第3章　　量子力学中的力学量

3.1 算符的起源

3.2 算符的性质

3.3 动量算符和角动量算符。

3.4厄密算符的本征值和本征函数

3.5 算符与力学量的关系

3.6 任意观测量的测不准关系

3.0. 薛定谔方程与算符

光子波函数： $\psi(x,t)=\psi_0\cos\left(\omega t-\frac{2\pi}{\lambda}x\right)\rightarrow\psi_0 e^{-i\left(\omega t-\frac{2\pi}{\lambda}x\right)}$

$$\begin{cases} E_{能量}=h\nu=h\dfrac{1}{\dfrac{2\pi}{\omega}}=h\dfrac{\omega}{2\pi}=\hbar\omega \\ p_{动量}=\dfrac{h}{\lambda} \end{cases}\rightarrow\begin{cases} \omega=\dfrac{E_{能量}}{\hbar} \\ \lambda=\dfrac{h}{p_{动量}} \end{cases}$$

光子的波函数 $\rightarrow\psi(x,t)=\psi_0 e^{-i\left(\omega t-\frac{2\pi}{\lambda}x\right)}=\psi_0 e^{\frac{i}{\hbar}(px-Et)}$

自由粒子的波函数 $\rightarrow\psi(x,t)=\psi_0 e^{-i\left(\omega t-\frac{2\pi}{\lambda}x\right)}=\psi_0 e^{\frac{i}{\hbar}(px-Et)}$

$$\psi(x,t)=\psi_0 e^{\frac{i}{\hbar}(p_x x-Et)}$$

对波函数时间微分 $\rightarrow \dfrac{\partial\psi(x,t)}{\partial t}=-\dfrac{i}{\hbar}E\psi(x,t) \quad \rightarrow i\hbar\dfrac{\partial\psi(x,t)}{\partial t}=E\psi(x,t)$

对波函数的空间二阶导数 $\rightarrow \dfrac{\partial^2\psi(x,t)}{\partial x^2}=-\dfrac{p_x^2}{\hbar^2}\psi(x,t)$

利用动量 $E=\dfrac{P^2}{2m}, \rightarrow -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi(x,t)}{\partial x^2}=E\psi(x,t)$

$$\begin{cases} i\hbar\dfrac{\partial\psi(x,t)}{\partial t}=E\psi(x,t) \\ -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi(x,t)}{\partial x^2}=E\psi(x,t) \end{cases}$$

$\rightarrow$ 自由粒子的薛定锷方程：$i\hbar\dfrac{\partial\psi(x,t)}{\partial t}=-\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}\psi(x,t)$

$$i\hbar\frac{\partial\psi\ (x,t)}{\partial t}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}\psi\ (x,t)$$

$$\begin{cases} i\hbar\dfrac{\partial\psi(x,t)}{\partial t}=E\psi(x,t) \\ -\dfrac{\hbar^2}{2m}\dfrac{\partial^2\psi\ (x,t)}{\partial x^2}=E\psi(x,t) \end{cases} \rightarrow \begin{cases} i\hbar\dfrac{\partial}{\partial t}=E \\ -\dfrac{\hbar^2}{2m}\dfrac{\partial^2}{\partial x^2}=E \end{cases}$$

把自由粒子运动算符推广到非自由粒子运动，粒子所处的势场为U(x, t)，粒子的能量

$$E=\frac{p_x^2}{2m}+U(x,t)\rightarrow E=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x,t)$$

$$\rightarrow i\hbar\frac{\partial\psi(x,t)}{\partial t}=\left(-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x,t)\right)\psi(x,t)$$ 令： $$H=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+U(x,t)$$

$$i\hbar\frac{\partial\psi(\vec{x},t)}{\partial t}=\hat{H}\psi(\vec{x},t)$$ —这就是含时薛定谔方程

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

H称为哈密顿算符

- 三维势场U(r, t) 中

$$E=\frac{p_x^2+p_y^2+p_z^2}{2m}+U(\vec{r},t)\rightarrow\hat{H}=-\frac{\hbar^2}{2m}\left(\frac{\partial^2}{\partial x^2}+\frac{\partial^2}{\partial y^2}+\frac{\partial^2}{\partial z^2}\right)+U(\vec{r},t)$$

$$\nabla=\frac{\partial}{\partial x}\vec{i}+\frac{\partial}{\partial y}\vec{j}+\frac{\partial}{\partial z}\vec{k}\rightarrow\text{哈密顿算符：}\hat{H}=-\frac{\hbar^2}{2m}\nabla^2+U(\vec{r},t)$$

薛定谔方程形式不变

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

$$-\frac{\hbar^2}{2m}\frac{\partial^2\psi\ (x,t)}{\partial x^2}=E\psi(x,t)\rightarrow -\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}=E_k\rightarrow \text{定义为动能算符}$$

$$\psi(x,t)=\psi_0 e^{\frac{i}{\hbar}(p_x x-Et)}\rightarrow\frac{\partial\psi(x,t)}{\partial x}=i\frac{p_x}{\hbar}\psi(x,t)$$

$$-i\hbar\frac{\partial\psi(x,t)}{\partial x}=p_x\psi(x,t)\rightarrow\hat{p}_x=-i\hbar\frac{\partial}{\partial x}\rightarrow\text{定义为动量算符}$$

$$\text{角动量算符}\rightarrow\hat{\vec{L}}=\vec{r}\times\hat{\vec{p}}=\begin{vmatrix}\vec{i} & \vec{j} & \vec{k}\\ x & y & z\\ \hat{p}_x & \hat{p}_y & \hat{p}_z\end{vmatrix}\quad\text{展开得到}\rightarrow\begin{cases}\hat{L}_x=y\hat{p}_z-z\hat{p}_y\\ \hat{L}_y=z\hat{p}_x-x\hat{p}_z\\ \hat{L}_z=x\hat{p}_y-y\hat{p}_x\end{cases}$$

$$\rightarrow\hat{L}^2=\hat{\vec{L}}\bullet\hat{\vec{L}}=\hat{L}_x^2+\hat{L}_y^2+\hat{L}_z^2$$

3.1 算符的性质

1.算符的基本概念

什么是算符？算符是指作用在一个函数上得出另一个函数的运算符号。

$\hat{F}\ u = \upsilon \rightarrow \hat{F}$统称为算符

例如：$\dfrac{d}{dx}u = \upsilon,\quad \dfrac{d}{dx}$是微商算符，$\sqrt{\ }$为开方算符等

线性算符 $\hat{F}(\alpha_1 u_1 + \alpha_2 u_2) = \alpha_1 \hat{F} u_1 + \alpha_2 \hat{F} u_2$

位置算符和动量算符 $\hat{x} = x,\quad \hat{p}_x = -i\hbar\dfrac{\partial}{\partial x}$ 均为线性算符。

典型的非线性算符为 $\sqrt{\alpha_1 u_1 + \alpha_2 u_2} \neq \alpha_1\sqrt{u_1} + \alpha_2\sqrt{u_2}$

坐标和动量算符 $\hat{r}=r,\quad \hat{p}=-i\hbar\nabla$

哈密顿算符： $\hat{H}=-\frac{\hbar^2}{2\mu}\nabla^2+U(\mathrm{r})$

角动量算符： $\hat{L}=\hat{r}\times\hat{p}=-i\hbar r\times\nabla$

2.算符的物理意义

若一个算符 $\hat{F}$ 作用于一个函数ψ

$$\hat{F}\psi = \lambda\psi$$

λ称为算符$\hat{F}$的本征值，ψ称为本征函数，方程称为算符的本征值方程。

3.厄密算符

两个波函数ψ和φ，满足下列等式

$$\int \psi^* \hat{F} \varphi d\tau = \int (\hat{F}\psi)^* \varphi d\tau$$ 的算符 $\hat{F}$ 称为厄密算符

厄密算符的本征值为实数

$$\hat{F}\psi = \lambda\psi \rightarrow \int \psi^* \hat{F}\psi d\tau = \lambda \int \psi^* \psi d\tau$$

如果$\hat{F}$是呃密算符，则$\rightarrow \int \psi^* \hat{F}\psi d\tau = \int (\hat{F}\psi)^* \psi d\tau = \int (\lambda\psi)^* \psi d\tau = \lambda^* \int \psi^* \psi d\tau$

则有 $\rightarrow \lambda = \lambda^*$

在量子力学中，为了使所描述的力学量具有意义，我们要求它们的平均值为实数，即量子力学中表示力学量的算符都是厄密算符。

证明动量算符 $\hat{p}_x = -i\hbar\partial / \partial x$ 的厄密性

$$\int_{-\infty}^{+\infty} \psi^* \hat{p}_x \phi d\tau = \int_{-\infty}^{+\infty} \psi^* \hat{p}_x \phi dx = \int_{-\infty}^{+\infty} \psi^* (-i\hbar \frac{\partial}{\partial x}) \phi dx = -i\hbar (\phi\psi) \Big|_{-\infty}^{+\infty} + i\hbar \int_{-\infty}^{+\infty} \phi \frac{\partial}{\partial x} \psi^* dx$$

因为ψ和φ是有限的 $-i\hbar(\varphi\psi)\Big|_{-\infty}^{+\infty} = 0$

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

4.算符运算初步

1）算符之和： $\hat{A}+\hat{B}=\hat{C} \rightarrow \hat{C}\psi=(\hat{A}+\hat{B})\psi=\hat{A}\psi+\hat{B}\psi$

2）算符之积：$\hat{A}\hat{B}=\hat{C} \rightarrow \hat{C}\psi=(\hat{A}\hat{B})\psi=\hat{A}(\hat{B}\psi)$

$$\hat{F}\hat{F}\hat{F}\hat{F}\ldots=\hat{F}^{n}$$

一般情况下，算符之积不满足交换律

$$\hat{A}\hat{B} \neq \hat{B}\hat{A}$$

$x\dfrac{\partial}{\partial x}u \neq \dfrac{\partial}{\partial x}(xu) \rightarrow \dfrac{\partial}{\partial x}$ 和 x 不 对 易

例 $[\hat{x}, \hat{p}_x] = ?$

$$(\hat{x}\hat{p}_x - \hat{p}_x\hat{x})\psi = -i\hbar x\frac{\partial}{\partial x}\psi + i\hbar\frac{\partial}{\partial x}(x\psi)$$

$$= -i\hbar x\frac{\partial}{\partial x}\psi + i\hbar\psi + i\hbar x\frac{\partial}{\partial x}\psi = i\hbar\psi$$

ψ是体系的任意波函数，所以 $[\hat{x}, \hat{p}_x] = i\hbar$ 这两算符不对易

$$\left\{\begin{array}{l} [\hat{x}, \hat{p}_x] = x\hat{p}_x - \hat{p}_x x = i\hbar \\ [\hat{y}, \hat{p}_y] = y\hat{p}_y - \hat{p}_y y = i\hbar \rightarrow \text{不对易} \\ [\hat{z}, \hat{p}_z] = z\hat{p}_z - \hat{p}_z z = i\hbar \end{array}\right.$$

不对易算符不能同时有确定值。

3） 算符的对易性

$\hat{A}\hat{B}-\hat{B}\hat{A}=0 \to \hat{A},\hat{B}$算符对易　记为 $[\hat{A},\hat{B}] \equiv \hat{A}\hat{B}-\hat{B}\hat{A}=0$

$\frac{\partial}{\partial x}\frac{\partial}{\partial y}u=\frac{\partial}{\partial y}\frac{\partial}{\partial x}u \to \frac{\partial}{\partial x}$和$\frac{\partial}{\partial y}$对易

$$\begin{cases} xy-yx=0 \\ xz-zx=0 \\ yz-zy=0 \end{cases} \to$$ 三个坐标分量相互对易

$$\begin{cases} [\hat{z},\hat{p}_x]=z\hat{p}_x-\hat{p}_x z=0 \\ [\hat{y},\hat{p}_z]=y\hat{p}_z-\hat{p}_z y=0 \to z\hat{p}_x \text{等对易} \\ [\hat{x},\hat{p}_y]=x\hat{p}_y-\hat{p}_y x=0 \end{cases}$$

例：

$$\begin{cases} \hat{p}_x = -i\hbar \dfrac{\partial}{\partial x} \\ \hat{p}_y = -i\hbar \dfrac{\partial}{\partial y} \end{cases} \rightarrow \begin{cases} \hat{p}_y \hat{p}_x \psi = -\hbar^2 \dfrac{\partial^2 \psi}{\partial y \partial x} \\ \hat{p}_x \hat{p}_y \psi = -\hbar^2 \dfrac{\partial^2 \psi}{\partial x \partial y} \end{cases}$$

$$\begin{cases} [\hat{p}_y, \hat{p}_x] = \hat{p}_y \hat{p}_x - \hat{p}_x \hat{p}_y = 0 \\ [\hat{p}_x, \hat{p}_z] = \hat{p}_x \hat{p}_z - \hat{p}_z \hat{p}_x = 0 \\ [\hat{p}_z, \hat{p}_y] = \hat{p}_z \hat{p}_y - \hat{p}_y \hat{p}_z = 0 \end{cases} \rightarrow \hat{p}_x \hat{p}_x \text{两两等对易}$$

对易算符有共同的本征函数系。

对易式满足下列恒等式

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

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

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

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

3.2 动量和角动量算符

动量算符 $$\hat{p} = -i\hbar\nabla$$

分量形式 $$\hat{p}_x = -i\hbar\frac{\partial}{\partial x},\ \hat{p}_y = -i\hbar\frac{\partial}{\partial y},\ \hat{p}_z = -i\hbar\frac{\partial}{\partial z}$$

动量算符各分量与坐标算符各分量之间的对易关系

$$[\hat{x}_i, \hat{p}_j] = i\hbar\delta_{ij} = \begin{cases} 0, & i \neq j \\ i\hbar, & i = j \end{cases}$$

动量平方算符 $$\hat{p}^2 = \hat{p}_x{}^2 + \hat{p}_y{}^2 + \hat{p}_z{}^2 = -\hbar^2\nabla^2$$

动量算符的本征值方程 $$-i\hbar\nabla\psi_p(\mathbf{r})=\mathbf{p}\psi_p(\mathbf{r})$$

P是动量算符的本征值，ψ_p（r）是动量算符的本征函数。

三个分量形式：
$$\begin{cases}-i\hbar\dfrac{\partial}{\partial x}\psi_p(r)=p_x\psi_p(r)\\ -i\hbar\dfrac{\partial}{\partial y}\psi_p(r)=p_y\psi_p(r)\\ -i\hbar\dfrac{\partial}{\partial z}\psi_p(\mathbf{r})=p_z\psi_p(\mathbf{r})\end{cases}$$

动量算符的本征函数 $$\psi_p(r)=Ce^{\frac{i}{\hbar}(p\cdot r)}$$

2）动量算符本征函数的“归一化”

