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例: $t=0$ 时, $\psi(x)=(\sin kx+\frac{1}{3}\cos^2 kx)$, 求 $\bar{p}$, $\bar{E}$

解: $\psi(x)=[\frac{1}{2i}(e^{ikx}-e^{-ikx})+\frac{1}{12}(e^{2ikx}+2+e^{-2ikx})]$

$=\frac{1}{12}[e^{-2ikx}+6ie^{-ikx}+2-6ie^{ikx}+e^{2ikx}]$

$\because \psi_p=\frac{C_i}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px}$ $\therefore$ $p_1=-2k\hbar$, $p_2=-k\hbar$, $p_3=0$; $p_4=k\hbar$, $p_5=2k\hbar$

$C_1=\frac{A}{12}\sqrt{2\pi\hbar}$, $C_2=\frac{Ai}{2}\sqrt{2\pi\hbar}$, $C_3=\frac{A}{6}\sqrt{2\pi\hbar}$, $C_4=-\frac{Ai}{2}\sqrt{2\pi\hbar}$, $C_5=\frac{A}{12}\sqrt{2\pi\hbar}$

$\therefore \sum|C_i|^2=1 \Rightarrow A=\frac{6}{\sqrt{34\pi\hbar}}$ $\therefore$ $\bar{p}=\sum|C_i|^2p_i$, $\bar{E}=\sum|C_i|^2\frac{p_i^2}{2m}$.

例: 一维无限深, $\phi(x)=Axe^{-\lambda x}$ $(x\geq 0, \lambda>0)$ 1) 求 p 的分布 2) $\bar{p}$

解: 先求 A: $\int_0^\infty\phi(x)\phi^*(x)dx=1 \Rightarrow A=2\lambda^{\frac{3}{2}}$, $\phi(x)=\sum C_p\psi_p(x)$, $\psi_p(x)=\frac{1}{\sqrt{2\pi\hbar}}e^{\frac{i}{\hbar}px}$

$\therefore C_p=\int\frac{1}{\sqrt{2\pi\hbar}}e^{-\frac{i}{\hbar}px}\cdot 2\lambda^{\frac{3}{2}}xe^{-\lambda x}dx=\cdots$

2) $\bar{p}=\int\phi^*\hat{p}\phi dx$, $\hat{p}=-i\hbar\frac{\partial}{\partial x}$

例: $\phi(r,\theta,\varphi)=\frac{1}{2}R_{2,1}(r)Y_{1,0}(\theta,\varphi)-\frac{\sqrt{2}}{2}R_{2,1}(r)Y_{1,-1}(\theta,\varphi)$, 求 E, L^2, L_z 的可能值

解: $\phi_{n,l,m}=R_{n,l}\cdot Y_{l,m}$ $\therefore n=2, l=1, m=0,-1$

$C_1^2=\frac{\frac{1}{4}}{\frac{1}{4}+\frac{1}{2}}=\frac{1}{3}$, $C_2^2=1-C_1^2=\frac{2}{3}$, $E=\frac{1}{n^2}E_1=\frac{1}{n^2}(-13.6)eV$, $L^2=l(l+1)\hbar^2$.

$\therefore E=\frac{1}{4}(-13.6)$, $P=1$. $L^2=2\hbar^2$, $P=1$ $\quad L_z=m\hbar$

$L_z=0,-\hbar$, $P=\frac{1}{3},\frac{2}{3}$

例: 求 $[\hat{H}_x,\hat{x}]$

解: $\hat{H}=-\frac{\hbar^2}{2m}\frac{\partial^2}{\partial x^2}+V(x)=\frac{1}{2m}\hat{p}_x^2+V(x)$, $[\hat{p}_x,x]=-i\hbar=\hat{p}_xx-x\hat{p}_x$

$[\hat{H},\hat{x}]=\hat{H}x-x\hat{H}=\frac{1}{2m}(\hat{p}_x^2x-x\hat{p}_x^2)=\frac{1}{2m}(\hat{p}\cdot\hat{p}x-x\hat{p}\cdot\hat{p})$

