

I.

以 \hat{p}_x 为例,

$$\begin{aligned}\int_{-\infty}^{\infty} \psi^*(\hat{p}_x \phi) dx &= -i\hbar \int_{-\infty}^{\infty} \psi^* \frac{\partial \phi}{\partial x} dx \\ &= -i\hbar \int_{-\infty}^{\infty} d(\psi^* \phi) + i\hbar \int_{-\infty}^{\infty} \frac{\partial \psi^*}{\partial x} \phi dx\end{aligned}$$

不妨令 $\psi(x) = C_1 e^{ik_1 x}$, $\phi(x) = C_2 e^{ik_2 x}$,

$$\begin{aligned}\int_{-\infty}^{\infty} d(\psi^* \phi) &= \int_{-\infty}^{\infty} iC_1^* C_2 (k_2 - k_1) e^{i(k_2 - k_1)x} dx \\ &= 2i\pi C_1^* C_2 (k_2 - k_1) \delta(k_2 - k_1)\end{aligned}$$

对 $\forall k_1, k_2$, $(k_2 - k_1)\delta(k_2 - k_1) = 0$, 所以对 $\forall \psi(x), \phi(x)$,

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

所以 \hat{p}_x 是厄密算符, 同理, \hat{p}_y 和 \hat{p}_z 也是厄密算符

II.

转置算符定义为:

$$(\psi, \hat{A}^T \phi) = (\phi^*, \hat{A} \psi^*)$$

则

$$(\psi, \hat{A}^{T*} \phi) = (\phi^*, \hat{A}^* \psi^*)$$

厄密共轭算符定义为:

$$(\psi, \hat{A}^+ \phi) = (\hat{A} \psi, \phi)$$

因此

$$(\psi, \hat{A}^+ \phi) = (\phi, \hat{A} \psi)^* = (\phi^*, \hat{A}^* \psi^*)$$

即

$$(\psi, \hat{A}^{T*} \phi) = (\psi, \hat{A}^+ \phi)$$

$$\hat{A}^+ = \hat{A}^{T*}$$

III.

$$\vec{r} = r \cdot \vec{e}_r = r \sin \theta \cos \varphi \vec{e}_x + r \sin \theta \sin \varphi \vec{e}_y + r \cos \theta \vec{e}_z$$

$$\begin{cases} \vec{e}_r = \sin \theta \cos \varphi \vec{e}_x + \sin \theta \sin \varphi \vec{e}_y + \cos \theta \vec{e}_z \\ \vec{e}_\theta = \cos \theta \cos \varphi \vec{e}_x + \cos \theta \sin \varphi \vec{e}_y - \sin \theta \vec{e}_z \\ \vec{e}_\varphi = -\sin \varphi \vec{e}_x + \cos \varphi \vec{e}_y \end{cases}$$

代入 $\vec{L} = -i\hbar(e_\varphi \frac{\partial}{\partial \theta} - \vec{e}_\theta \frac{1}{\sin \theta} \frac{\partial}{\partial \varphi})$, 有:

$$\vec{L} = -i\hbar[(-\sin \varphi \frac{\partial}{\partial \theta} - \cot \theta \cos \varphi \frac{\partial}{\partial \varphi})\vec{e}_x + (\cos \varphi \frac{\partial}{\partial \theta} - \cot \theta \sin \varphi \frac{\partial}{\partial \varphi})\vec{e}_y - (\frac{\partial}{\partial \varphi})\vec{e}_z]$$

所以

$$\hat{L}_z = -i\hbar \frac{\partial}{\partial \varphi}$$

IV.

因为 $A^+ = A, B^+ = B$, 所以

$$\frac{1}{2}(AB + BA)^+ = \frac{1}{2}(B^+A^+ + A^+B^+) = \frac{1}{2}(BA + AB) = \frac{1}{2}(AB + BA)$$

$$[\frac{1}{2i}(AB - BA)]^+ = -\frac{1}{2i}(B^+A^+ - A^+B^+) = -\frac{1}{2i}(BA - AB) = \frac{1}{2i}(AB - BA)$$

即 $\frac{1}{2}(AB + BA)$ 和 $-\frac{1}{2i}(AB - BA)$ 均为厄密算符

$$F = \frac{F}{2} + \frac{F}{2} = \frac{1}{2}(F + F^+) + \frac{1}{2}(F - F^+) = F_+ + iF_-$$

而 F_+ 和 F_- 显然均为厄密算符

V.