本征值是分立的

考虑粒子限制在一维[-L/2, L/2]中运动，动量的本征态为

$$\psi_{p_x}(x) = Ce^{ip_x x/\hbar}$$

边界条件：$\psi_{px}(-L/2)=\psi_{px}(L/2)\to e^{-ip_xL/2\hbar}=e^{ip_xL/2\hbar}$

$$\frac{p_x L}{\hbar} = 2n\pi, \qquad (n = 0, \pm 1, \pm 2, \ldots)$$

粒子只在-L/2到L/2之间运动，所以可以认为两侧的外侧区域没有粒子出现，及边界出现频率相等且均为0

$$\to p_x = p_n = \frac{2n\pi\hbar}{L} = \frac{nh}{L}$$

$$\rightarrow p_x = p_n = \frac{2n\pi\hbar}{L} = \frac{nh}{L} \qquad \rightarrow \psi_{px}(x) = Ce^{inhx/L\hbar} = Ce^{in2\pi x/L}$$

可以看出，动量取值是不连续的，相应的归一化本征函数为

$$\rightarrow \int_0^L \psi_{plx}^2(x)dx = \int_0^L C^2 \cos^2 \frac{2\pi nx}{L} dx = 1$$

$$\rightarrow \int_0^L C^2 \cos^2 \frac{2\pi nx}{L} dx = \int_0^L C^2 \left(\frac{1+\cos\frac{4\pi nx}{L}}{2} \right) dx = 1$$

$$\rightarrow LC^2 = 1 \rightarrow C = \frac{1}{\sqrt{L}}$$

$$\psi_{px}(x) = \frac{1}{\sqrt{L}} e^{ip_x x/\hbar} \rightarrow \psi_p(r) = \frac{1}{L^{3/2}} e^{ip\cdot r/\hbar}$$

3）角动量算符

$$\hat{L} = \hat{r} \times \hat{p} = -i\hbar(r \times \nabla)$$

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

角动量平方算符

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$$

角动量算符的各分量之间是不对易的

$$[\hat{L}_x,\hat{L}_y]=\hat{L}_x\hat{L}_y-\hat{L}_y\hat{L}_x$$

$$=(y\hat{p}_z-z\hat{p}_y)(z\hat{p}_x-x\hat{p}_z)-(z\hat{p}_x-x\hat{p}_z)(y\hat{p}_z-z\hat{p}_y)$$

$$=y\hat{p}_z z\hat{p}_x\cancel{-y\hat{p}_z x\hat{p}_z}\cancel{-z\hat{p}_y z\hat{p}_x}+z\hat{p}_y x\hat{p}_z$$

$$-z\hat{p}_x y\hat{p}_z\cancel{+z\hat{p}_x z\hat{p}_y}\cancel{+x\hat{p}_z y\hat{p}_z}-x\hat{p}_z z\hat{p}_y$$

$$=(\hat{p}_z z-z\hat{p}_z)y\hat{p}_x+(z\hat{p}_z-\hat{p}_z z)x\hat{p}_y$$

$$=-i\hbar y\hat{p}_x+i\hbar x\hat{p}_y=i\hbar\hat{L}_z$$

$$[\hat{L}_x,\hat{L}_y]=i\hbar\hat{L}_z \rightarrow \begin{cases}[\hat{L}_x,\hat{L}_y]=i\hbar\hat{L}_z\\[\hat{L}_y,\hat{L}_z]=i\hbar\hat{L}_x\\[\hat{L}_z,\hat{L}_x]=i\hbar\hat{L}_y\end{cases}$$

三个角动量不能同时有确定的值，一个确定，其它两个就不能确定。

角动量平方算符与其各分量之间是对易的

$$[\hat{L}^2,\hat{L}_x]=[\hat{L}_x^2+\hat{L}_y^2+\hat{L}_z^2,\hat{L}_x]=[\hat{L}_y^2,\hat{L}_x]+[\hat{L}_z^2,\hat{L}_x]$$

$$=\hat{L}_y[\hat{L}_y,\hat{L}_x]+[\hat{L}_y,\hat{L}_x]\hat{L}_y+\hat{L}_z[\hat{L}_z,\hat{L}_x]+[\hat{L}_z,\hat{L}_x]\hat{L}_z$$

$$=i\hbar(-\hat{L}_y\hat{L}_z-\hat{L}_z\hat{L}_y+\hat{L}_z\hat{L}_y+\hat{L}_y\hat{L}_z)=0$$

$$\rightarrow\begin{cases}[\hat{L}^2,\hat{L}_x]=0\\ [\hat{L}^2,\hat{L}_y]=0\\ [\hat{L}^2,\hat{L}_z]=0\end{cases}$$

右手螺旋定正方向

L平方算符和每一个分量的算符同时有确定的值，有共同本征函数。

例：求 $\hat{L}_z = -i\hbar\frac{\partial}{\partial\varphi}$ **算符的本征值和本征函数**

解：本征方程表示为：

$$\hat{L}_z\psi = l_z\psi \rightarrow -i\hbar\frac{\partial}{\partial\phi}\psi = l_z\psi$$ 得到 $\rightarrow \psi(\phi) = C\exp(\frac{i}{\hbar}l_z\phi)$

C由周期性边界条件φ→φ+2π，体系回到原来位置，要求 $L_z = m\hbar$，$m=0$，±1，±2，…

$$\rightarrow \int_0^{2\pi}\left|\psi_m(\phi)\right|^2 d\phi = 1, \qquad C = \frac{1}{\sqrt{2\pi}}$$

算符L_z的归一化本征函数表示为

$$\rightarrow \psi_m(\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}, \quad m = 0,\ \pm 1,\ \pm 2,\ \ldots$$ 相应的本征值为 $m\hbar$

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 \qquad \hat{L}^2 = -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)$$

$$\rightarrow -\hbar^2\left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right)Y = L^2 Y$$

$$\lambda = \frac{\hbar^2}{L^2} \rightarrow \left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right) = -\lambda Y$$

$$\rightarrow \left(\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right) = -\lambda Y(\theta,\phi) = -\lambda\Phi(\phi)\Theta(\theta)$$

$\hat{L}^2$和L_z共同的本征函数

在Y_{lm}态中，体系角动量在z方向上的投影为$m\hbar$

前面几个球函数 $\rightarrow$

$$
\begin{cases}
Y_{00} = \dfrac{1}{\sqrt{4\pi}} \\[2ex]
Y_{1,1} = \dfrac{3}{\sqrt{8\pi}} \sin\theta e^{i\phi} \\[2ex]
Y_{1,0} = \dfrac{3}{\sqrt{4\pi}} \cos\theta \\[2ex]
Y_{1,-1} = \dfrac{3}{\sqrt{8\pi}} \sin\theta e^{-i\phi}
\end{cases}
$$

3.3 厄密算符本征函数的性质

$$\int \psi^* \hat{F} \varphi d\tau = \int (\hat{F}\psi)^* \varphi d\tau$$

如果两个函数ψ_1和ψ_2满足 $\int \psi_1^* \psi_2 dV = 0$ ψ_1和ψ_2正交

属于不同本征值的厄密算符本征函数正交

$$\begin{cases} \hat{L}\psi_m = l_m \psi_m \\ \hat{L}\psi_n = l_n \psi_n \end{cases} \rightarrow \begin{cases} \psi_m^* \hat{L}\psi_n = \psi_m^* l_n \psi_n = l_n \psi_m^* \psi_n \\ (\hat{L}\psi_m)^* \psi_n = l_m^* \psi_m^* \psi_n = l_m \psi_m^* \psi_n \end{cases}$$

两式相减 $\rightarrow \psi_m^* \hat{L}\psi_n - (\hat{L}^* \psi_m^*)\psi_n = \psi_n \psi_m^* (l_n - l_m)$

对整个体积空间进行积分 $\int_{-\infty}^{+\infty} \psi_m^* \hat{L}\psi_n dV - \int_{-\infty}^{+\infty} (\hat{L}\psi_m)^* \psi_n dV = (l_n - l_m) \int_{-\infty}^{+\infty} \psi_n \psi_m^* dV$

$$\int_{-\infty}^{+\infty} \psi_{\mathrm{m}}^{*} \hat{L}\psi_{n} dV - \int_{-\infty}^{+\infty} (\hat{L}\psi_{m})^{*} \psi_{n} dV = (l_{n} - l_{m}) \int_{-\infty}^{+\infty} \psi_{n} \psi_{m}^{*} dV$$

由于 $\hat{L}$ 是厄密算符，左边积分在整个空间的积分相等

$$0 = (l_{n} - l_{m}) \int_{-\infty}^{+\infty} \psi_{n} \psi_{m}^{*} dV$$

因为 $l_n \neq l_m$ $\rightarrow \int_{-\infty}^{+\infty} \psi_{n} \psi_{m}^{*} dV = 0 \rightarrow \int_{-\infty}^{+\infty} \psi_{n} \psi_{m}^{*} dV = \delta_{mn}$

从而证明了两波函数是正交的

如果厄密算符的本征值是连续分布的，则 $\int_{-\infty}^{+\infty} \psi_{\lambda} \psi_{\lambda'}^{*} dV = \delta(\lambda - \lambda')$

例题　对下面两个氢原子的未归一化的1s和2s电子的波函数

$$\psi_{1s}(r,\theta,\varphi)=\psi_{1s}(r)=e^{-r/a},$$

$$\psi_{2s}(r,\theta,\varphi)=\psi_{2s}(r)=(1-\frac{r}{2a})e^{-r/2a},a=\frac{\hbar^2}{me^2}$$

证明它们的正交性

解 根据正交性的定义，有 $\int\psi_{1s}^*\psi_{2s}d^3r=4\pi\int_0^\infty r^2(1-\frac{r}{2a})e^{-r/a}e^{-r/2a}dr$

$$=4\pi\int_0^\infty(r^2-\frac{r^3}{2a})e^{-3r/2a}dr$$

$$=4\pi[(\frac{2a}{3})^3 2!-\frac{1}{2a}(\frac{2a}{3})^4 3!]=0$$

说明两波函数是正交.

3.4 叠加态原理

叠加态定义：一般情况下，如果Ψ_1和Ψ_2 是体系的可能状态，那末它们的线性叠加$\Psi = C_1\Psi_1 + C_2\Psi_2$ 也是该体系的一个可能状态.其中C1和 C2 是复常数，这就是量子力学的态叠加原理。

态叠加原理一般表述 :若Ψ_1，$\Psi_2,\ldots,\Psi_n,\ldots$是体系的一系列可能的状态，则这些态的线性叠加$\Psi = C_1\Psi_1 + C_2\Psi_2 + \ldots + C_n\Psi_n + \ldots$（其中 $C_1, C_2,\ldots,C_n,\ldots$为复常数），也是体系的一个可能状态，处于Ψ态的体系，部分的处于 Ψ_1态，部分的处于Ψ_2态. . . ，部分的处于Ψ_n，…

1. 叠加态是粒子存在的状态

$$\hat{F}\psi_n(r)=\lambda_n\psi_n(r)\rightarrow\begin{cases}\hat{F}\psi_1(r)=\lambda_1\psi_1(r)\\ \hat{F}\psi_2(r)=\lambda_2\psi_2(r)\\ \hat{F}\psi_3(r)=\lambda_3\psi_3(r)\\ \cdots\cdots\cdots\cdots\cdots\cdots\\ \hat{F}\psi_n(r)=\lambda_n\psi_n(r)\end{cases}\rightarrow\begin{cases}\Phi_1=c_{11}\psi_1(r)+c_{12}\psi_2(r)+c_{13}\psi_3(r)+\ldots+c_{1n}\psi_n(r)\\ \Phi_2=c_{21}\psi_1(r)+c_{22}\psi_2(r)+c_{23}\psi_3(r)+\ldots+c_{2n}\psi_n(r)\\ \Phi_3=c_{31}\psi_1(r)+c_{32}\psi_2(r)+c_{33}\psi_3(r)+\ldots+c_{3n}\psi_n(r)\\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\ \Phi_n=c_{n1}\psi_1(r)+c_{n2}\psi_2(r)+c_{n3}\psi_3(r)+\ldots+c_{nn}\psi_n(r)\end{cases}$$

$$\rightarrow\begin{cases}\hat{F}\Phi_1(r)=c_{11}\lambda_1\psi_1(r)+c_{12}\lambda_2\psi_2(r)+\ldots+c_{1n}\lambda_n\psi_n(r)\\ \hat{F}\Phi_2(r)=c_{21}\lambda_1\psi_1(r)+c_{22}\lambda_2\psi_2(r)+\ldots+c_{2n}\lambda_n\psi_n(r)\\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\ \hat{F}\Phi_n(r)=c_{n1}\lambda_1\psi_1(r)+c_{n2}\lambda_2\psi_2(r)+\ldots+c_{n1}\lambda_{nn}\psi_n(r)\end{cases}\rightarrow\begin{cases}\hat{F}\Phi_1(r)=\lambda_{11}\psi_1(r)+\lambda_{12}\psi_2(r)+\ldots+\lambda_{1n}\psi_n(r)\\ \hat{F}\Phi_2(r)=\lambda_{21}\psi_1(r)+\lambda_{22}\psi_2(r)+\ldots+\lambda_{2n}\psi_n(r)\\ \cdots\cdots\cdots\cdots\cdots\cdots\cdots\cdots\\ \hat{F}\Phi_n(r)=\lambda_{n1}\psi_1(r)+\lambda_{n2}\psi_2(r)+\ldots+\lambda_{nn}\psi_n(r)\end{cases}$$

$$\rightarrow \begin{cases} \hat{F}\Phi_1(r) = \lambda_{11}\psi_1(r) + \lambda_{12}\psi_2(r) + \ldots + \lambda_{1n}\psi_n(r) \\ \hat{F}\Phi_2(r) = \lambda_{21}\psi_1(r) + \lambda_{22}\psi_2(r) + \ldots + \lambda_{2n}\psi_n(r) \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ \hat{F}\Phi_n(r) = \lambda_{n1}\psi_1(r) + \lambda_{n2}\psi_2(r) + \ldots + \lambda_{nn}\psi_n(r) \end{cases} \quad \rightarrow \hat{F}\begin{bmatrix} \Phi_1(r) \\ \Phi_2(r) \\ \ldots\ldots \\ \Phi_n(r) \end{bmatrix} = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \ldots & \lambda_{1n} \\ \lambda_{21} & \lambda_{22} & \ldots & \lambda_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ \lambda_{n1} & \lambda_{n2} & \ldots & \lambda_{nn} \end{bmatrix} \begin{bmatrix} \psi_1(r) \\ \psi_2(r) \\ \ldots \\ \psi_n(r) \end{bmatrix}$$