$=\frac{1}{2m}(\hat{p}\cdot(x\hat{p}_x-i\hbar)-(\hat{p}_xx+i\hbar)\hat{p})=-\frac{i\hbar}{m}\hat{p}$

$\therefore \hat{p}=\frac{im}{\hbar}[\hat{H},x]$, $\bar{p}=\int\psi^*\hat{p}\psi d\tau=\int\psi^*[\hat{H},x]\psi d\tau$

$\bar{p}=\frac{im}{\hbar}(\int\psi^*\hat{H}x\psi d\tau-\int\psi^*x\hat{H}\psi d\tau)=\frac{im}{\hbar}(\int(\hat{H}\psi)^*x\psi d\tau-\int\psi^*xE\psi d\tau)$

$=\frac{im}{\hbar}(\int\psi^*Ex\psi dx-\int\psi^*xE\psi dx)=0$

$\therefore$ 在 E 确定时, $\bar{p}\equiv 0$

力学测不准定理

两个力学量有共同本征态 $\Leftrightarrow [\hat F,\hat G]=0$

若 $[\hat F,\hat G]\neq 0$，一般不能同时有确定值.

记 $\Delta F = F-\bar F$，$\Delta G = G-\bar G$，则有 $\overline{\Delta F^2} = \overline{F^2}-\bar F^2$，$\overline{\Delta G^2} = \overline{G^2}-\bar G^2$

且 $\Delta F\cdot\Delta G \geq \frac{1}{2}|\overline{[\hat F,\hat G]}|$

proof: $\overline{\Delta F^2} = \int\psi^*\Delta F^2\psi\, d\tau = \int\psi^*(F^2-2F\bar F+\bar F^2)\psi\, d\tau = \overline{F^2}-\bar F^2$

令 $\psi = (\hat F + i\alpha\hat G)\phi$，$|\psi|^2 = \psi\cdot\psi^* \geq 0$

$|\psi|^2 = \int(\hat F+i\alpha\hat G)^*\phi^*\cdot(\hat F+i\alpha\hat G)\phi\, d\tau = \alpha^2\overline{G^2} - \alpha\overline{[\hat F,\hat G]} + \overline{F^2} \geq 0$

∴ $\Delta\leq 0 \Rightarrow [\hat F,\hat G] = \hat C \Rightarrow \bar C^2 \leq 4\overline{G^2}\,\overline{F^2} \Rightarrow \bar G\bar F \geq \frac{1}{2}\bar C$

上式对 $\Delta F,\Delta G$ 也成立.

例: 证明 $\Delta x\cdot\Delta p_x \geq \frac{\hbar}{2}$

proof: $\Delta x\cdot\Delta p_x \geq \frac{1}{2}|\overline{[\Delta x,\Delta p_x]}| = \frac{1}{2}|[x\, i\hbar\frac{\partial}{\partial x} + i\hbar]| = \frac{1}{2}\hbar$

例: 证明: 在 $\hat L_z$ 的本征态下，$\bar L_x, \bar L_y = 0$，并求 $\Delta\overline{L_x^2}$

proof: ∵ $[\hat L_y,\hat L_z] = i\hbar\hat L_x$，∵ $\bar L_x = \int\phi^*\hat L_x\phi\, dx$，$\hat L_z\phi = m\hbar\phi$

∴ $\bar L_x = \frac{1}{i\hbar}\int\phi^*(\hat L_y\hat L_z - \hat L_z\hat L_y)\phi\, d\tau = \frac{1}{i\hbar}\left(\int\phi^*\hat L_y\hat L_z\phi\, d\tau - \int\phi^*\hat L_z\hat L_y\phi\, d\tau\right)$

$= \frac{1}{i\hbar}\left(\int m\hbar\phi^*\hat L_y\phi\, d\tau - \int(\hat L_z\phi)^*\hat L_y\phi\, d\tau\right)$ $\hat L_z$是厄密算符

$= 0$

同理 $\bar L_y = 0$

$\Delta\overline{L_x^2} = \overline{L_x^2} - \bar L_x^2 = \overline{L_x^2}$，由对称性 $\overline{L_x^2} = \overline{L_y^2}$，$\overline{L^2} = \overline{L_x^2}+\overline{L_y^2}+\overline{L_z^2}$

