partial}{\partial\omega}$
频率	$i\frac{\partial}{\partial t}$	ω
统计量 高阶矩	…	…

基本对易关系

$[\hat{x},\hat{p}_x]=i\hbar$, $[\hat{y},\hat{p}_y]=i\hbar$, $[\hat{z},\hat{p}_z]=i\hbar$, 其它为0

$\Leftrightarrow [\hat{r}_j,\hat{p}_k]=i\hbar\delta_{jk}, [\hat{r}_j,\hat{r}_k]=0, [\hat{p}_j,\hat{p}_k]=0$

克罗内克符号$\delta_{jk} \stackrel{\text{def}}{=} \begin{cases}1, & j=k;\\ 0, & j\neq k.\end{cases}$

海森堡矩阵力学的基本假设

基本对易关系

$$[\hat{r}_j,\hat{p}_k]=i\hbar\delta_{jk},[\hat{r}_j,\hat{r}_k]=0,[\hat{p}_j,\hat{p}_k]=0$$

海森堡运动方程

$$i\hbar\frac{d\hat{A}}{dt}=i\hbar\frac{\partial\hat{A}}{\partial t}+[\hat{A},\hat{H}]$$

$$\boxed{\text{矩阵力学的基本假设}}$$

由波动力学证明矩阵力学：对任意波函数$|\psi\rangle,|\varphi\rangle$，矩阵元的变化为

$$\frac{d}{dt}\langle\psi|\hat{A}(t)|\varphi\rangle=\left\langle\frac{d}{dt}\psi\middle|\hat{A}\middle|\varphi\right\rangle+\left\langle\psi\middle|\frac{\partial\hat{A}(t)}{\partial t}\middle|\varphi\right\rangle+\left\langle\psi\middle|\hat{A}\middle|\frac{d}{dt}\varphi\right\rangle$$

$$=\left\langle\frac{\hat{H}}{i\hbar}\psi\middle|\hat{A}\middle|\varphi\right\rangle+\left\langle\psi\middle|\frac{\partial\hat{A}(t)}{\partial t}\middle|\varphi\right\rangle+\left\langle\psi\middle|\hat{A}\middle|\frac{\hat{H}}{i\hbar}\varphi\right\rangle$$

$$=-\frac{1}{i\hbar}\langle\psi|\hat{H}\hat{A}|\varphi\rangle+\left\langle\psi\middle|\frac{\partial\hat{A}(t)}{\partial t}\middle|\varphi\right\rangle+\frac{1}{i\hbar}\langle\psi|\hat{A}\hat{H}|\varphi\rangle$$

$$=-\frac{1}{i\hbar}\langle\psi|\hat{H}\hat{A}|\varphi\rangle+\left\langle\psi\middle|\frac{\partial\hat{A}(t)}{\partial t}\middle|\varphi\right\rangle+\frac{1}{i\hbar}\langle\psi|\hat{A}\hat{H}|\varphi\rangle$$

$$=\left\langle\psi\middle|\frac{\partial\hat{A}}{\partial t}+\frac{1}{i\hbar}[\hat{A},\hat{H}]\middle|\varphi\right\rangle$$

经典对易关系（泊松括号）

$$[A,B]_{PB}\overset{\text{def}}{=}\sum_\gamma\left(\frac{\partial A}{\partial q_\gamma}\frac{\partial B}{\partial p_\gamma}-\frac{\partial A}{\partial p_\gamma}\frac{\partial B}{\partial q_\gamma}\right)$$

哈密顿力学的泊松括号表示

$$\dot{q}_\alpha=[q_\alpha,H]_{PB}\Leftrightarrow\dot{q}_\alpha=\partial H/\partial p_\alpha$$
$$\dot{p}_\alpha=[p_\alpha,H]_{PB}\Leftrightarrow\dot{p}_\alpha=-\partial H/\partial q_\alpha$$