$$\rightarrow \begin{cases} \psi_1(r) = C'_{11}\Phi_1(r) + C'_{12}\Phi_2(r) + \ldots + C'_{1n}\Phi_n(r) \\ \psi_2(r) = C'_{21}\Phi_1(r) + C'_{22}\Phi_2(r) + \ldots + C'_{2n}\Phi_n(r) \\ \ldots\ldots\ldots\ldots\ldots\ldots\ldots \\ \psi_n(r) = C'_{n1}\Phi_1(r) + C'_{n2}\Phi_2(r) + \ldots + C'_{nn}\Phi_n(r) \end{cases} \quad \rightarrow \begin{bmatrix} \psi_1(r) \\ \psi_2(r) \\ \ldots \\ \psi_n(r) \end{bmatrix} = \begin{bmatrix} C'_{11} & C'_{12} & \ldots & C'_{1n} \\ C'_{21} & C'_{22} & \ldots & C'_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ C'_{n1} & C'_{n2} & \ldots & C'_{nn} \end{bmatrix} \begin{bmatrix} \Phi_1(r) \\ \Phi_2(r) \\ \ldots \\ \Phi_n(r) \end{bmatrix}$$

$$\rightarrow \hat{F}\begin{bmatrix} \Phi_1(r) \\ \Phi_2(r) \\ \ldots\ldots \\ \Phi_n(r) \end{bmatrix} = \begin{bmatrix} \lambda_{11} & \lambda_{12} & \ldots & \lambda_{1n} \\ \lambda_{21} & \lambda_{22} & \ldots & \lambda_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ \lambda_{n1} & \lambda_{n2} & \ldots & \lambda_{nn} \end{bmatrix} \begin{bmatrix} C'_{11} & C'_{12} & \ldots & C'_{1n} \\ C'_{21} & C'_{22} & \ldots & C'_{2n} \\ \ldots & \ldots & \ldots & \ldots \\ C'_{n1} & C'_{n2} & \ldots & C'_{nn} \end{bmatrix} \begin{bmatrix} \Phi_1(r) \\ \Phi_2(r) \\ \ldots \\ \Phi_n(r) \end{bmatrix}$$

$$\rightarrow \hat{F}\begin{bmatrix}\Phi_1(r)\\ \Phi_2(r)\\ \cdots\cdots\\ \Phi_n(r)\end{bmatrix}=\begin{bmatrix}\lambda_{11} & \lambda_{12} & \cdots & \lambda_{1n}\\ \lambda_{21} & \lambda_{22} & \cdots & \lambda_{2n}\\ \cdots & \cdots & \cdots & \cdots\\ \lambda_{n1} & \lambda_{n2} & \cdots & \lambda_{nn}\end{bmatrix}\begin{bmatrix}C'_{11} & C'_{12} & \cdots & C'_{1n}\\ C'_{21} & C'_{22} & \cdots & C'_{2n}\\ \cdots & \cdots & \cdots & \cdots\\ C'_{n1} & C'_{n2} & \cdots & C'_{nn}\end{bmatrix}\begin{bmatrix}\Phi_1(r)\\ \Phi_2(r)\\ \cdots\\ \Phi_n(r)\end{bmatrix}$$

$$\rightarrow \hat{F}\begin{bmatrix}\Phi_1(r)\\ \Phi_2(r)\\ \cdots\cdots\\ \Phi_n(r)\end{bmatrix}=\begin{bmatrix}A_{11} & A_{12} & \cdots & A_{1n}\\ A_{21} & A_{22} & \cdots & A_{2n}\\ \cdots & \cdots & \cdots & \cdots\\ A_{n1} & A_{n2} & \cdots & A_{nn}\end{bmatrix}\begin{bmatrix}\Phi_1(r)\\ \Phi_2(r)\\ \cdots\\ \Phi_n(r)\end{bmatrix}$$

类似于 $\rightarrow \hat{F}\Phi(r)=A\Phi(r)$，则叠加态也是粒子存在的状态

3.5 叠加态与力学量的展开

$$\hat{F}\psi_n(r)=\lambda_n\psi_n(r) \quad \rightarrow \begin{cases} \hat{F}\psi_1(r)=\lambda_1\psi_1(r) \\ \hat{F}\psi_2(r)=\lambda_2\psi_2(r) \\ \hat{F}\psi_3(r)=\lambda_3\psi_3(r) \\ \cdots\cdots\cdots\cdots\cdots\cdots \\ \hat{F}\psi_n(r)=\lambda_n\psi_n(r) \end{cases}$$

如果算符F是厄密算符，它的正交归一化本征函数为$\psi_n(r)$，对应的本征值为λ_n，则任意函数$\psi(r)$可以按$\psi_n(x)$展开，则得到叠加态

$$\psi_1(r)=c_1\psi_1(r)+c_2\psi_2(r)+c_3\psi_3(r)+\ldots+c_n\psi_n(r)$$

$$\psi(r)=c_1\psi_1(r)+c_2\psi_2(r)+c_3\psi_3(r)+\ldots+c_n\psi_n(r)$$

$$\psi(r)=\sum_n c_n\psi_n(r)\rightarrow\psi_n(x)\text{组成完全系:}$$

在量子力学中，"表示力学量的算符为厄密算符，它们的本征函数组成完全系。

$$\int\psi(r)\bullet\psi*(r)dr$$

$$=\int[c_1\psi_1(r)+c_2\psi_2(r)+\ldots+c_n\psi_n(r)]\bullet[c_1\psi*_1(r)+c_2\psi_2*(r)+\ldots+c_n\psi*_n(r)]dr$$

由$\psi_n(x)$的正交归一化性，系数c_n为

$$\int\psi(r)\bullet\psi*(r)dr$$

$$=\int\left[c_1^2\psi_1(r)\bullet\psi*_1(r)dr+c_2^2\psi_2(r)\bullet\psi_2*(r)dr+\ldots+c_n^2\psi_n(r)\bullet\psi*_n(r)dr\right]$$

$$\int \psi(r) \bullet \psi^*(r) dr = \int \left[c_1^2 \psi_1(r) \bullet \psi^*_1(r) dr + c_2^2 \psi_2(r) \bullet \psi_2^*(r) dr + \ldots + c_n^2 \psi_n(r) \bullet \psi^*_n(r) dr \right]$$

$$\rightarrow 1 = \int \psi^*(r) \psi(r) dr = \sum_{m,n} c_m^* c_n \int \psi_m^*(r) \psi_n(r) dr = \sum_{m,n} c_m^* c_n \delta_{mn} = \sum_n |c_n|^2$$

$$1 = c_1^2 + c_2^2 + \ldots\ldots + c_n^2$$

C的物理意义：表示在$\psi(x)$态中测量力学量F得到的结果是算符F的本征态λ_n的几率，也被称为几率振幅。

叠加系数的计算

$$\psi(r) = c_1\psi_1(r) + c_2\psi_2(r) + c_3\psi_3(r) + \ldots + c_n\psi_n(r)$$

$$\rightarrow \psi_1{*}(r)\bullet\psi(r) = \psi_1{*}(r)\bullet\left[c_1\psi_1(r) + c_2\psi_2(r) + c_3\psi_3(r) + \ldots + c_n\psi_n(r)\right]$$

对全空间积分 $\rightarrow \int\left[\psi_1{*}(r)\bullet\psi(r)\right]dr$

$$= \int\left[c_1\psi_1{*}(r)\bullet\psi_1(r) + c_2\psi_1{*}(r)\bullet\psi_2(r) + \ldots + c_n\psi_1{*}(r)\bullet\psi_n(r)\right]dr$$

考虑正交性 $\rightarrow \int\left[\psi_1{*}(r)\bullet\psi(r)\right]dr = \int\left[c_1\psi_1{*}(r)\bullet\psi_1(r) + 0 + 0 + \ldots 0\right]dr$

$$\rightarrow \int\left[\psi_1{*}(r)\bullet\psi(r)\right]dr = c_1 \quad \rightarrow \int\left[\psi_2{*}(r)\bullet\psi(r)\right]dr = c_2$$

$$\rightarrow c_n = \int\left[\psi_n{*}(r)\bullet\psi(r)\right]dr$$

例：设体系处于 $\psi = c_1 Y_{11} + c_2 Y_{20}$

求 $\hat{L}_z$ 和 $\hat{L}^2$ 的可能测值及相应的几率。

解：根据 Y_{lm} 的正交归一化性，得到

$$\int \psi^* \psi dV = \int (c_1^* Y_{11}^* + c_2^* Y_{20}^*)(c_1 Y_{11} + c_2 Y_{20}) dV$$
$$= |c_1|^2 + |c_2|^2$$

由于 $\begin{cases} \hat{L}_z Y_{lm} = m\hbar Y_{lm} \\ \hat{L}^2 Y_{lm} = l(l+1)\hbar^2 Y_{lm} \end{cases}$

$\hat{L}_z$ 和 $\hat{L}^2$ 的可能测值为及相应的几率为：

	可能测值	相应的几率
$\hat{L}_z$	$0,\ \hbar$	$\dfrac{\lvert c_1\rvert^2}{\lvert c_1\rvert^2 + \lvert c_2\rvert^2},\quad \dfrac{\lvert c_2\rvert^2}{\lvert c_1\rvert^2 + \lvert c_2\rvert^2}$
$\hat{L}^2$	$2\hbar^2,\ 6\hbar^2$	$\dfrac{\lvert c_1\rvert^2}{\lvert c_1\rvert^2 + \lvert c_2\rvert^2},\quad \dfrac{\lvert c_2\rvert^2}{\lvert c_1\rvert^2 + \lvert c_2\rvert^2}$

例题2：　氢原子处于基态时的波函数为 $\psi_{100}(r)=\frac{1}{\sqrt{\pi a_0^3}}e^{-\frac{r}{a_0}}$

求电子动量的几率分布

解：首先将ψ_{100}按动量算符的本征值ψ_p展开，由于动量算符组成连续谱，则

$$\psi_{100}(r)=\int c_p\psi_p(\mathbf{r})d^3p$$

几率振幅为　$c_p=\int\psi_p^*\psi_{100}(\mathbf{r})d^3r$

动量本征值为p的本征函数　$\psi_p(r)=\frac{1}{(2\pi\hbar)^{3/2}}e^{\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}$

$$c_p=\frac{1}{\sqrt{\pi a_0^3}}\frac{1}{(2\pi\hbar)^{3/2}}\int e^{-\frac{r}{a_0}}e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}}d^3r$$

球坐标比较好！

$$c_p = \frac{1}{\sqrt{\pi a_0^3}} \frac{1}{(2\pi\hbar)^{3/2}} \int e^{-\frac{r}{a_0}} e^{-\frac{i}{\hbar}\mathbf{p}\cdot\mathbf{r}} d^3 r$$

$$c_p = \frac{1}{\pi^2} \frac{1}{(2a_0\hbar)^{3/2}} \int_0^\infty \int_0^\pi \int_0^{2\pi} e^{-\frac{r}{a_0}} e^{-\frac{i}{\hbar}pr\cos\theta} r^2 \sin\theta dr d\theta d\varphi$$

先对ψ积分，再对θ积分，最后再对r积分。

$$c_\mathbf{p} = \frac{2}{\pi(2a_0\hbar)^{3/2}} \int_0^\infty \int_0^\pi e^{-\frac{r}{a_0}} e^{-\frac{i}{\hbar}pr\cos\theta} r^2 \sin\theta dr d\theta = \frac{2i\hbar}{\pi p(2a_0\hbar)^{3/2}} \int_0^\infty e^{-\frac{r}{a_0}} (e^{-\frac{i}{\hbar}pr} - e^{\frac{i}{\hbar}pr}) r dr$$

$$= \frac{(2a_0\hbar)^{3/2}\hbar}{\pi(a_0^2 p^2 + \hbar^2)^2}$$

动量的几率密度为 $$\left|\mathrm{c}_{\mathrm{p}}\right|^2 = \frac{8a_0^{\ 3}\hbar^5}{\pi^2(a_0^{\ 2}p^2+\hbar^2)^4}$$

当氢原子处于基态时，电子动量的绝对值在***p→p+dp***范围内的几率为：

$$w(p)dp = \left|c_p\right|^2 4\pi p^2 dp$$

可以证明各种可能的几率之和为1， 即

$$\int w(p)dp^3 = 1$$

3.6 力学量测量结果的几率的平均值

对算符和算符的本征函数

$$\hat{F}\psi_n(r)=\lambda_n\psi_n(r)\rightarrow\begin{cases}\lambda_1(\text{本征值}) & \rightarrow\quad \psi_1(r)(\text{本征波函数})\\ \lambda_2(\text{本征值}) & \rightarrow\quad \psi_2(r)(\text{本征波函数})\\ \cdots\cdots\cdots\cdots & \\ \lambda_n(\text{本征值}) & \rightarrow\quad \psi_{n(r)}(\text{本征波函数})\end{cases}$$

则存在一个态(叠加态),也是状态波函数

$$\psi(r)=c_1\psi_1(r)+c_2\psi_2(r)+c_3\psi_3(r)+\ldots+c_n\psi_n(r)$$

$$\psi(r) = c_1\psi_1(r) + c_2\psi_2(r) + c_3\psi_3(r) + \ldots + c_n\psi_n(r)$$

叠加态不是本征态

$$\hat{F}\psi(r) = c_1\hat{F}\psi_1(r) + c_2\hat{F}\psi_2(r) + c_3\hat{F}\psi_3(r) + \ldots + c_n\hat{F}\psi_n(r)$$

根据本征态方程 $\hat{F}\psi_n(r) = \lambda_n\psi_n(r)$

$$\hat{F}\psi(r) = c_1\lambda_1\psi_1(r) + c_2\lambda_2\psi_2(r) + c_3\lambda_3\psi_3(r) + \ldots + c_n\lambda_n\psi_n(r)$$

$$\psi^*(r)\hat{F}\psi(r)$$

$$= \left[c_1\psi_1^*(r) + c_2\psi_2^*(r) \ldots + c_n\psi^*_n(r)\right] \bullet \left[c_1\lambda_1\psi_1(r) + c_2\lambda_2\psi_2(r) \ldots + c_n\lambda_n\psi_n(r)\right]$$

$$= c_1^2\lambda_1 + c_2^2\lambda_2 + c_3^2\lambda_3 + \ldots + c_n^2\lambda_n$$

每一个本征值对应于一个状态，故这个式子表示的是所有状态出现的均值，即期望值

$$\psi^*(r)\hat{F}\psi(r)$$
$$=\left[c_1\psi_1^*(r)+c_2\psi_2^*(r)\ldots+c_n\psi^*_n(r)\right]\bullet\left[c_1\lambda_1\psi_1(r)+c_2\lambda_2\psi_2(r)\ldots+c_n\lambda_n\psi_n(r)\right]$$
$$=c_1^2\lambda_1+c_2^2\lambda_2+c_3^2\lambda_3+\ldots.+c_n^2\lambda_n$$
$$\rightarrow\psi^*(r)\hat{F}\psi(r)=c_1^2\lambda_1+c_2^2\lambda_2+c_3^2\lambda_3\ldots.+c_n^2\lambda_n=\overline{\lambda}$$