∴ $l(l+1)\hbar^2 = 2\overline{L_x^2} + m^2\hbar^2 \Rightarrow \overline{L_x^2} = \frac{1}{2}(l(l+1)-m^2)\hbar^2 = \Delta\overline{L_x^2}$

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例：$\hat{F}$不含时，求证 $\frac{d\overline{F}}{dt} = \frac{1}{i\hbar}\overline{[\hat{F},\hat{H}]}$

proof: $\frac{d\overline{F}}{dt} = \frac{d}{dt}\int \psi^*\hat{F}\psi dx = \int \frac{\partial}{\partial t}\psi^* \cdot \hat{F}\psi dx + \int \psi^*\hat{F}\frac{\partial}{\partial t}\psi dx + \int \psi^*\frac{d\hat{F}}{dt}\psi dx$

$\because$ $\hat{F}$不含时 $\therefore$ $\frac{d\hat{F}}{dt}=0$，又$\because$ $i\hbar\frac{d\psi}{dt} = \hat{H}\psi$ $\therefore$ $-i\hbar\frac{d\psi^*}{dt} = \hat{H}\psi^*$

$\therefore$ 原式 $= \frac{1}{i\hbar}\left(\int \psi^*\hat{F}\hat{H}\psi dx - \int \hat{H}\psi^*\hat{F}\psi dx\right)$

$= \frac{1}{i\hbar}\left(\int \psi^*\hat{F}\hat{H}\psi dx - \int \psi^*\hat{H}\hat{F}\psi dx\right)$ $\quad (\hat{H}\psi^* = (\hat{H}\psi)^* = \psi^*\hat{H})$

$= \frac{1}{i\hbar}(\overline{[\hat{F},\hat{H}]})$

$\therefore$ 用$\hat{P}$代入$\hat{F}$，有 $\frac{d\overline{P}}{dt}=0$，表明E确定的$\psi$动量守恒

用$\hat{L}^2$代入$\hat{F}$，有 $\frac{d\overline{F}}{dt}=0$

表象变换

表象.

$\psi = \sum c_i\phi_i$，$c_i = \int \phi_i^*\psi d\tau$，那么在基矢$\phi_i$下，用 $C=\{c_i\}$ 向量表征ψ

其中$\{\phi_i\}$是正交归一基矢组，$\{c_i\}$称为ψ在$\hat{F}$下的表象（$\hat{F}\phi_i = \lambda_i\phi_i$）

记 $\psi(F) = (c_1, c_2, \cdots, c_n, \cdots)^T$，$\psi^+(F) = (c_1^*, c_2^*, \cdots, c_n^*, \cdots)$

$\therefore$ $\psi^+\cdot\psi = \sum c_i^* c_i = \sum |c_i|^2 = 1$

基矢 $\phi_i(F) = (0, 0, \cdots, 1, 0\cdots, 0\cdots)^T$ 第i个元素为1

算符的表象

设 $\Psi = \hat{F}\Phi$，$\Psi = \sum a_i\phi_i$，$\Phi = \sum b_i\phi_i$，其中ϕ_i是基矢.

$\therefore$ $\sum a_i\phi_i = \hat{F}\sum b_i\phi_i$ $\quad$ 由于表象都在$\hat{G}$下，故ϕ_i相同.

$\therefore$ $a_i = \int \phi_i^*\Psi d\tau = \int \phi_i^*\hat{F}\Phi d\tau \Rightarrow \int \phi_i^* a_i\phi_i d\tau = \int \phi_i^*\hat{F}\sum b_j\phi_j d\tau$.

由于不知道 $\int \phi_i^*\hat{F}b_j\phi_j = ?0$，故记 $\int \phi_i^*\hat{F}\phi_j d\tau = F_{ij}$

$\therefore$ $a_i = \sum_j F_{ij}b_j \Rightarrow \{a_i\}^T = F_{n\times n} = (F_{ij})_{n\times n}\{b_i\}^T$

注意：首先指定基矢的表象，这里令 $\hat{G}\phi_i = \lambda_i\phi$，即在$\hat{G}$下的表象

则$\hat{F}$在$\hat{G}$下的表象为 $F_{n\times n} = \{F_{ij}\} = \{\int \phi_i^*\hat{F}\phi_j d\tau\}$.