任何一个力学量$A(t,q,p)$随时间的演化

$$\frac{dA}{dt}=\frac{\partial A}{\partial t}+[A,H]_{PB}$$

正则量子化*

$$[\cdot,\cdot]_{PB}\rightarrow\frac{1}{i\hbar}[\cdot,\cdot]$$

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对易子运算的形式规则

- 反对称（或幂零）

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

- 双线性

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

- 导数规则

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

- 雅可比恒等式

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

李积 李代数

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例：计算对易子

角动量的对易关系

$$[\hat{L}_j, \hat{L}_k] = i\hbar\varepsilon_{jkl}\hat{L}_l, \qquad \hat{\vec{L}} \times \hat{\vec{L}} = i\hbar\hat{\vec{L}}$$

普通矢量$\vec{a} \times \vec{a} = \vec{0}$

求和约定

$$a_j b_j \stackrel{\text{def}}{=} \sum_{j=1}^{3} a_j b_j$$

$$[\hat{L}_j, \hat{r}_k] = i\hbar\varepsilon_{jkl}\hat{r}_l$$

$$[\hat{L}_j, \hat{p}_k] = i\hbar\varepsilon_{jkl}\hat{p}_l$$

$$[\hat{L}_j, \hat{T}] = 0$$

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动量是否守恒

动量期望值

$$\bar{p}(t) = \langle\psi|\hat{p}|\psi\rangle$$
$$= \int_{-\infty}^{+\infty} \psi^*(x,t)\hat{p}\psi(x,t)dx$$

$$\frac{d}{dt}\bar{p}(t) = \frac{d}{dt}\int_{-\infty}^{+\infty} \psi^*(x,t)\hat{p}\psi(x,t)dx$$
$$= \int_{-\infty}^{+\infty}\left(\frac{\partial}{\partial t}\psi^*\right)\hat{p}\psi dx + \int_{-\infty}^{+\infty}\psi^*\left(\frac{\partial}{\partial t}\hat{p}\right)\psi dx + \int_{-\infty}^{+\infty}\psi^*\hat{p}\left(\frac{\partial}{\partial t}\psi\right)dx$$
$$= \int_{-\infty}^{+\infty}\psi^*\left\{-\frac{1}{i\hbar}\hat{H}\hat{p} + \frac{\partial}{\partial t}\hat{p} + \frac{1}{i\hbar}\hat{p}\hat{H}\right\}\psi dx$$

$$\hat{p} = -i\hbar\frac{\partial}{\partial x}$$

$$\frac{\partial\hat{p}}{\partial t} = 0$$ （ $\hat{p}$ 中不含时间参数）

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

$$[\hat{p},\hat{H}] = -i\hbar\frac{\partial V}{\partial x} = i\hbar F(x)$$

$$\frac{d}{dt}\bar{p} = \left\langle\psi\left|\frac{\partial}{\partial t}\hat{p} + \frac{1}{i\hbar}[\hat{p},\hat{H}]\right|\psi\right\rangle$$

$$\boxed{\frac{d}{dt}\bar{A} = \left\langle\psi\left|\frac{\partial\hat{A}}{\partial t} + \frac{1}{i\hbar}[\hat{A},\hat{H}]\right|\psi\right\rangle}$$

$$\frac{d}{dt}A_{fi} = \left\langle\psi_f\left|\frac{\partial\hat{A}}{\partial t} + \frac{1}{i\hbar}[\hat{A},\hat{H}]\right|\psi_i\right\rangle$$

$$\boxed{\frac{d\hat{A}}{dt} = \frac{\partial\hat{A}}{\partial t} + \frac{1}{i\hbar}[\hat{A},\hat{H}]}$$

可用于检验是否守恒量

$$\Rightarrow \frac{d\bar{p}}{dt} = \bar{F}$$

埃伦费斯特定理
Ehrenfest's theorem

补：不确定关系的证明

$$\int \left|\xi\hat{A}\psi + i\hat{B}\psi\right|^2 dx \geq 0, \qquad \hat{A}^\dagger = \hat{A}, \hat{B}^\dagger = \hat{B}, \forall\xi \in \boldsymbol{R}.$$

$$\int \left|\xi\hat{A}\psi + i\hat{B}\psi\right|^2 dx = \xi^2\overline{A^2} - \xi\bar{C} + \overline{B^2} = \overline{A^2}\left(\xi - \frac{\bar{C}}{2\overline{A^2}}\right)^2 + \left(\overline{B^2} - \frac{\bar{C}^2}{4\overline{A^2}}\right)$$