物理量的平均值$\rightarrow\overline{F}=\int\psi^*(r)\hat{F}\psi(r)dr$

例题：已知波函数，计算平均动量与平均动能

$$\psi(x) = A\left[\sin^2 kx + \frac{1}{2}\cos kx\right]$$

解：

$$-i\hbar\frac{\partial\psi(x)}{\partial x} = p\psi(x)$$

$$\overline{p} = \frac{\int_0^\infty \psi^*(x) p_x \psi(x)\,dx}{\int_0^\infty \psi^*(x)\psi(x)\,dx}$$

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

注意归一化！

$$\overline{p} = \frac{\int_0^\infty \psi^*(x)\left[-i\hbar\frac{\partial}{\partial x}\psi(x)\right]dx}{\int_0^\infty \psi^*(x)\psi(x)\,dx}$$

$$\hat{p}_x = -i\hbar Ak\left(2\sin kx\cos kx - \frac{1}{2}\sin kx\right)$$

$$\overline{p} = \frac{\int_0^\infty A\left[\sin^2 kx + \frac{1}{2}\cos kx\right]\left(-i\hbar Ak\left(2\sin kx\cos kx - \frac{1}{2}\sin kx\right)\right)dx}{\int_0^\infty A^2\left[\sin^2 kx + \frac{1}{2}\cos kx\right]^2 dx}$$

例题：已知波函数，计算平均动量与平均动能

$$\psi(x) = A\left[\sin^2 kx + \frac{1}{2}\cos kx\right]$$

解：

$$\hat{E}_k = \frac{-\hbar^2\nabla^2}{2m}$$

$$\overline{E} = \frac{\int_0^\infty \psi^*(x) E_x \psi(x)\,dx}{\int_0^\infty \psi^*(x)\psi(x)\,dx} = \frac{\int_0^\infty \psi^*(x) \hat{E}_x \psi(x)\,dx}{\int_0^\infty \psi^*(x)\psi(x)\,dx} = \frac{\int_0^\infty \psi^*(x)\left[\frac{-\hbar^2\nabla^2\psi(x)}{2m}\right]dx}{\int_0^\infty \psi^*(x)\psi(x)\,dx}$$

$$\nabla^2\psi(x) = Ak\left[2k\cos 2kx - \frac{k}{2}\cos kx\right]$$

$$\overline{E} = \frac{\int_0^\infty \psi^*(x)\left[\frac{-\hbar^2}{2m}Ak\left[2k\cos 2kx - \frac{k}{2}\cos kx\right]\right]dx}{\int_0^\infty \psi^*(x)\psi(x)\,dx}$$

3.6 动量表征中的波函数

$$\psi(r,t)=c_1(p_1)\psi_{p_1}(r,t)+c_2(p_2)\psi_{p_2}(r,t)+\ldots+c_n(p_n)\psi_{p_n}(r,t)$$
$$=\sum_p c(p)\psi_p(r,t)$$

利用指数函数特性

利用波函数的特征 $\rightarrow \psi_{p_1}(r,t)=\psi_{p_1}(r)\psi_{p_1}(t)$

$$\rightarrow\psi(r,t)=c_1(p_1)\psi_{p_1}(t)\psi_{p_1}(r)+c_2(p_2)\psi_{p_2}(t)\psi_{p_2}(r)+\ldots+c_n(p_n)\psi_{p_n}(t)\psi_{p_n}(r)$$

再利用 $\rightarrow C_{p_1}(p_1,t)=\mathrm{C}_1(p_1)\psi_{p_1}(t)$

$$\rightarrow\psi(r,t)=c_1(p_1,t)\psi_{p_1}(r)+c_2(p_2,t)\psi_{p_2}(r)+\ldots+c_n(p_n,t)\psi_{p_n}(r_n)=\sum_p c(p,t)\psi_p(r)$$

$$\to \psi(r,t) = c_1(p_1,t)\psi_{p_1}(r) + c_2(p_2,t)\psi_{p_2}(r) + \ldots + c_n(p_n,t)\psi_{p_n}(r_n) = \sum_p c(p,t)\psi_p(r)$$

$$\sum_r \psi^*_{p_1}(r) \bullet \psi(r,t) = \sum \psi^*_{p_1}(r) \bullet \left[c_1(p_1,t)\psi_{p_1}(r) + c_2(p_2,t)\psi_{p_2}(r) + \ldots + c_n(p_n,t)\psi_{p_n}(r)\right]$$

$$\sum_r \psi(r,t) \bullet \psi_{p_1} * (r) = \sum \psi_{p_1} * (r) \bullet c_1(p_1,t)\psi_{p_1}(r) = c_1(p_1,t)$$

$$c_1(p_1,t) = \int \psi^*_{p_1} \psi(r,t) dr$$

与前面提到的处理几率振幅方法类似

$$\psi(r,t)=c_1\left(p_1,t\right)\psi_{p_1}\left(r\right)+c_2\left(p_2,t\right)\psi_{p_2}\left(r\right)+\ldots+c_n\left(p_n,t\right)\psi_{p_n}\left(r\right)=\sum_p c\left(p,t\right)\psi_p\left(r\right)$$

$$\sum_r \psi^*(r,t)\bullet\psi(r,t)=\sum_r\left[c_1\left(p_1,t\right)\psi_{p_1}\left(r\right)+c_2\left(p_2,t\right)\psi_{p_2}\left(r\right)+\ldots+c_n\left(p_n,t\right)\psi_{p_n}\left(r\right)\right]$$

$$\bullet\left[c_1^*\left(p_1,t\right)\psi_{p_1}^*\left(r\right)+c_2^*\left(p_2,t\right)\psi_{p_2}^*\left(r\right)+\ldots+c_n^*\left(p_n,t\right)\psi_{p_n}^*\left(r\right)\right]$$

$$\sum_r \psi^*(r,t)\bullet\psi(r,t)=c_1\left(p_1,t\right)\bullet c_1^*\left(p_1,t\right)+c_2\left(p_2,t\right)c_2^*\left(p_2,t\right)+\ldots+c_n\left(p_n,t\right)\bullet c_n^*\left(p_n,t\right)=1$$

$$\int c_1\left(p_1,t\right)\bullet c_1^*\left(p_1,t\right)dp=1$$

$$\psi(r,t)=\int C(p,t)\psi_p(r)dp$$ 用动量状态来描述位置状态

$|\Psi(r,t)|^2 dr$ 是在$\Psi(r,t)$所描写的状态中，测量粒子的位置所得结果在 $r \to r+dr$ 范围内的几率。

$$c_1(p_1,t)=\int \psi_{p_1}^*\psi(r,t)dr$$ 用位置状态来描述动量信息

$|C(p,t)|^2 dp$是在$\Psi(x,t)$所描写的状态中，测量粒子的动量所得结果在 $p \to p+dp$ 范围内的几率。

$\Psi(x,t)$ 与 $C(p,t)$ 一一对应，描述同一状态。

$\Psi(x,t)$ 是该状态在坐标表象中的波函数；

而 $C(p,t)$ 就是该状态在动量表象中的波函数。

例题2： 一粒子的波函数为 $\psi(x)=\frac{1}{(2\pi)^{\frac{1}{4}}a}e^{-\frac{x^2}{4a^2}}$

求电子动量的几率分布

解：首先将ψ_{100}按动量算符的本征值ψ_p展开，由于动量算符组成连续谱，则

$$\begin{cases}-i\hbar\frac{\partial}{\partial x}\psi_p(x)=p_x\psi_p(x)\\-i\hbar\frac{\partial}{\partial y}\psi_p(y)=p_y\psi_p(y)\\-i\hbar\frac{\partial}{\partial z}\psi_p(z)=p_z\psi_p(z)\end{cases}\rightarrow\begin{cases}\psi_p(x)=C_1e^{\frac{i}{\hbar}p_x x}\\\psi_p(y)=C_1e^{\frac{i}{\hbar}p_y y}\\\psi_p(z)=C_1e^{\frac{i}{\hbar}p_z z}\end{cases}$$

$$\rightarrow\psi_p(r)=\psi_p(x)\psi_p(y)\psi_p(z)=Ce^{\frac{i}{\hbar}\overline{p}_r\bullet\vec{x}}$$

C的计算

$$\psi_p(r)=\psi_p(x)\psi_p(y)\psi_p(z)=Ce^{\frac{i}{\hbar}\overline{p}_r\bullet\vec{x}}$$

$$\int_{-\infty}^{\infty}\psi*_{p'}(r)\psi_p(r)d\tau=C^2\iiint_{\infty}e^{\frac{i}{\hbar}\left[(p_x-p_x')\bullet x+\left(p_y-p_y'\right)\bullet y+\left(p_z-p_z'\right)\bullet z\right]}dxdydz$$

$$\int_{-\infty}^{\infty}e^{\frac{i}{\hbar}\left[(p_x-p_x')\bullet x\right]}dx=2\pi\hbar\delta\left(p_x-p_y'\right)\qquad\rightarrow\int_{-\infty}^{\infty}\psi*_{p'}(r)\psi_p(r)d\tau=C^2\left(2\pi\hbar\right)^3\delta\left(p-p'\right)$$

$$\rightarrow\delta\left(p-p'\right)=C^2\left(2\pi\hbar\right)^3\delta\left(p-p'\right)\qquad\rightarrow C=\frac{1}{\left(2\pi\hbar\right)^{\frac{3}{2}}}$$

这个式子左边式子是利用动量的连续性得到的

$$\psi_p(r)=\frac{1}{\left(2\pi\hbar\right)^{\frac{3}{2}}}e^{\frac{i}{\hbar}\overline{p}_r\bullet\vec{r}}\qquad\psi_p(x)=\frac{1}{\left(2\pi\hbar\right)^{\frac{1}{2}}}e^{\frac{i}{\hbar}\overline{p}_x\bullet\vec{x}}$$

$$\begin{cases} \psi_p(x) = \dfrac{1}{(2\pi\hbar)^{\frac{1}{2}}} e^{\frac{i}{\hbar} p_x \bullet x} \\ \psi(x) = \dfrac{1}{(2\pi)^{\frac{1}{4}} a} e^{-\frac{x^2}{4a^2}} \end{cases}$$

$$\rightarrow c(p,t) = \int_{-\infty}^{\infty} \psi *_p (x) \psi(x) dp = \int_{-\infty}^{+\infty} \frac{1}{(2\pi\hbar)^{\frac{1}{2}}} e^{-\frac{i}{\hbar} p_x \bullet x} \frac{1}{(2\pi)^{\frac{1}{4}} a} e^{-\frac{x^2}{4a^2}} dx$$

$$\rightarrow \frac{\partial}{\partial p} c^2(p,t) =$$

3.7 希尔伯特空间

$$\psi(r,t)=c_1(p_1,t)\psi_{p_1}(r)+c_2(p_2,t)\psi_{p_2}(r)+\ldots+c_n(p_n,t)\psi_{p_n}(r)$$

考虑到：厄米算符波函数的正交性

C（p，t）为态矢

$$\begin{cases}\psi^*_{p_1}(r)\bullet\psi_{p_2}(r)=0\\ \psi^*_{p_1}(r)\bullet\psi_{p_3}(r)=0\\ \cdots\cdots\cdots\\ \psi^*_{p_2}(r)\bullet\psi_{p_3}(r)=0\\ \psi^*_{p3}(r)\bullet\psi_{p_2}(r)=0\end{cases}\Rightarrow\begin{cases}\vec{i}\bullet\vec{j}=0\\ \vec{i}\bullet\vec{k}=0\\ \vec{j}\bullet\vec{k}=0\end{cases}$$

$$\begin{cases}\psi_{p_1}(r)\\ \psi_{p_2}(r)\\ \cdots\cdots\\ \psi_{p_n}(r)\end{cases}\Rightarrow \text{基矢}$$

$\left[\psi_{p_1}(r),\psi_{p_2}(r),\ldots\ldots\psi_{p_n}(r)\right]$由此构成的空间为希尔伯特空间

3.8态的表象

1.基本概念

x, p都是力学量，分别对应有坐标表象和动量表象，

因此可以对任何力学量Q都建立一种表象，称为力学量 Q 表象。

$$\begin{cases}\psi(r,t)=\sum_n a_n(t)\psi_n(r) \\ a(t)=\sum_n \psi_n^*(r)\psi(r,t)\end{cases} \qquad \psi \leftrightarrow \begin{pmatrix} a_1(t) \\ a_2(t) \\ \cdots\cdots \\ a_n(t) \end{pmatrix}$$

所以我们可以把状态ψ看成是一个矢量——态矢量。 选取一个特定力学量 Q 表象，相当于选取特定的坐标系，

$\psi_1(r)$， $\psi_2(r)$， ...，$\psi_n(r)$， 是Q表象 的基本矢量简称基矢。

2. 波函数

$$\psi = \begin{pmatrix} a_1(t) \\ a_2(t) \\ \cdots \\ a_n(t) \end{pmatrix}$$

是态矢量Ψ在Q表象中沿各基矢方向上的“分量”。Q表象的基矢有无限多个，所以态矢量所在的空间是一个无限维的抽象的函数空间，称为Hilbert空间。

$$\psi = \begin{pmatrix} a_1(t) \\ a_2(t) \\ \cdots \\ a_n(t) \end{pmatrix} \quad \text{共轭矩阵} \rightarrow \psi^{+} = \begin{pmatrix} a_1(t)^* & a_2(t)^* & \ldots & a_n(t)^* \end{pmatrix}$$

归一化可写为 $\psi^{+}\psi = \begin{pmatrix} a_1(t)^* & a_2(t)^* & \ldots & a_n(t)^* \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \\ \cdots \\ a_n(t) \end{pmatrix} = \sum_n a_n(t)^* a_n(t) = 1$

2.力学量算符的矩阵表示

$$\Phi(x,t)=\hat{F}(x,\hat{p})\psi(x,t)=\hat{F}(x,-i\hbar\frac{\partial}{\partial x})\psi(x,t)$$

假设只有分立本征值，将Φ， Ψ按{$u_n(x)$}展开：

$$\begin{cases}\psi(x,t)=\sum_m a_m(t)u_m(x)\\ \Phi(x,t)=\sum_m b_m(t)u_m(x)\end{cases}\qquad \sum_m b_m(t)u_m(x)=\hat{F}(x,-i\hbar\frac{\partial}{\partial x})\sum_m a_m(t)u_m(x)$$

两边左乘 $u^*_n(x)$ 并对 x 积分

$$\sum_m b_m(t)\int u_n{}^*u_m(x)dx=\sum_m\int u_n{}^*\hat{F}(x,-i\hbar\frac{\partial}{\partial x})u_m(x)dx]a_m(t)$$

令： $F_{nm}\equiv\int u_n{}^*(x)\hat{F}(x,-i\hbar\frac{\partial}{\partial x})u_m(x)dx$

$$\sum_m b_m(t)\delta_{nm}=\sum_m F_{nm}a_m(t)$$ Q表象的达方式 $$b_n(t)=\sum_m F_{nm}a_m(t)$$