本征值方程

很显然，在$\hat{G}$下$\hat{F}$的本征值方程为 $\hat{F}\Phi_i = \lambda_i \Phi_i$，写为矩阵有

$$\begin{pmatrix} F_{11} & F_{12} & \cdots & F_{1n} & \cdots \\ F_{21} & F_{22} & \cdots & F_{2n} & \cdots \\ \vdots & & & & \\ F_{n1} & \cdots & \cdots & F_{nn} & \\ \vdots & & & & \end{pmatrix}\begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \\ \vdots \end{pmatrix} = \lambda \begin{pmatrix} c_1 \\ c_2 \\ \vdots \\ c_n \\ \vdots \end{pmatrix}$$ 显然λ有多解，变换得

$$\begin{pmatrix} F_{11}-\lambda & F_{12} & \cdots \\ F_{21} & F_{22}-\lambda & \cdots \\ & & \ddots \end{pmatrix}\begin{pmatrix} \\ \\ \end{pmatrix} = 0$$

要使之有非0解，$r(A) \neq n$

$\therefore \det(F-\lambda I)=0$

上式为久期方程，解得λ_i为$\hat{F}$在$\hat{G}$下的本征值

解得λ_i后代回方程组，解得$\{c_j\}_i$

当$\hat{G}=\hat{F}$，即在$\hat{F}$表象下的$\hat{F}$矩阵，很显然为对角阵，$F_{mn}=\mathrm{diag}(\lambda_1, \lambda_2, \cdots, \lambda_n)$

例：$\hat{A}^2=1$，求$\hat{A}$在$\hat{A}$下的表示。

解：$\hat{A}\phi = \alpha\phi \Rightarrow \hat{A}^2\phi = \alpha^2\phi = \phi \Rightarrow \alpha = \pm 1 \quad \therefore \hat{A} = \mathrm{diag}(1,-1)$

薛定谔方程的矩阵表示

$i\hbar\dot{\Psi} = \hat{H}\Psi$，$\Psi = \sum c_i\phi_i$ $\therefore$两边左乘ϕ_m^*并积分，有

$i\hbar\frac{\partial}{\partial t}c_m = \int \phi_m^* \hat{H} \sum c_i\phi_i \, d\tau = \sum H_{mi}c_i$ H_{mi}为H矩阵的第mi个元素

$\therefore i\hbar\frac{\partial}{\partial t}\{c_i\}^T = H\cdot\{c_i\}^T$，在$\hat{H}$表象下 $H=\mathrm{diag}(E_1, E_2, \cdots, E_n)$

$\therefore i\hbar\frac{\partial}{\partial t}c_m = E_m c_m \Rightarrow c_m = c_m(0)e^{-\frac{i}{\hbar}E_m t}$.

例：已知$\hat{L}_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$，求其本征值和对应本征矢（矩阵形式的波函数）

解：$\hat{L}_z\phi = \lambda\phi \Rightarrow |\hat{L}_z - \lambda E| = 0 \Rightarrow \lambda = \hbar, 0, -\hbar$

当$\lambda=\hbar$时，$(\hat{L}_z - \hbar E)\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix} = 0 \Rightarrow a_1=1, a_2=0, a_3=0$ 即$(1,0,0)^T$

当$\lambda=0$时，$a_1=0, a_2=1, a_3=0$ 即$(0,1,0)^T$

当$\lambda=-\hbar$时，$(0,0,1)^T$

注意 $\phi = (Y_{1,1}, Y_{1,0}, Y_{1,-1})\begin{pmatrix} a_1 \\ a_2 \\ a_3 \end{pmatrix}$，由归一化条件 $\sum a_i^2 = 1$

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例: $\hat{L}_x=\hbar\frac{\sqrt{2}}{2}\begin{pmatrix}0&1&0\\1&0&1\\0&1&0\end{pmatrix}$，求本征值、矢