令$\xi = \frac{\bar{C}}{2\overline{A^2}} \Rightarrow \overline{B^2} - \frac{\bar{C}^2}{4\overline{A^2}} \geq 0 \Leftrightarrow \overline{A^2}\cdot\overline{B^2} \geq \frac{1}{4}\bar{C}^2$

$$[\hat{A}, \hat{B}] = i\hat{C} \Rightarrow \boxed{\overline{A^2}\cdot\overline{B^2} \geq \frac{1}{4}\bar{C}^2}$$

可用于任何算符
可用于信号理论

取$\hat{A} = \hat{x} - \bar{x}, \hat{B} = \hat{p}_x - \bar{p}_x \Rightarrow \hat{C} = \hbar$

$$\Rightarrow \Delta x^2 \cdot \Delta p_x^2 \geq \frac{1}{4}\hbar^2,$$

$$\Delta x\Delta p_x \geq \frac{\hbar}{2}$$

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等式成立的条件

$$\Delta x \Delta p_x = \frac{\hbar}{2} \Leftrightarrow \xi - \frac{\bar{C}}{2\overline{A^2}} = 0\text{时，}\int \left|\xi \hat{A}\psi + i\hat{B}\psi\right|^2 dx = 0$$

$$\Leftrightarrow \frac{\bar{C}}{2\overline{A^2}}\hat{A}\psi + i\hat{B}\psi = 0$$

$$\Leftrightarrow \frac{\hbar}{2(\Delta x)^2}(x - \bar{x})\psi(x) + i\left(-i\hbar\frac{\partial}{\partial x} - \bar{p}_x\right)\psi(x) = 0$$

$$\frac{\partial}{\partial x}\psi(x) = \left\{\frac{i}{\hbar}\bar{p}_x - \frac{1}{2(\Delta x)^2}(x - \bar{x})\right\}\psi(x)$$

$$\psi(x) \propto \exp\left\{\frac{i}{\hbar}\bar{p}_x x - \frac{1}{(2\Delta x)^2}(x - \bar{x})^2\right\}$$

最小测不准波包

压缩态squeezed state:

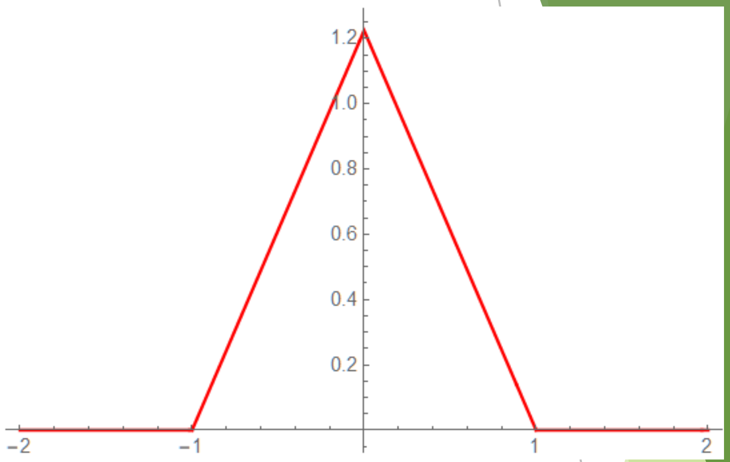
压缩时域或频域信号宽度，精确测量，激光

相干态$\Delta q^2 = \frac{1}{2}, \Delta p^2 = \frac{1}{2}$

检验不确定关系

- 不确定关系对任意波函数均成立
- 例如取三角形波，

$$\psi(x)=\begin{cases}\left(\frac{3}{2}\right)^{\frac{1}{2}}(1-|x|), & \text{if } |x|<1;\\ 0, & \text{if } |x|\geq 1.\end{cases}$$