令：$F_{nm} \equiv \int u_n{}^*(x)\hat{F}(x,-i\hbar\frac{\partial}{\partial x})u_m(x)dx$

$$F_{nm} = \int u_n{}^*(x)\hat{F}(x,-i\hbar\frac{\partial}{\partial x})u_m(x)dx \rightarrow \begin{bmatrix} F_{11} & F_{12} & \dots & F_{1m} \\ F_{21} & F_{21} & & F_{2m} \\ & & & \\ F_{n1} & F_{22} & \dots & F_{nm} \end{bmatrix}$$

$$b_n(t) = \sum_m F_{nm} a_m(t) \rightarrow \begin{pmatrix} b_1(t) \\ b_2(t) \\ \dots \\ b_n(t) \end{pmatrix} = \begin{pmatrix} F_{11} & F_{12} & \cdots & F_{1m} \\ F_{21} & F_{22} & \cdots & F_{2m} \\ \cdots & \cdots & \cdots & \dots \\ F_{n1} & F_{n2} & \cdots & F_{nm} \end{pmatrix} \begin{pmatrix} a_1(t) \\ a_2(t) \\ \dots \\ a_m(t) \end{pmatrix}$$

F 在 Q 表象中是一个矩阵，F_{nm} 是其矩阵元

$$b_n(t)=\sum_m F_{nm}a_m(t)\rightarrow\begin{pmatrix}b_1(t)\\b_2(t)\\\cdots\\b_n(t)\end{pmatrix}=\begin{pmatrix}F_{11}&F_{12}&\cdots&F_{1m}\\F_{21}&F_{22}&\cdots&F_{2m}\\\cdots&\cdots&\cdots&\cdots\\F_{n1}&F_{n2}&\cdots&F_{nm}\end{pmatrix}\begin{pmatrix}a_1(t)\\a_2(t)\\\cdots\\a_m(t)\end{pmatrix}$$

$$\hat{F}\psi(x)=\lambda\psi(x)\rightarrow\begin{pmatrix}F_{11}&F_{12}&&F_{1m}\\F_{21}&F_{22}&&F_{2m}\\\cdots&\cdots&\cdots&\cdots\\F_{n1}&F_{n2}&&F_{nm}\end{pmatrix}\begin{pmatrix}a_1(t)\\a_2(t)\\\cdots\\a_m(t)\end{pmatrix}=\lambda\begin{pmatrix}a_1(t)\\a_2(t)\\\cdots\\a_m(t)\end{pmatrix}$$

$$\rightarrow\begin{pmatrix}F_{11}-\lambda&F_{12}&\cdots&F_{1n}\\F_{21}&F_{22}-\lambda&\cdots&F_{2n}\\\cdots&\cdots&\cdots&\cdots\\F_{n1}&F_{n2}&\cdots&F_{nn}-\lambda\end{pmatrix}\begin{pmatrix}a_1\\a_2\\\cdots\\a_n\end{pmatrix}=0$$

这里的λ是一个向量

$$\begin{pmatrix} F_{11}-\lambda & F_{12} & \cdots & F_{1n} \\ F_{21} & F_{22}-\lambda & \cdots & F_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ F_{n1} & F_{n2} & \cdots & F_{nn}-\lambda \end{pmatrix} \begin{pmatrix} a_1 \\ a_2 \\ \cdots \\ a_n \end{pmatrix} = 0$$

方程组有不完全为零解的条件是系数行列式等于零

$$\begin{vmatrix} F_{11}-\lambda & F_{12} & \cdots & F_{1n} \\ F_{21} & F_{22}-\lambda & \cdots & F_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ F_{n1} & F_{n2} & \cdots & F_{nn}-\lambda \end{vmatrix} = 0$$

求解此久期方程得到一组λ值：λ_1，λ_2，…，λ_n，….就是F的本征值。

$$\begin{pmatrix} F_{11}-\lambda & F_{12} & \cdots & F_{1n} \\ F_{21} & F_{22}-\lambda & \cdots & F_{2n} \\ \cdots & \cdots & \cdots & \cdots \\ F_{n1} & F_{n2} & \cdots & F_{nn}-\lambda \end{pmatrix} = 0$$

求解此久期方程得到一组λ值：λ_1, λ_2, ..., λ_n, ...就是F的本征值.将其分别代入原齐次线性方程组就能得到相应于各λ_i的本征矢

$$\begin{pmatrix} a_{1i} \\ a_{2i} \\ \cdots \\ a_{ni} \end{pmatrix} \qquad i = 1, 2, \cdots, n \cdots$$

薛定锷方程

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

$$\begin{cases}\psi(x,t)=\sum_m a_m(t)u_m(x)\\ \Phi(x,t)=\sum_m b_m(t)u_m(x)\end{cases}$$

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

两边左乘 $u*_n(x)$ 并对 x 积分

$$i\hbar\frac{\partial}{\partial t}\sum_m a_m(t)\int u_m^*(x)u_m(x)dx=\int u_m^*(x)\hat{H}(x,\frac{\hbar}{i}\frac{\partial}{\partial x})u_m(x)dx\sum_m a_m(t)$$

$$i\hbar\frac{\partial}{\partial t}\sum_m a_m(t)\int u_m^*(x)u_m(x)dx=\int u_m^*(x)\hat{H}(x,\frac{\hbar}{i}\tfrac{\partial}{\partial x})u_m(x)dx\sum_m a_m(t)$$

$$\rightarrow i\hbar\frac{\partial}{\partial t}\sum_m a_m(t)=\int u_m^*(x)\hat{H}(x,\frac{\hbar}{i}\tfrac{\partial}{\partial x})u_m(x)dx\sum_m a_m(t)$$

令 $H_{mn}=\int u_m^*(x)\hat{H}(x,\frac{\hbar}{i}\tfrac{\partial}{\partial x})u_n(x)dx$

$$i\hbar\frac{d}{dt}\begin{pmatrix}a_1(t)\\a_2(t)\\\dots\\a_m(t)\end{pmatrix}=\begin{pmatrix}H_{11}&H_{12}&&H_{1m}\\H_{21}&H_{22}&&H_{2m}\\\dots&\dots&\dots&\dots\\H_{n1}&H_{n2}&&H_{nm}\end{pmatrix}\begin{pmatrix}a_1(t)\\a_2(t)\\\dots\\a_m(t)\end{pmatrix}\qquad i\hbar\frac{d}{dt}\psi=H\psi$$

3.狄拉克算符极其表征

$$\begin{cases}\psi(x,t)=\sum_m a_m(t)u_m(x)\\ \Phi(x,t)=\sum_m b_m(t)u_m(x)\end{cases}$$ 对应的关系 $\rightarrow\begin{cases}\psi(x,t)=a_1(t)u_1(x)+a_2(t)u_2(x)+\ldots+a_m(t)u_m(x)\\ \Phi(x,t)=b_1(t)u_1(x)+b_2(t)u_2(x)+\ldots+b_m(t)u_m(x)\end{cases}$

$\boxed{\text{态矢的狄拉克算符}}$ $\boxed{\text{基矢的狄拉克算符}}$

$$\begin{cases}|\varphi(t)\rangle=[a_1(t)\quad a_2(t)\quad \ldots\ldots\quad a_m(t)]\\ |\phi(t)\rangle=[b_1(t)\quad b_2(t)\quad \ldots\ldots\quad b_m(t)]\end{cases}\quad\begin{cases}\langle u(x)=[u^*{}_1(x)\quad u^*{}_2(x)\quad \ldots\quad u^*{}_m(x)]\\ u(x)\rangle=[u_1(x)\quad u_2(x)\quad \ldots\quad u_m(x)]\end{cases}$$

$$\rightarrow\langle u(x)|u(x)\rangle\rangle=\int[u^*{}_1(x)\quad u^*{}_2(x)\quad\ldots\quad u^*{}_m(x)][u_1(x)\quad u_2(x)\quad\ldots\quad u_m(x)]dx=1$$

$$\rightarrow\begin{cases}\langle u^*(x)|\varphi(t)\rangle=u^*{}_1(x)a_1(t)+u^*{}_2(x)a_2(t)+u^*{}_m(x)a_m(t)\\ \langle u^*(x)|\phi(t)\rangle=u^*{}_1(x)b_1(t)+u^*{}_2(x)b_2(t)+u^*{}_m(x)b_m(t)\end{cases}$$

$$\langle u(x) = \left[u^*_1(x) \quad u^*_2(x) \quad \ldots \quad u^*_m(x) \right]$$

$$\rightarrow \begin{cases} |\varphi(t)\rangle = u_1(x)\left[u^*_1(x)a_1(t)\right] + u_2(x)\left[u^*_2(x)a_2(t)\right] + \ldots + u_m(x)\left[u^*_m(x)a_m(t)\right] \\ |\phi(t)\rangle = u_1(x)\left[u^*_1(x)b_1(t)\right] + u_2(x)\left[u^*_2(x)b_2(t)\right] + \ldots + u_m(x)\left[u^*_m(x)b_m(t)\right] \end{cases}$$

$$\rightarrow \begin{cases} \sum |u_i(x)\rangle\langle u^*_i(x)|\varphi(t)\rangle = u_1(x)\left[u^*_1(x)a_1(t)\right] + u_2(x)\left[u^*_2(x)a_2(t)\right] + \ldots + u_m(x)\left[u^*_m(x)a_m(t)\right] \\ \sum |u_i(x)\rangle\langle u^*_i(x)|\phi(t)\rangle = u_1(x)\left[u^*_1(x)b_1(t)\right] + u_2(x)\left[u^*_2(x)b_2(t)\right] + \ldots + u_m(x)\left[u^*_m(x)b_m(t)\right] \end{cases}$$

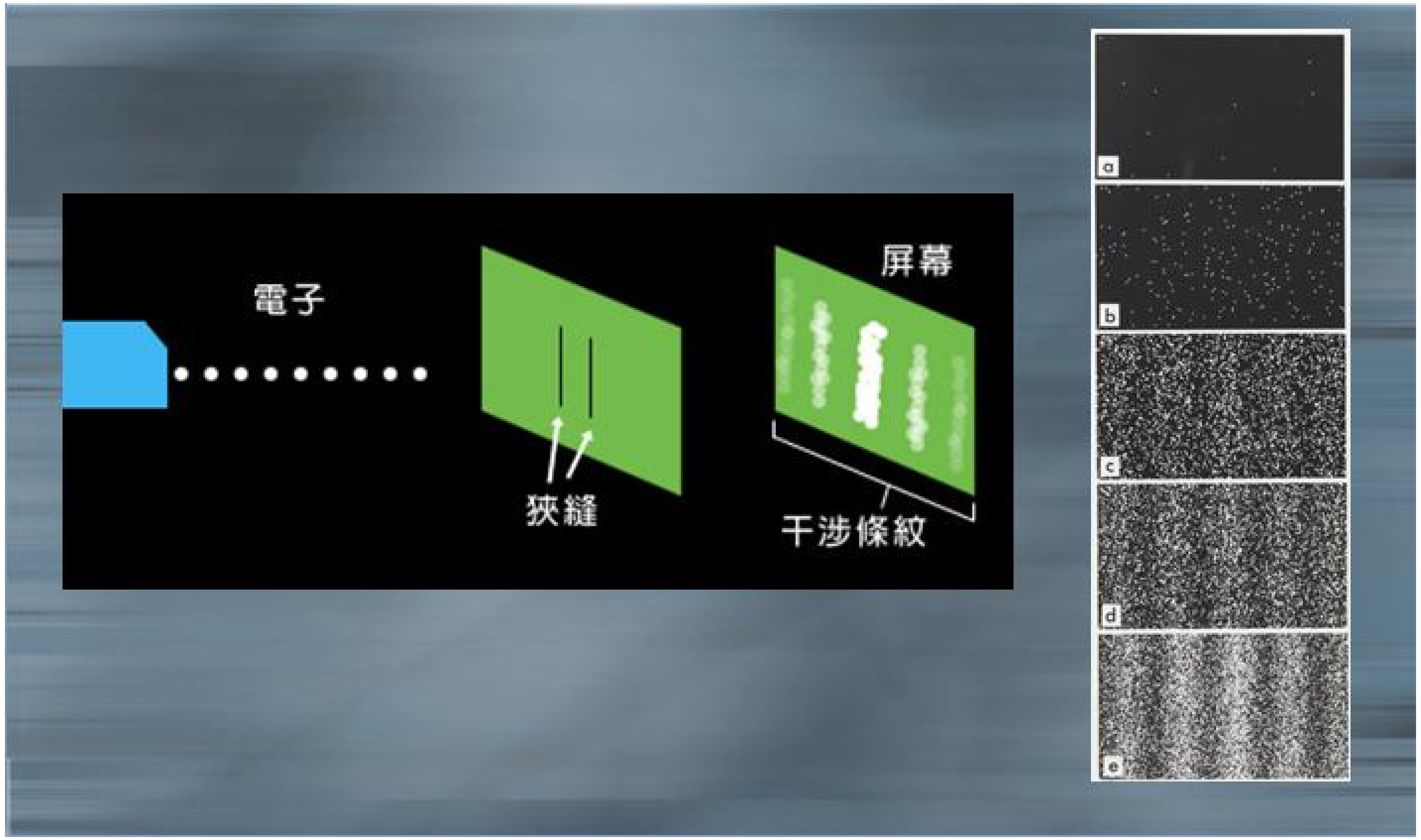
$$\rightarrow \begin{cases} |\varphi(t)\rangle = \sum |u_i(x)\rangle\langle u^*_i(x)|\varphi(t)\rangle \\ |\phi(t)\rangle = \sum |u_i(x)\rangle\langle u^*_i(x)|\phi(t)\rangle \end{cases}$$