对于 $\vec{l} = \vec{r} \times \vec{p}$, 有

$$l_x = yp_z - zp_y$$

$$l_x^+ = (yp_z - zp_y)^+ = (p_z^+ y^+ - p_y^+ z^+) = (p_z y - p_y z) = yp_z - zp_y = l_x$$

同理,

$$l_y^+ = l_y, l_z^+ = l_z$$

所以, $\vec{l} = \vec{r} \times \vec{p} = \vec{l}^+$ 是厄密算符

对于 $\vec{r} \cdot \vec{p}$, 有

$$\begin{aligned} (\vec{r} \cdot \vec{p})^+ &= (xp_x + yp_y + zp_z)^+ = p_x^+ x^+ + p_y^+ y^+ + p_z^+ z^+ \\ &= p_x x + p_y y + p_z z \neq xp_x + yp_y + zp_z \end{aligned}$$

所以 $\vec{r} \cdot \vec{p}$ 不是厄密算符, 而

$$(\vec{r} \cdot \vec{p})^+ = \vec{p} \cdot \vec{r} = p_x x + p_y y + p_z z = (xp_x - i\hbar) + (yp_y - i\hbar) + (zp_z - i\hbar) = \vec{r} \cdot \vec{p} - 3i\hbar$$

可构造相应的厄密算符为 $\frac{1}{2}[\vec{r} \cdot \vec{p} + \vec{p} \cdot \vec{r}] = \vec{r} \cdot \vec{p} - 3i\hbar/2$

对于 $\vec{p} \times \vec{l}$,

$$(\vec{p} \times \vec{l})_x^+ = (p_y l_z - p_z l_y)^+ = l_z p_y - l_y p_z = (xp_y - yp_x)p_y - (zp_x - xp_z)p_z = xp_y^2 + xp_z^2 - yp_x p_y - zp_x p_z$$

$$(\vec{p} \times \vec{l})_x = p_y l_z - p_z l_y = p_y(xp_y - yp_x) - p_z(zp_x - xp_z) = xp_y^2 + xp_z^2 - p_y yp_x + p_z zp_x$$

利用 $[x, p] = i\hbar$, 得到

$$\begin{aligned} (\vec{p} \times \vec{l})_x &= xp_y^2 + xp_z^2 - (yp_y - i\hbar)p_x + (zp_z - i\hbar)p_x \\ &= xp_y^2 + xp_z^2 - yp_x p_y - zp_x p_z + 2i\hbar p_x = (\vec{p} \times \vec{l})_x^+ + 2i\hbar p_x \end{aligned}$$

同理,

$$\begin{aligned} (\vec{p} \times \vec{l})_y &= (\vec{p} \times \vec{l})_y^+ + 2i\hbar p_y, \\ (\vec{p} \times \vec{l})_z &= (\vec{p} \times \vec{l})_z^+ + 2i\hbar p_z \end{aligned}$$

所以

$$(\vec{p} \times \vec{l})^+ = \vec{p} \times \vec{l} - 2i\hbar \vec{p}$$

故 $\vec{p} \times \vec{l}$ 不是厄密算符, 但可构造相应的厄密算符为

$$\frac{1}{2}[(\vec{p} \times \vec{l}) + (\vec{p} \times \vec{l})^+] = \vec{p} \times \vec{l} - i\hbar \vec{p}$$

对于 $\vec{r} \times \vec{l}$, 类似的可证明:

$$(\vec{r} \times \vec{l})^+ = \vec{r} \times \vec{l} - 2i\hbar \vec{r}$$

即 $\vec{r} \times \vec{l}$ 也不是厄密算符, 但可构造相应的厄密算符为

$$\frac{1}{2}[(\vec{r} \times \vec{l}) + (\vec{r} \times \vec{l})^+] = \vec{r} \times \vec{l} - i\hbar \vec{r}$$