$$\bar{x}=\int_{-\infty}^{+\infty} x\psi^*(x)\psi(x)dx=0$$

$$\Delta x^2=\int_{-\infty}^{+\infty}(x-\bar{x})\psi^*(x)\psi(x)dx=1/10$$

$$\bar{p}=\int_{-\infty}^{+\infty}\psi^*(x)\hat{p}\psi(x)dx=(-i\hbar)\int_{-\infty}^{\infty}\psi\frac{\partial\psi}{\partial x}dx=\frac{1}{2}(-i\hbar)(\psi^2|_{-1}^{0}+\psi^2|_{0}^{1})=0$$(后面章节证明)

$$\Delta p^2=\int_{-\infty}^{+\infty}\psi^*(x)(\hat{p}-\bar{p})^2\psi(x)dx=(-i\hbar)^2\int_{-\infty}^{\infty}\psi\frac{\partial^2\psi}{\partial x^2}dx$$

$$=\frac{3}{2}(-i\hbar)^2\int_{-\infty}^{\infty}\psi(x)\{\delta(x+1)-2\delta(x)+\delta(x-1)\}dx=\frac{3}{2}(-i\hbar)^2\{-2\psi(0)\}=3\hbar^2$$

$$\Delta x\Delta p=\sqrt{\frac{3}{10}}\hbar>\frac{1}{2}\hbar$$

例题：估算谐振子基态能量

- 哈密顿算符

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

- 能量的期望值

$$\bar{E}=\langle\hat{H}\rangle=\left\langle\frac{\hat{p}^2}{2m}+\frac{1}{2}m\omega^2\hat{x}^2\right\rangle$$

$$\hat{A}\stackrel{\text{def}}{=}\frac{1}{\sqrt{2m}}\hat{p},\qquad \hat{B}\stackrel{\text{def}}{=}\sqrt{\frac{m}{2}}\omega\hat{x}$$

$$\hat{C}=[\hat{A},\hat{B}]=\frac{1}{2}\omega(-i\hbar),\qquad \bar{C}=-\frac{i}{2}\hbar\omega$$

$$\langle\hat{H}\rangle=\left\langle\hat{A}^2+\hat{B}^2\right\rangle=\overline{A^2}+\overline{B^2}\geq2\sqrt{\overline{A^2}\cdot\overline{B^2}}\geq2\sqrt{\frac{1}{4}\bar{C}^2}=\frac{1}{2}\hbar\omega$$

能量最低的基态为$\hbar\omega/2$

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量子力学中物理状态

- 与线性代数中的概念对比：

状态矢量（波函数）	↔	矢量（矢量的坐标分量）
力学量（算符）	↔	线性变换（矩阵）
态矢的内积	↔	矢量的内积

- 量子力学的状态空间是一个复线性空间
- 状态空间是投影几何projective geometry
- 状态空间是扩展的Hilbert空间（{平方可积函数}=$\mathcal{H}$）

态矢(state vector)

- 对偶矢量：Dirac左矢和右矢

$$|\psi\rangle \to \psi(\vec{r},t), \qquad \langle\psi| \to \psi^*(\vec{r},t)$$

- 力学量作用在态矢量上，是线性变换，

$$\boldsymbol{A}|\psi\rangle \to \hat{A}\psi(\vec{r},t)$$

- 态矢的内积

$$\langle\psi_1|\psi_2\rangle \equiv \iiint \psi_1^*(\vec{r},t)\psi_2(\vec{r},t)dxdydz$$

- 力学量的矩阵元

$$\langle\psi_1|\boldsymbol{A}|\psi_2\rangle \equiv \iiint \psi_1^*(\vec{r},t)\hat{A}\psi_2(\vec{r},t)dxdydz$$