解:

$\hat{L}_x\phi=\lambda\phi$，$\phi=(Y_{1,1},Y_{1,0},Y_{1,-1})(a_1,a_2,a_3)^T$ // m取3个值，3阶matrix，$l=1$

$\Rightarrow$ 令 $\lambda=\frac{\sqrt{2}}{2}\hbar k$ ∴ $\begin{vmatrix}-k&1&0\\1&-k&1\\0&1&-k\end{vmatrix}=-k^3+2k=0\Rightarrow k=0,\pm\sqrt{2}$

∴ 当 $k=0$ 时，$\lambda=0$

$(\hat{L}_x-\lambda E)\alpha=0\Rightarrow\alpha=(\frac{\sqrt{2}}{2},0,-\frac{\sqrt{2}}{2})^T$

当 $k=\sqrt{2}$ 时，$\frac{\sqrt{2}}{2}\hbar\begin{pmatrix}-\sqrt{2}&1&0\\1&-\sqrt{2}&1\\0&1&-\sqrt{2}\end{pmatrix}\begin{pmatrix}a_1\\a_2\\a_3\end{pmatrix}=0_{1\times3}\Rightarrow\alpha=(\frac{1}{2},\frac{\sqrt{2}}{2},\frac{1}{2})^T$

同理 $k=-\sqrt{2}$ 时，$\alpha=(\frac{1}{2},-\frac{\sqrt{2}}{2},\frac{1}{2})^T$

例: $\hat{L}_y=\frac{\sqrt{2}}{2}\hbar\begin{pmatrix}0&-i&0\\i&0&-i\\0&i&0\end{pmatrix}$，求本征值、矢

过程同上题，$\lambda=\frac{\sqrt{2}}{2}\hbar\cdot k$，$k=0,\pm\sqrt{2}$

当 $k=0$ 时，$\alpha=(\frac{\sqrt{2}}{2},0,\frac{\sqrt{2}}{2})^T$

当 $k=\sqrt{2}$ 时，$\alpha=(\frac{1}{2},\frac{\sqrt{2}}{2}i,-\frac{1}{2})^T$ 当 $k=-\sqrt{2}$ 时，$\alpha=(\frac{1}{2},-\frac{\sqrt{2}}{2}i,-\frac{1}{2})^T$

注: 上面的 $\hat{L}_x,\hat{L}_y,\hat{L}_z$ 的矩阵在 $Y_{1,1},Y_{1,0},Y_{1,-1}$ 下才成立。

例: 在 $\hat{L}^2,\hat{L}_z$ 的本征函数体系上，$L^2=2\hbar^2$，已知 $P(L_y=0)=\frac{1}{2}$，求 $\hat{L}_y=\hbar$ 的概率。

解: $L^2=2\hbar^2\Rightarrow l=1$ ∴ $m=1,0,-1$，$\hat{L}_y$ 的矩阵如上。

当 $L_y=0$ 时，$\psi_1=\frac{\sqrt{2}}{2}Y_{1,1}+\frac{\sqrt{2}}{2}Y_{1,-1}$ ∴ $P(\phi=\psi_1)=0.5$

又∵ ϕ 是 L^2 和 L_z 的本征态，不是叠加态，故 $\phi=(1,0,0)^T$ 或 $(0,1,0)^T$ 或 $(0,0,1)^T$

视 ϕ 为 ψ_i 的叠加，$\phi=\sum c_i\psi_i\Rightarrow$ ~~$c_i=\int\phi\,\psi_i^*d\tau$~~ $c_i=\int\phi\psi_i^*d\tau$

∴ $c_i=\int\phi(\sum d_i\phi_i)^*d\tau$，而 $\phi=\sum a_i\phi_i$，a_i 为本征矢 $\psi_i=\sum d_i\phi_i$

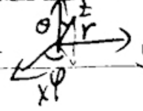
$=(a_1,a_2,\cdots,a_n)(d_1^*,d_2^*,\cdots,d_n^*)^T$