VI.

$$\begin{aligned} \hat{P}_r &= \frac{1}{2}(\frac{\vec{r}}{r} \cdot \vec{p} + \vec{p} \cdot \frac{\vec{r}}{r}) \\ \hat{P}_r^+ &= \frac{1}{2}(\frac{\vec{r}}{r} \cdot \vec{p} + \vec{p} \cdot \frac{\vec{r}}{r})^+ = \frac{1}{2}[\hat{p}^+ \hat{r}^+ (\frac{1}{r})^+ + (\frac{1}{r})^+ \hat{r}^+ \hat{p}^+] \\ &= \frac{1}{2}(\vec{p} \cdot \frac{\vec{r}}{r} + \frac{\vec{r}}{r} \cdot \vec{p}) = \hat{P}_r \end{aligned}$$

所以 \hat{P}_r 是厄密算符

$$\hat{P}_r = \frac{1}{2}(\frac{\vec{r}}{r} \cdot \vec{p} + \vec{p} \cdot \frac{\vec{r}}{r}) = -\frac{i\hbar}{2}(\vec{\nabla} \cdot \frac{\vec{r}}{r} + \frac{\vec{r}}{r} \cdot \vec{\nabla})$$

对一任意波函数 ψ ,

$$\begin{aligned} \hat{P}_r \psi &= -\frac{i\hbar}{2}[\vec{\nabla} \cdot (\frac{\vec{r}}{r} \psi) + \frac{\vec{r}}{r} \cdot \vec{\nabla} \psi] \\ \vec{\nabla} \cdot (\frac{\vec{r}}{r} \psi) &= \frac{\partial}{\partial x}(x \frac{\psi}{r}) + \frac{\partial}{\partial y}(y \frac{\psi}{r}) + \frac{\partial}{\partial z}(z \frac{\psi}{r}) \end{aligned} \tag{1}$$

又

$$\frac{\partial}{\partial x}(x \frac{\psi}{r}) = \frac{x}{r} \frac{\partial \psi}{\partial x} + \psi \frac{\partial}{\partial x}(\frac{x}{r}) = \frac{x}{r} \frac{\partial \psi}{\partial x} + (\frac{1}{r} - \frac{x^2}{r^3})\psi$$

代入(1)式,

$$\vec{\nabla} \cdot (\frac{\vec{r}}{r} \psi) = \frac{x}{r} \frac{\partial \psi}{\partial x} + \frac{y}{r} \frac{\partial \psi}{\partial y} + \frac{z}{r} \frac{\partial \psi}{\partial z} + [\frac{3}{r} - (\frac{x^2}{r^3} + \frac{y^2}{r^3} + \frac{z^2}{r^3})]\psi$$

$$= \frac{\vec{r}}{r} \cdot \vec{\nabla} \psi + \left(\frac{3}{r} - \frac{r^2}{r^3} \right) \psi = \frac{\vec{r}}{r} \cdot \vec{\nabla} \psi + \frac{2}{r} \psi$$

所以，

$$\vec{\nabla} \cdot \frac{\vec{r}}{r} = \frac{\vec{r}}{r} \cdot \vec{\nabla} + \frac{2}{r}$$

在球坐标中：

$$\vec{\nabla} = \vec{e}_r \frac{\partial}{\partial r} + \vec{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} + \vec{e}_\varphi \frac{1}{r \sin \theta} \frac{\partial}{\partial \varphi}$$

故

$$\vec{r} \cdot \vec{\nabla} = r \frac{\partial}{\partial r}$$

所以，

$$\begin{aligned} \hat{P}_r &= -\frac{i\hbar}{2} \left(\vec{\nabla} \frac{\vec{r}}{r} + \frac{\vec{r}}{r} \cdot \vec{\nabla} \right) = -\frac{i\hbar}{2} \left(2 \frac{\vec{r}}{r} \cdot \vec{\nabla} + \frac{2}{r} \right) \\ &= -i\hbar \left(\frac{\partial}{\partial r} + \frac{1}{r} \right) \end{aligned}$$