- 波函数相当于坐标分量，

$$\psi(\vec{r},t) = \langle\vec{r},t|\psi\rangle, \qquad |\psi\rangle = \iiint \psi(\vec{r},t)|\vec{r},t\rangle d^3\vec{r}$$

力学量的本征值

- 力学量是矩阵，所以有本征值eigen value、本征矢（本征态eigen state ）

$$\boldsymbol{A}|\psi\rangle = a|\psi\rangle \Leftrightarrow \hat{A}\psi(\vec{r},t) = a\psi(\vec{r},t)$$

- 能量本征态

$$\boldsymbol{H}|\psi\rangle = E|\psi\rangle \Leftrightarrow \widehat{H}\psi(\vec{r},t) = E\psi(\vec{r},t)$$

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right\}\psi(\vec{r},t) = E\psi(\vec{r},t)$$

$$\psi(\vec{r},t) \stackrel{\text{def}}{=} f(t)u(\vec{r})$$

$$\left\{-\frac{\hbar^2}{2m}\nabla^2 + V(\vec{r})\right\}u(\vec{r}) = Eu(\vec{r})$$

动量的本征态

一维空间

$$\hat{p}_x\psi(x,t) = p_x\psi(x,t)$$

$$\hat{p}_x u(x) = p_x u(x)$$

$$-i\hbar\,\partial_x u(x) = p_x u(x)$$

$$u(x) = \frac{1}{\sqrt{2\pi\hbar}} e^{\frac{i}{\hbar}p_x x}$$

三维空间

$$u(\vec{r}) = \frac{1}{(2\pi\hbar)^{3/2}} e^{\frac{i}{\hbar}(p_x x + p_y y + p_z z)}$$

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力学量对应的算符是厄米算符

- 可测物理量的所有本征值都是实数
  →力学量对应的算符是厄米算符

- 定理：同一力学量的不同本征值对应的本征矢正交

$$\left.\begin{aligned}\mathbf{A}|\alpha\rangle &= \alpha|\alpha\rangle\\ \mathbf{A}|\beta\rangle &= \beta|\beta\rangle\end{aligned}\right\} \Rightarrow \langle\alpha|\mathbf{A}|\beta\rangle = \alpha\langle\alpha|\beta\rangle = \beta\langle\alpha|\beta\rangle$$

$$\Rightarrow (\alpha-\beta)\langle\alpha|\beta\rangle = 0 \Rightarrow \langle\alpha|\beta\rangle = 0$$

- 定理：力学量的所有本征矢，构成态空间的完备基

（谱分解定理）下列条件等价：
1. 算符是规范的（$\hat{A}^{\dagger}\hat{A} = \hat{A}\hat{A}^{\dagger}$）
2. 算符的本征矢构成正交完备基（规范基、标准基）
3. 算符在某组正交完备基下是对角化的

测量

- 测量是在仪器所决定的态矢上的投影
- 测量即制备　　电子的双缝干涉
- 物理态空间

$$H_{\text{phys}}=\{\psi|\forall f\in H,(\psi,f)<\infty\}$$

类比

能量信号：信号总能量为有限值而信号平均功率为零；

功率信号：平均功率为有限值而信号总能量为无限大。

- 测量公理 冯·诺依曼1930年
- 公理化量子力学
- 自然科学的黄金时期：量子光学、量子电子学、量子化学……
- 量子力学与各学科的关系：生物物理（光合、细胞、意识），量子信息，量子通信，量子计算机，量子雷达……

量子力学的基本假设

- 每一个可观测量A，对应物理状态空间的一个自伴算符$\hat{A}$。
- 观测物理量A的结果，只能是算符$\hat{A}$的本征值之一。
- 如果波函数展开为

$$\psi \equiv \sum_a c_a \psi_a$$

其中ψ_a是$\hat{A}$的归一化本征态，那么物理量A的测量值取a的概率是$|c_a|^2$。

- 测量即制备：如果测量A所得的值是a，那么在刚完成测量之后，系统的状态是ψ_a。
- 波函数随时间的演化满足薛定谔方程
- 全同粒子的假设（后面章节中介绍）