$P=|c_i|^2$，对本题，$\phi=(1,0,0)$ 时，$a=(1,0,0)$ ∵已知 $P_{\psi_1}=0.5$

$\psi_1=(\frac{\sqrt{2}}{2},0,\frac{\sqrt{2}}{2})$ ∴ $a=(1,0,0)^T$ 或 $(0,0,1)^T$

要求 $\hat{L}_y=\hbar$ 同理，$\psi_2=(\frac{1}{2},\frac{\sqrt{2}}{2}i,-\frac{1}{2})$ ∴ $P=\left[(\frac{1}{2},\frac{\sqrt{2}}{2}i,-\frac{1}{2})^*\begin{pmatrix}1\\0\\0\end{pmatrix}\right]^2=\frac{1}{4}$

例：$\psi = Ce^{-\alpha r}(x+y+2z)$，$\alpha$是正常数，C归一化用，求$L^2$的取值，$\overline{L_z}$，$L_z$为$\hbar$的P和$\hat{L}_x$的可能值与对应概率。

解：在球坐标  中（注意和高数不同）

$$\psi = Ce^{-\alpha r}\cdot r(\sin\theta\cos\varphi + \sin\theta\sin\varphi + 2\cos\theta)$$

$$= Ce^{-\alpha r} r\left(\frac{i-1}{2}\sin\theta e^{i\varphi} + \frac{1+i}{2}\sin\theta e^{-i\varphi} + 2\cos\theta\right)$$

$$= Ce^{-\alpha r} r\left(-\frac{i-1}{2}\sqrt{\frac{8\pi}{3}}Y_{1,1} + \frac{1+i}{2}\sqrt{\frac{8\pi}{3}}Y_{1,-1} + 2\sqrt{\frac{4\pi}{3}}Y_{1,0}\right)$$

$$Y_{l,m} \Rightarrow \begin{cases} Y_{1,1} = -\sqrt{\frac{3}{8\pi}}\sin\theta e^{i\varphi} \\ Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta \\ Y_{1,-1} = \sqrt{\frac{3}{8\pi}}\sin\theta e^{-i\varphi} \end{cases}$$

$\therefore L^2 = l(l+1)\hbar^2 = 2\hbar^2$，$\overline{L_z} = \sum \frac{|C_i|^2 m_i}{\sum |C_i|^2}\hbar$

$P(L_z = \hbar) = \frac{|C_1|^2}{\sum |C_i|^2}$　　$\hat{L}_x$见前一页，$(C_1, C_2, C_3)^T$见上。

当$L_x = 0$时，$\alpha_1 = (\frac{\sqrt{2}}{2}, 0, -\frac{\sqrt{2}}{2})$，　$P(L_x = 0) = |\alpha_1^* C|^2$

$L_x = \hbar$时，$\alpha_2 = (\frac{1}{2}, \frac{\sqrt{2}}{2}, \frac{1}{2})$，　$P(L_x = \hbar) = |\alpha_2^* C|^2$

$L_x = -\hbar$时，$\alpha_3 = (\frac{1}{2}, -\frac{\sqrt{2}}{2}, \frac{1}{2})$，　$P(L_x = -\hbar) = |\alpha_3^* C|^2$

例：$\psi = C_1 Y_{1,1} + C_2 Y_{1,0}$，$C_i$归一化，求$\hat{L}_z$和$\hat{L}^2$的值，P，$\hat{L}_x$的可能值和P。

解：$L_z = m\hbar = \hbar$，$P = |C_1|^2$；$= 0$，$P = |C_2|^2$

$L^2 = l(l+1)\hbar^2 = 2\hbar^2$，$P = 1$。

在$l=1$时，$\hat{L}_x$如前表，$C = (C_1, C_2, 0)$

$\therefore L_x = 0$时，$P = |\alpha_1^* \cdot C|^2 = \frac{1}{2}|C_1|^2$

$L_x = \hbar$时，$P = |\alpha_2^* \cdot C|^2 = \frac{1}{4}|C_1 + \sqrt{2}C_2|^2$

$L_x = -\hbar$时，$P = |\alpha_3^* \cdot C|^2 = \frac{1}{4}|C_1 - \sqrt{2}C_2|^2$