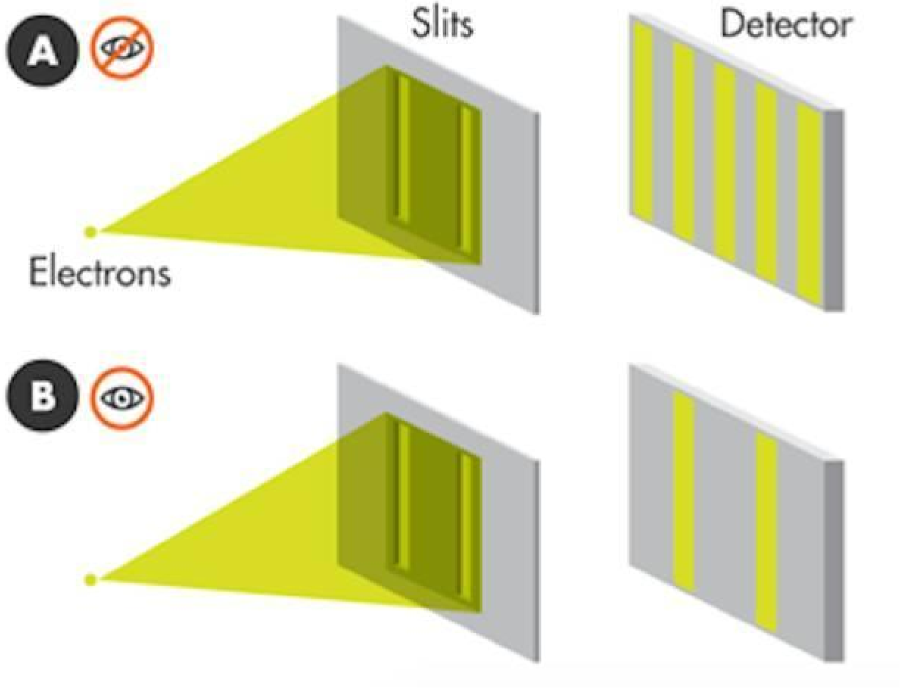
这里使用了：
u(x)*u*(x)的在
空间上的积分和
为1

诡异的叠加态实验

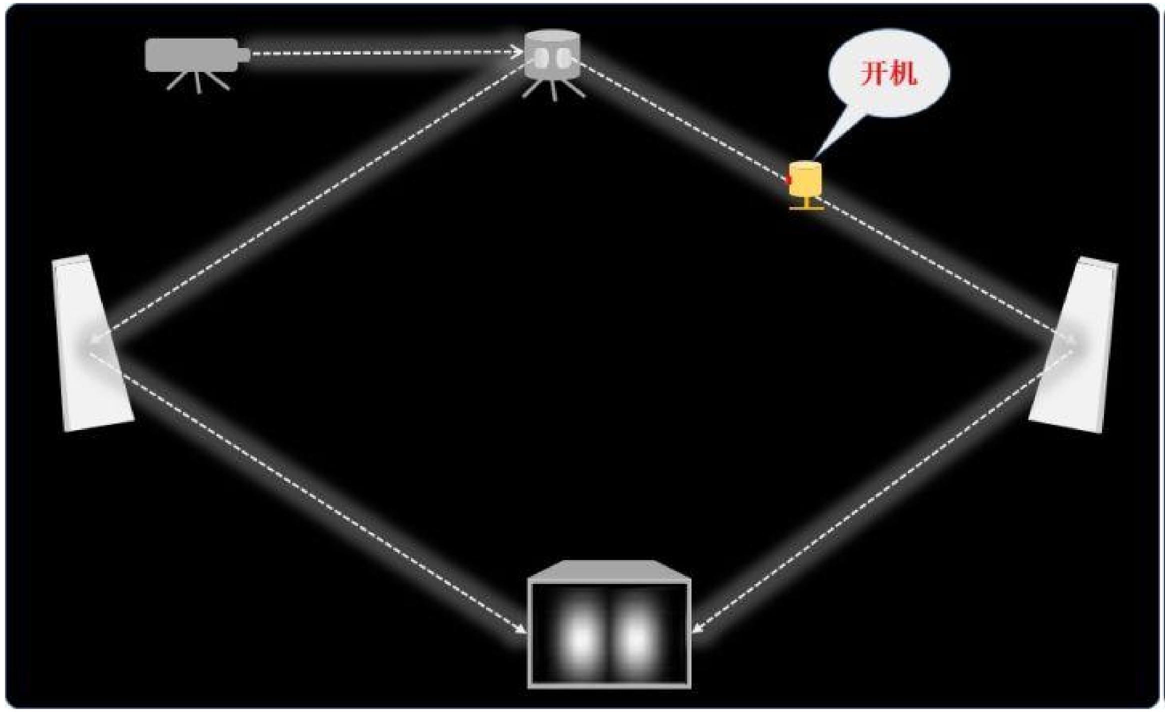
$$\psi(x)=\alpha\psi_1(x)+\beta\psi_2(x)$$

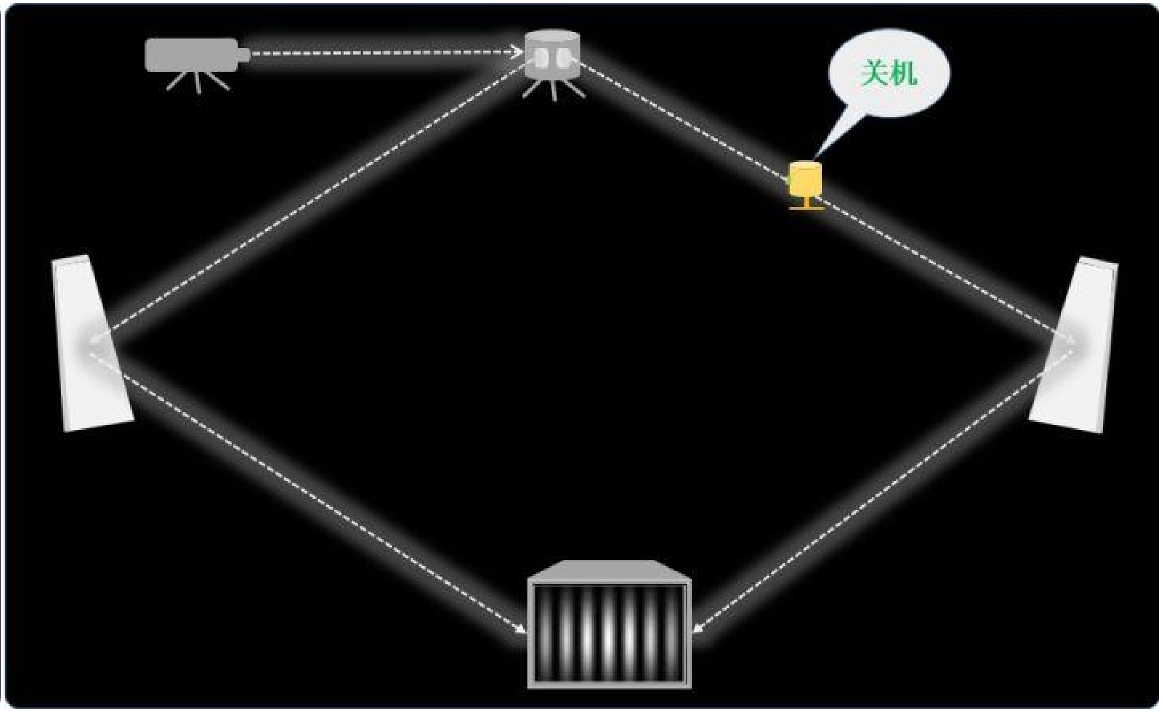
叠加态

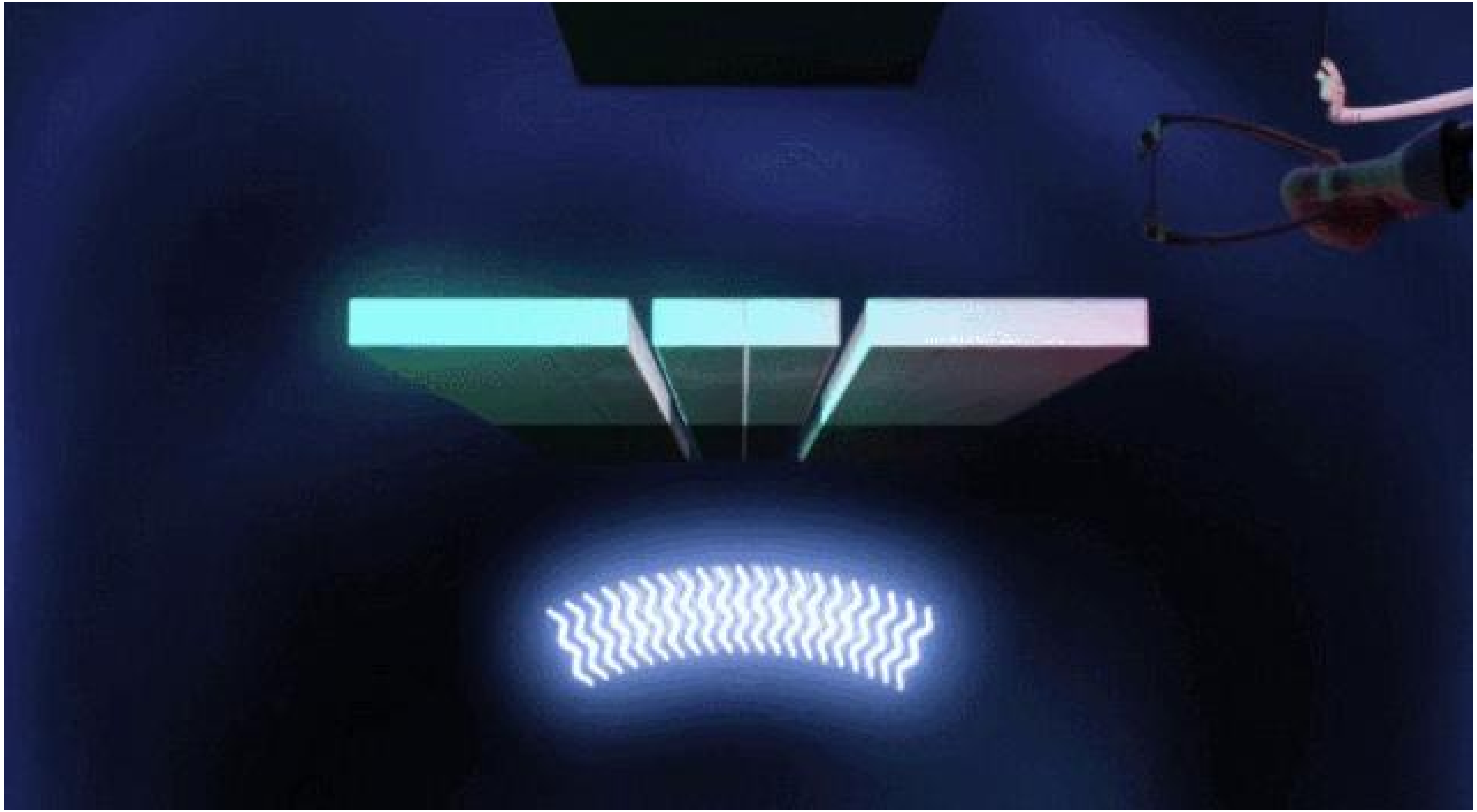


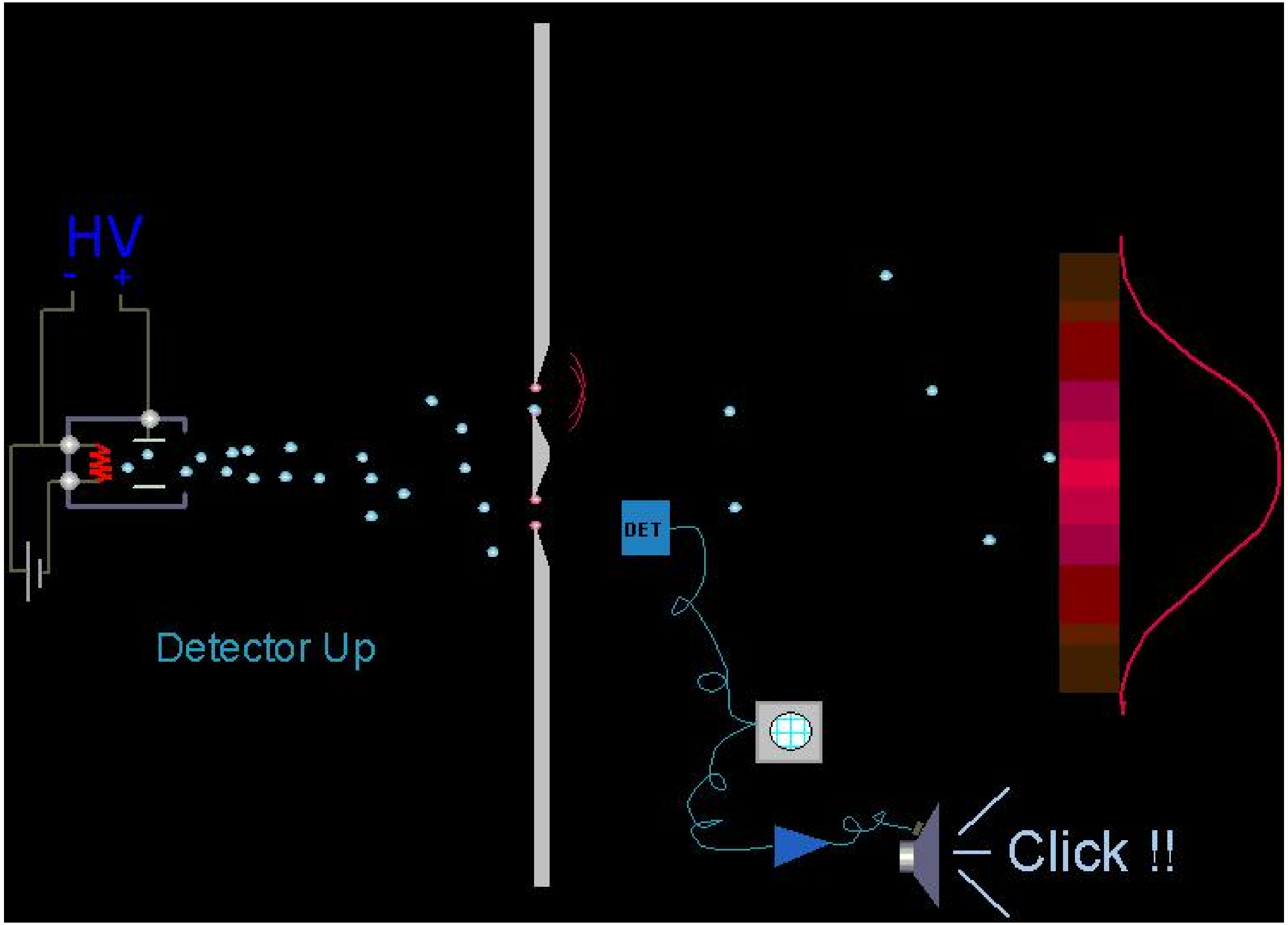


1984年马里兰大学的卡罗尔·阿雷和同事的一个小组完成了这个实验。

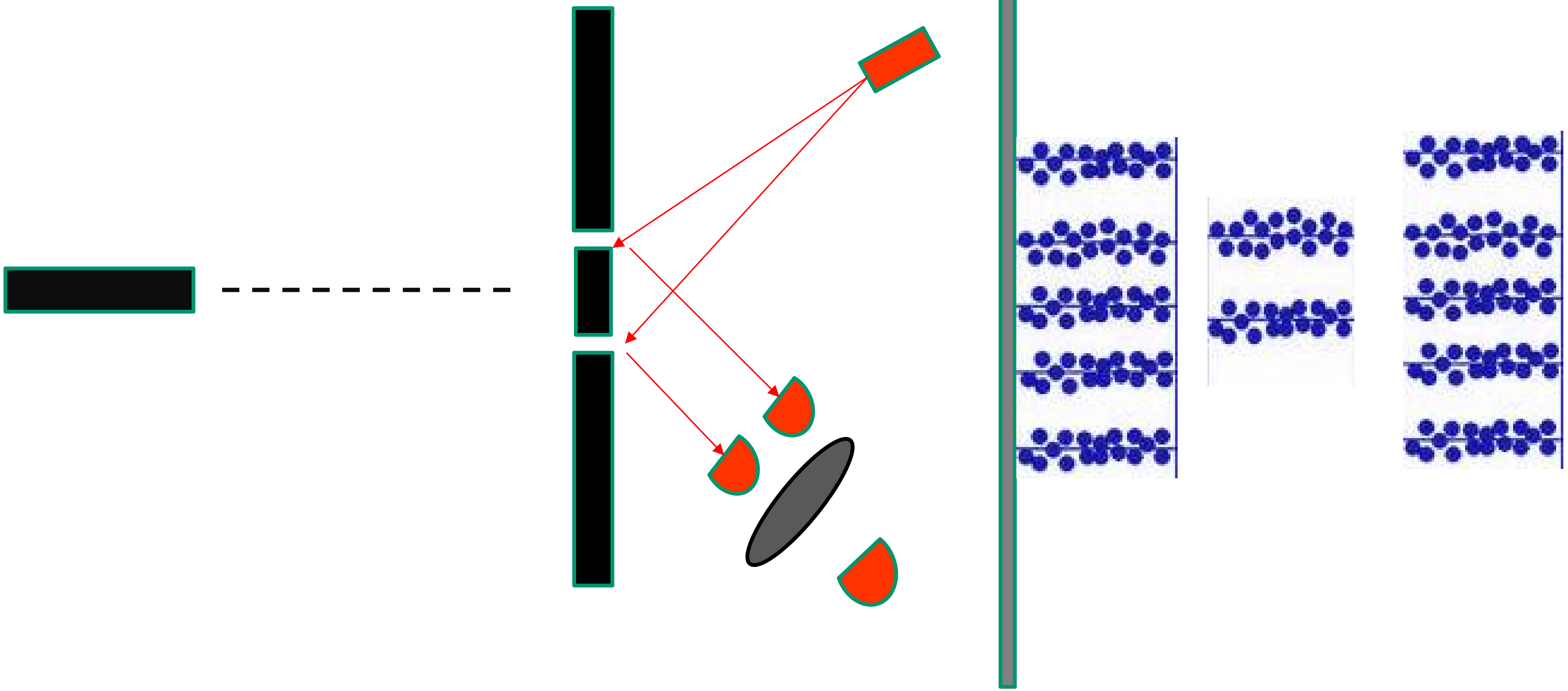




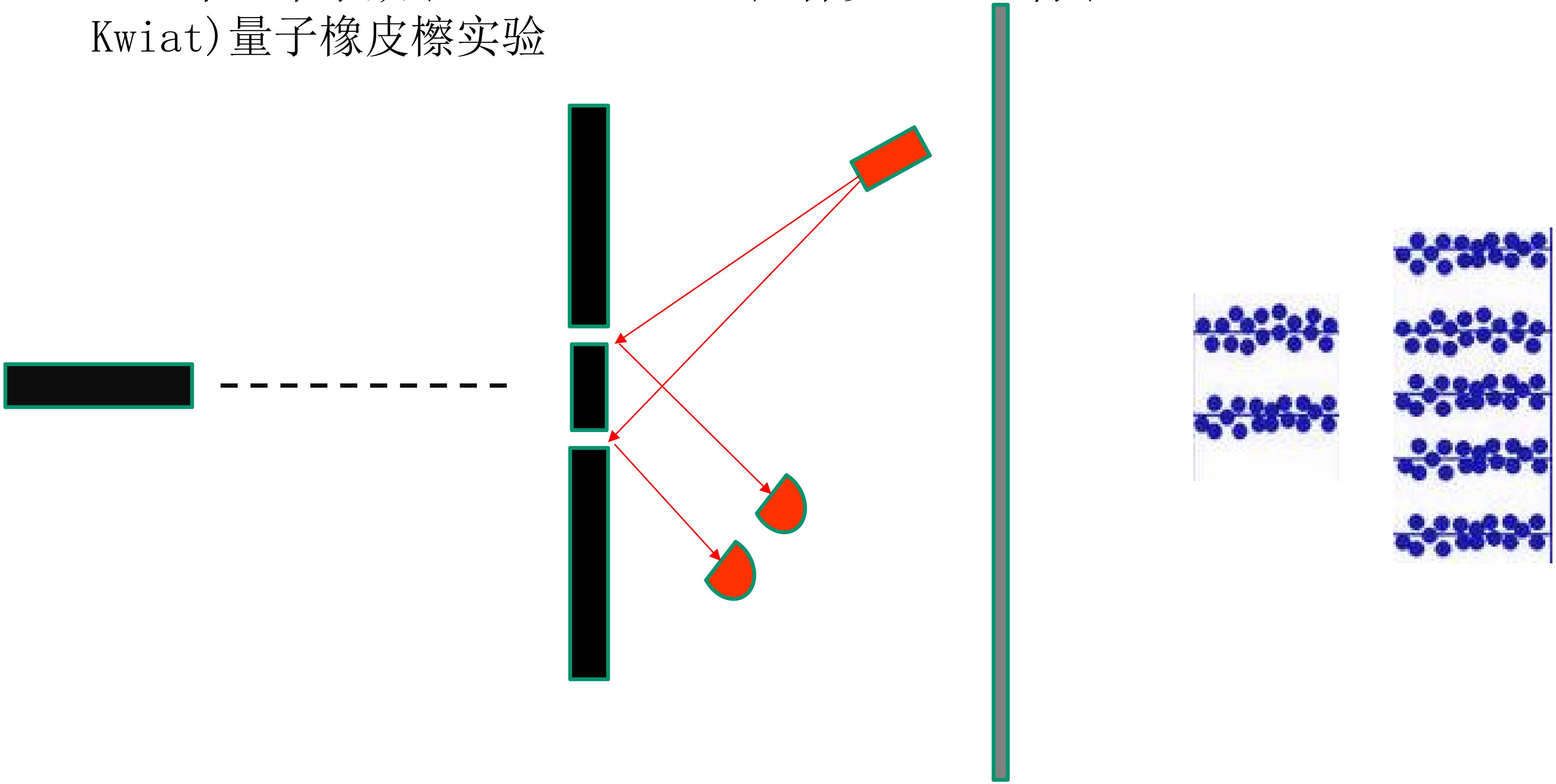



HV
-
+
Detector Up
DET
Click !!

2007年：希尔默(Rachel Hillmer) 保罗·奎亚特(Paul Kwiat)量子橡皮檫实验



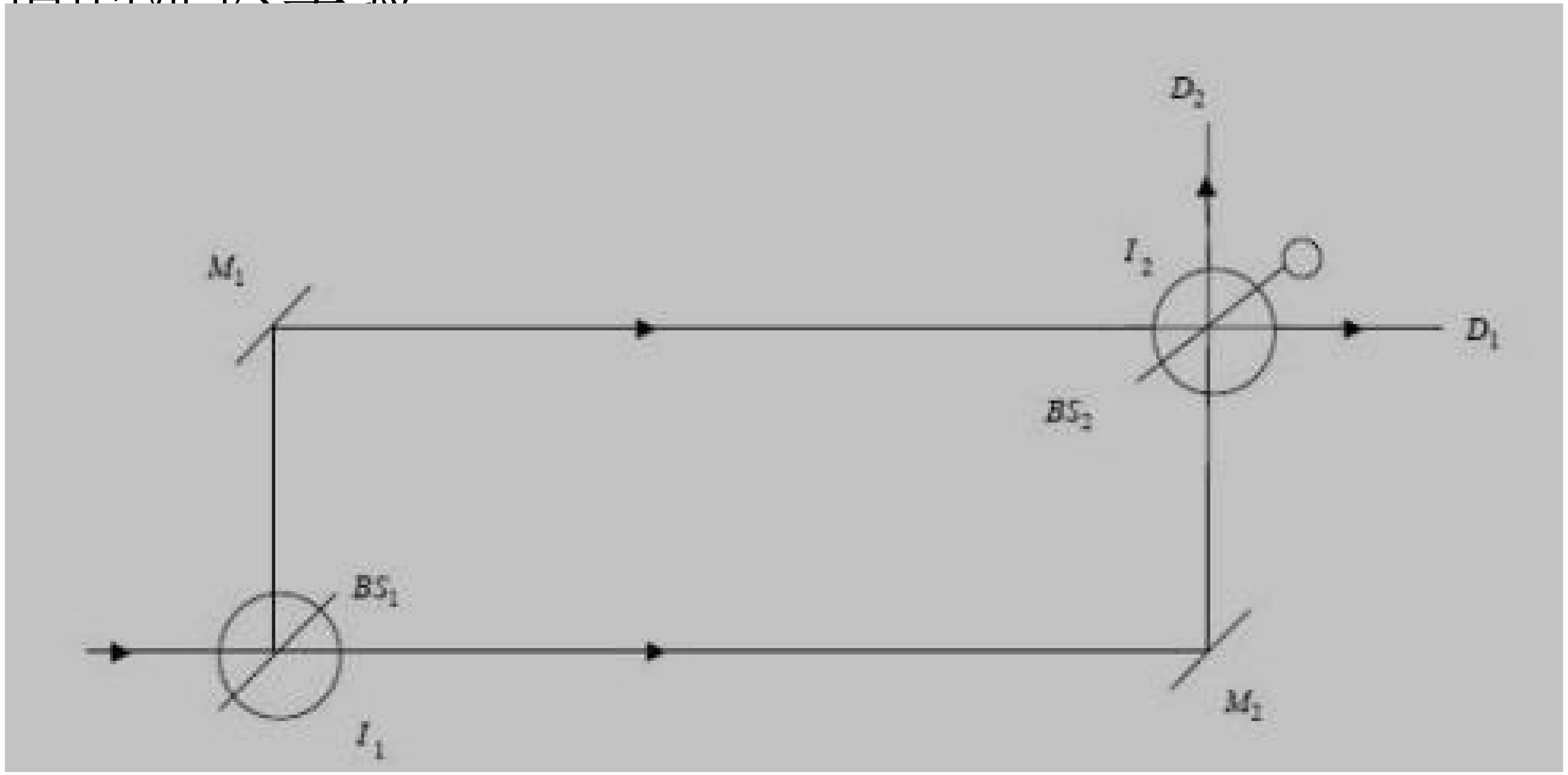
2007年：希尔默(Rachel Hillmer) 保罗·奎亚特(Paul Kwiat)量子橡皮檫实验



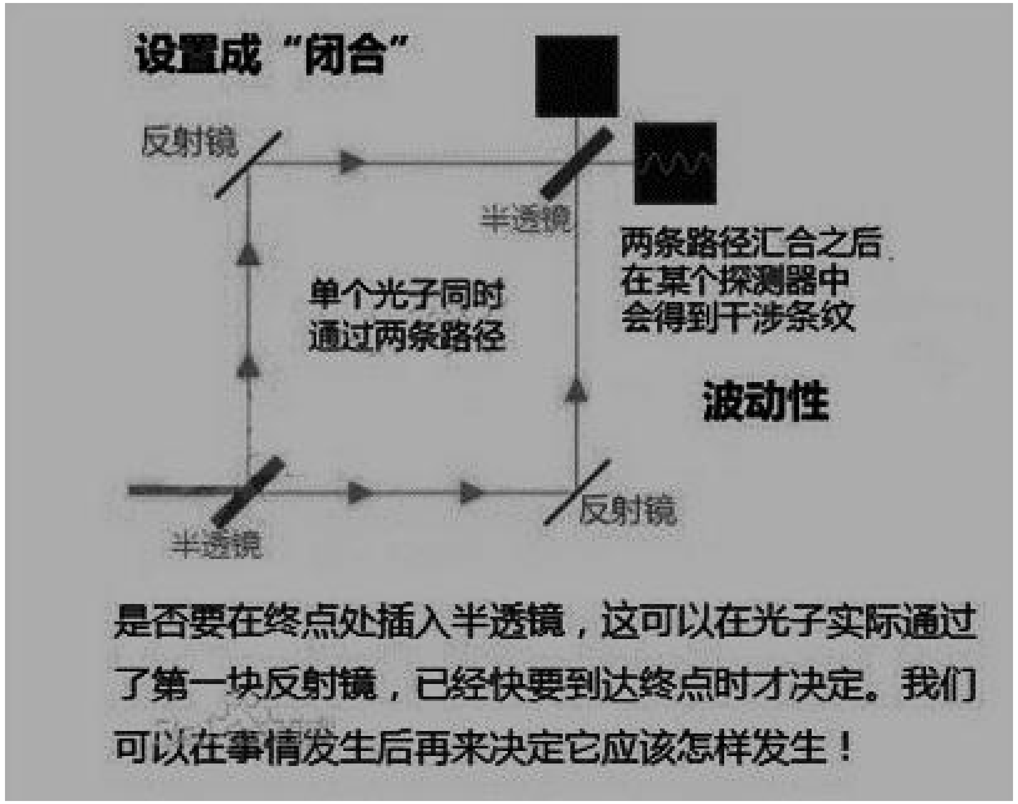
降低光的能量，会发生什么现象？

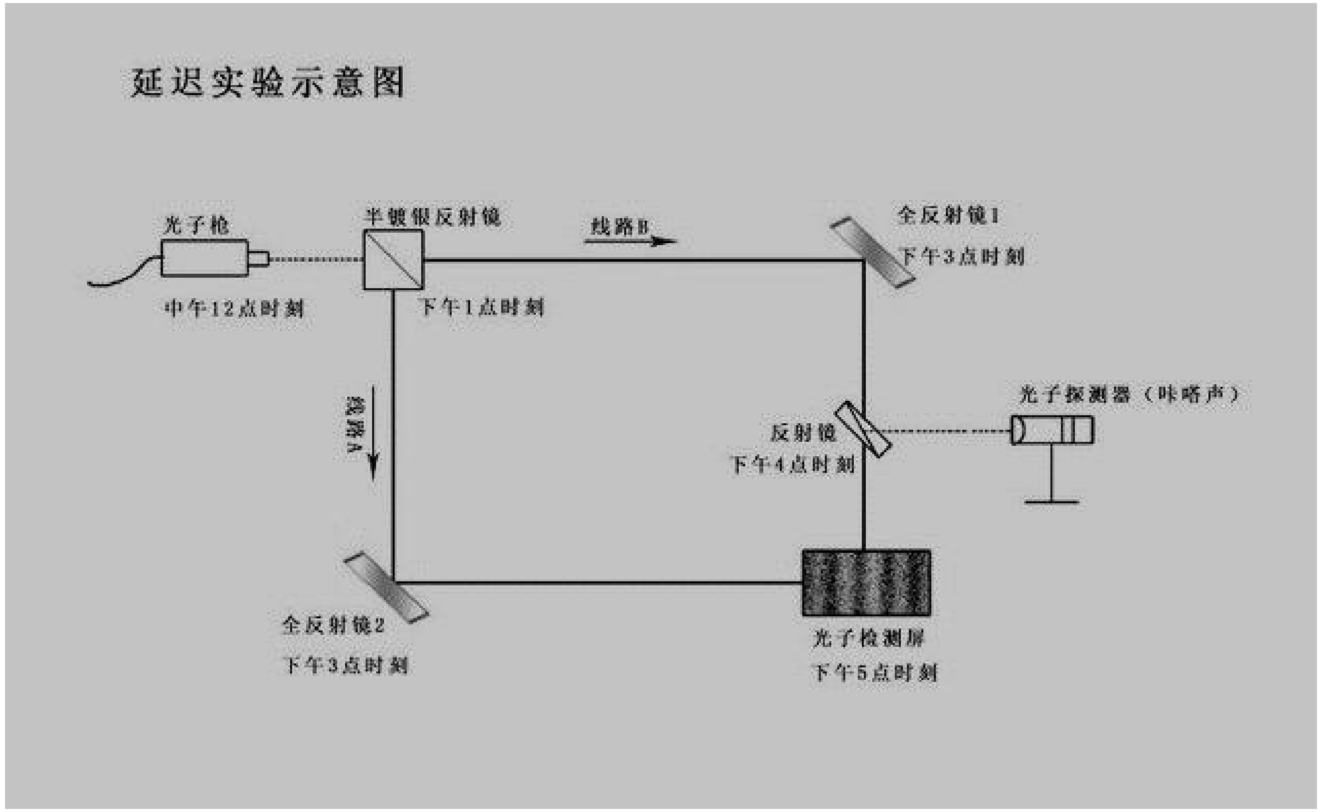
恐怖的延迟实验

1979年是爱因斯坦诞辰100周年，爱因斯坦的同事、玻尔的密切合作者之一约翰· 惠勒(John Wheeler)提出了一个相当令人吃惊的构想，也就是所谓的延迟实验



惠勒的构想提出5年后，马里兰大学的卡洛尔阿雷做了一个延迟实验






哈哈哈。。。
我告诉你啊，历史是
可以改变的！这次是
我总结经验，下次
赤壁之战我必胜
无疑！
丞相,赤壁之战
我们战败落荒而逃，
您为啥还这么开心？


电影已拍完，
现在可以选演员了。
可是,选杨幂当主演好，
还是刘亦菲当主演好呢？
这是个问题！


后悔药
——这个可以有

3.9 任意观测量的测不准关系

定理：如果两个算符有共同的本征函数，并组成完全系，则这两个算符对易

λ_n和μ_n分别是算符F和G的本征值，相应的本征值方程为：

$$\hat{F}\phi_n = \lambda_n\phi_n, \qquad \hat{G}\phi_n = \mu_n\phi_n$$

$$(\hat{F}\hat{G} - \hat{G}\hat{F})\phi_n = \lambda_n\mu_n\phi_n - \mu_n\lambda_n\phi_n = 0$$

由于ϕ_n组成完全系，$\psi = \sum_n a_n\phi_n$

$$(\hat{F}\hat{G}-\hat{G}\hat{F})\psi=\sum_n a_n(\hat{F}\hat{G}-\hat{G}\hat{F})\phi_n=0$$

因为ψ是任意波函数，所以 $\hat{F}\hat{G}-\hat{G}\hat{F}=0$

$\hat{p}_x,\hat{p}_y,\hat{p}_z$ 相互对易，有共同的本征函数ψ_p，且ψ_p组成完全系，三者能够同时精确测量

$\hat{H},\hat{L}^2,\hat{L}_z$ 在中心力场中，三者相互对易，有共同的本征函数。氢原子的定态波函数，三者能够同时精确测量， 确定的能量E_n，$l(l+1)\hbar^2$和$m\hbar$

具有共同本征函数的相互对易的力学量称为力学量完全集

2. 测不准关系

如果两个算符不对易，一般情况下，它们不能同时有确定值。

设两个物理量A和B都是厄密算符，它们的对易性为

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

一般C为厄密算符. 因为

$$\int \psi_1^*[\hat{A},\hat{B}]\psi_2 dx = \int \psi_1^*(\hat{A}\hat{B} - \hat{B}\hat{A})\psi_2 dx$$

$$= \int (\hat{B}^*\hat{A}^* - \hat{A}^*\hat{B}^*)\psi_1^*\psi_2 dx$$

$$= -\int [(\hat{A}\hat{B} - \hat{B}\hat{A})\psi_1]^*\psi_2 dx$$

注意这里，算符AB是厄米算符。

$$\int \psi_1^* i\hat{C}\psi_2 dx = -\int (i\hat{C}\psi_1)^* \psi_2 dx$$

$$\int \psi_1^* \hat{C}\psi_2 dx = \int (\hat{C}\psi_1)^* \psi_2 dx$$

所以C为厄密算符

任意态ψ中，对应算符A和B物理量的平均值为

$$\overline{A} = \int \psi^* \hat{A} \psi dx, \quad \overline{B} = \int \psi^* \hat{B} \psi dx$$

引入了平均值偏差

$$\Delta\hat{A} = \hat{A} - \overline{A}, \qquad \Delta\hat{B} = \hat{B} - \overline{B}$$

A和B的平均值是个常量，对算符的性质不会产生影响。

$\Delta\hat{A}$ 和 $\Delta\hat{B}$ 也是厄密算符

考察积分

α.为实参数

$$I(\alpha)=\int\left|(\alpha\Delta\hat{A}-\mathrm{i}\Delta\hat{B})\psi\right|^2 dx\geq 0$$

$$I(\alpha)=\int(\alpha\Delta\hat{A}-\mathrm{i}\Delta\hat{B})^*\psi^*(\alpha\Delta\hat{A}-\mathrm{i}\Delta\hat{B})\psi dx$$

$$=\alpha^2\int(\Delta\hat{A}\psi)^*(\Delta\hat{A}\psi)dx-i\alpha\int[(\Delta\hat{A}\psi)^*(\Delta\hat{B}\psi)-(\Delta\hat{B}\psi)^*(\Delta\hat{A}\psi)]dx+\int(\Delta\hat{B}\psi)^*(\Delta\hat{B}\psi)dx$$

$\boxed{\text{因为厄米算符！}}$

$$=\alpha^2\int\psi^*(\Delta\hat{A})^2\psi dx-\mathrm{i}\alpha\int\psi^*(\Delta\hat{A}\Delta\hat{B}-\Delta\hat{B}\Delta\hat{A})\psi dx+\int\psi^*(\Delta\hat{B})^2\psi dx$$

$$\Delta\hat{A}\Delta\hat{B}-\Delta\hat{B}\Delta\hat{A}=(\hat{A}-\overline{A})(\hat{B}-\overline{B})-(\hat{B}-\overline{B})(\hat{A}-\overline{A})=\hat{A}\hat{B}-\hat{B}\hat{A}=i\hat{C}$$

$$I(\alpha)=\overline{(\Delta\hat{A})^2}\alpha^2+\overline{C}\alpha+\overline{(\Delta\hat{B})^2}\geq 0$$

对每个实数 α，上式成立的条件为 $$\overline{(\Delta A)^2}\;\overline{(\Delta B)^2}\geq\frac{(\overline{C})^2}{4}$$

$$\Delta A \Delta B \geq \frac{1}{2}\left|\overline{[A,B]}\right|$$

这就是测不准关系

$$[x, \hat{p}_x] = i\hbar$$

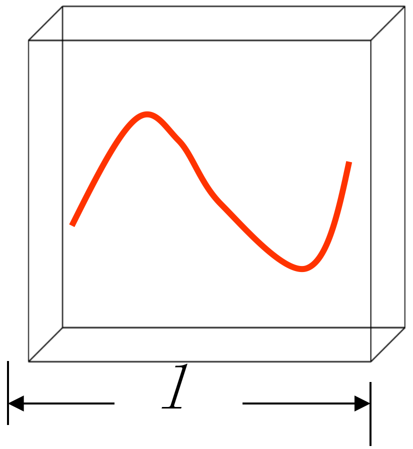
坐标和动量之间的测不准关系为 $\Delta p_x \Delta x \geq \frac{\hbar}{2}$

测不准关系表明，微观粒子的位置（坐标）和动量不能同时具有完全确定的值，这是粒子一波动两重性的反映。

物理上理解为：按照德布罗意关系$p=h/\lambda$，波长λ是描述波在空间变化快慢的量，与整个波相联系，因此，“在空间某点x的波长”的提法是没有意义的，同理，“粒子在空间某一点的动量”的提法也是没有意义的。

从宏观上看，h是一个非常小的量，测不准关系与日常生活并无矛盾。测不准关系指出了使用经典粒子运动概念的一个限度，即用h来表征. 当$h\to 0$，量子力学回到经典力学. 及量子效应可以忽略。

例题：确定箱中粒子的精确位置。



设箱的边长为l，$l=\Delta x$,

当$l=\Delta x\to 0$，则粒子动量的测不准性为

$$\Delta p \sim \frac{\hbar}{l}$$

由于粒子在箱中的运动为驻波的形式，其波长为l量级。

那么粒子的动能为：$E_{kin} = \frac{\Delta p^2}{2m} \sim \frac{\hbar^2}{2ml^2}$

由此可知，l越小，箱体越小， 动能和动量越大， 这正是实验得到的结果。

根据测不准关系，还可以计算线性谐振子的零点能量

$$E = \frac{\overline{p^2}}{2\mu} + \frac{1}{2}\mu\omega^2\overline{x^2}$$

$$\bar{x} = N_n^2 \int_{-\infty}^{+\infty} e^{-\alpha^2 x^2} H_n^2(\alpha x) x dx$$

$H_n^2(\alpha x)$是偶函数 $\quad \bar{x} = 0$

$$\overline{p} = \frac{\hbar}{i} N_n^{\ 2} \int_{-\infty}^{+\infty} e^{-\alpha^2 x^2/2} H_n(\alpha x) \frac{d}{dx} [e^{-\alpha^2 x^2/2} H_n(\alpha x)] dx$$

分部积分，得

$$\overline{p} = -\frac{\hbar}{i} N_n^{\ 2} \int_{-\infty}^{+\infty} \frac{d}{dx} [e^{-\alpha^2 x^2/2} H_n^2(\alpha x)] e^{-\alpha^2 x^2/2} H_n^2(\alpha x) dx = -\overline{p}$$

$$\overline{p} = 0$$

$$\overline{(\Delta x)^2} = \overline{(x - \overline{x})^2} = \overline{x^2}, \qquad \overline{(\Delta p)^2} = \overline{(p - \overline{p})^2} = \overline{p^2}$$

线性谐振子的平均能量为

$$\overline{E} = \frac{\overline{p^2}}{2\mu} + \frac{1}{2}\mu\omega^2\overline{x^2} = \frac{\overline{(\Delta p)^2}}{2\mu} + \frac{1}{2}\mu\omega^2\overline{(\Delta x)^2}$$

$$\overline{(\Delta p)^2} = \frac{\hbar^2}{4(\Delta x)^2}$$

$$\overline{E} = \frac{\hbar^2}{8\mu\overline{(\Delta x)^2}} + \frac{1}{2}\mu\omega^2\overline{(\Delta x)^2}$$

对Δx求最小值，得到 $\overline{E}_{\min} = \frac{1}{2}\hbar\omega$

例：已知能量函数 $E=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2$ 计算基态能量

解：

$$\psi(x)=\sqrt{\frac{\alpha}{\sqrt{\pi}}}e^{-\frac{1}{2}\alpha^2x^2} \qquad \overline{x^2}=\int_0^a x^2\psi^2(x,t)\,dx$$

$$\overline{x^2}=\int_{-\infty}^{+\infty}x^2\frac{\alpha}{\sqrt{\pi}}e^{-\alpha^2x^2}dx$$

$$\bar{x}=\int_{-\infty}^{+\infty}x\psi^2(x,t)\,dx=\int_{-\infty}^{\infty}x\frac{\alpha}{\sqrt{\pi}}e^{-\alpha^2x^2}dx$$

$$\overline{x^2}=\int_{-\infty}^{+\infty}x^2\frac{\alpha}{\sqrt{\pi}}e^{-\alpha^2x^2}dx=\frac{1}{2\alpha^2}$$

$$\bar{x}=\int_{-\infty}^{\infty}x\frac{\alpha}{\sqrt{\pi}}e^{-\alpha^2x^2}dx=0$$

奇函数在对称区间的积分。。。

$$\Delta x=\sqrt{\overline{x^2}-\bar{x}^2}=\sqrt{\frac{1}{2\alpha^2}}=\sqrt{\overline{x^2}}$$

$$\overline{p_x^{\;2}} = \int_{-\infty}^{+\infty} p^2 \psi^2(x,t)\,dx = \int_{-\infty}^{\infty} p^2 \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^2}\,dx$$

$$\overline{p_x^{\;2}} = \frac{1}{2}\alpha^2\hbar^2$$

$$\bar{p} = \int_{-\infty}^{\infty} p\psi^2(x,t)\,dx = \int_{-\infty}^{\infty} p \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^2}\,dx$$

$$\bar{p} = \int_{-\infty}^{\infty} p \frac{\alpha}{\sqrt{\pi}} e^{-\alpha^2 x^2}\,dx = 0$$

$$\Delta p_x = \sqrt{\overline{p^2} - \bar{p}^2}$$

$$\Delta p_x = \sqrt{\overline{p^2} - \bar{p}^2} = \frac{1}{\sqrt{2}}\alpha\hbar = \sqrt{\overline{p^2}}$$

$$E=\frac{p^2}{2m}+\frac{1}{2}m\omega^2x^2 \qquad E=\frac{\overline{p^2}}{2m}+\frac{1}{2}m\omega^2\overline{x^2}$$

$$\Delta x=\sqrt{\overline{x^2}-\overline{x}^2}=\sqrt{\frac{1}{2\alpha^2}}=\sqrt{\overline{x^2}}$$

$$\Delta p_x=\sqrt{\overline{p^2}-\overline{p}^2}=\frac{1}{\sqrt{2}}\alpha\hbar=\sqrt{\overline{p^2}}$$

$$E=\frac{\Delta p^2}{2m}+\frac{1}{2}m\omega^2\Delta x^2 \qquad \Delta p\Delta x=\frac{\hbar}{2}$$

注意平方的均值与均值的平方不是一个概念。

$$E=\frac{\hbar^2}{8m\Delta x^2}+\frac{1}{2}m\omega^2\Delta x^2 \qquad \frac{\partial E}{\partial \Delta x}=0$$

$$E=\frac{1}{2}\hbar\omega$$