

### 6.3 角動量量子化在軌道角動量上的應用

因軌道角動量是角動量中的一種特例，我們將應用上節角動量量子化的結果，來證明軌道角動量  $\hat{L}^2$  之固有值  $\ell(\ell+1)\hbar^2$  中之  $\ell$  必為整數。其固有狀態  $|j, m\rangle$ ，在位置空間上角度部分的振幅或投影值，將可以球面調和函數  $Y_\ell^m(\theta, \varphi)$  來表示，即

$$\langle \theta, \varphi | j, m \rangle = Y_\ell^m(\theta, \varphi) \quad (6.41)$$

其中  $\ell$ 、 $m$  均為整數，且  $-\ell \leq m \leq \ell$ 。

在位置空間  $|\vec{r}\rangle = |x, y, z\rangle = |r, \theta, \varphi\rangle$  中，位置與動量之運算子  $\hat{R}$ 、 $\hat{P}$  分別對應於

$$\hat{R} \rightarrow R, \quad \hat{P} \rightarrow -i\hbar\nabla \quad (6.42)$$

故軌道角動量運算子  $\hat{L} \rightarrow \hat{R} \times \hat{P}$  中各分量，由式(6.3)

$$\hat{L}_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right), \quad \hat{L}_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right), \quad \hat{L}_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right) \quad (6.43)$$

茲以球面坐標  $|r, \theta, \varphi\rangle$ ，而非直角坐標  $|x, y, z\rangle$ ，來表示軌道角動量  $\hat{L}_x$ 、 $\hat{L}_y$ 、 $\hat{L}_z$ ，因

$$x = r\sin\theta\cos\varphi, \quad y = r\sin\theta\sin\varphi, \quad z = r\cos\theta \quad (6.44)$$

其中  $r > 0$ ， $0 \leq \theta \leq \pi$ ， $0 \leq \varphi \leq 2\pi$ ；這是由球面坐標  $r, \theta, \varphi$  表示直角坐標  $x, y, z$  的關係式。又微小體積單元

$$d^3r = r^2 \sin\theta dr d\theta d\varphi = r^2 dr d\Omega \quad (6.45)$$

其中固體角  $d\Omega = \sin\theta d\theta d\varphi$ 。若以  $x, y, z$  表  $r, \theta, \varphi$ ，則有

$$r^2 = x^2 + y^2 + z^2, \quad \cos\theta = \frac{z}{r}, \quad \tan\varphi = \frac{y}{x} \quad (6.46)$$

故

$$\frac{\partial r}{\partial x} = \frac{1}{2}(x^2 + y^2 + z^2)^{-1/2} \cdot 2x = \frac{x}{r} \quad (6.47)$$

$$\text{同理} \quad \frac{\partial r}{\partial y} = \frac{y}{r}, \quad \frac{\partial r}{\partial z} = \frac{z}{r} \quad (6.48)$$

$$\begin{aligned} \text{又} \quad -\sin\theta \frac{\partial\theta}{\partial x} &= \frac{\partial\theta}{\partial x} \frac{\partial}{\partial\theta} \cos\theta = \frac{\partial}{\partial x} \cos\theta = z \frac{\partial}{\partial x} \left( \frac{1}{r} \right) \\ &= -\frac{z}{r^2} \frac{\partial r}{\partial x} = -\frac{zx}{r^3} = -\frac{1}{r} \cdot \frac{z}{r} \cdot \frac{x}{r} = -\frac{1}{r} \cos\theta \sin\theta \cos\varphi \end{aligned} \quad (6.48)$$

$$\text{所以} \quad \frac{\partial\theta}{\partial x} = \frac{\cos\theta \cos\varphi}{r} \quad (6.50)$$

$$\text{同理} \quad -\sin\theta \frac{\partial\theta}{\partial y} = \frac{1}{r} \cos\theta \sin\theta \sin\varphi, \quad -\sin\theta \frac{\partial\theta}{\partial z} = \frac{1}{r} (1 - \cos^2\theta) \quad (6.51)$$

$$\text{故} \quad \frac{\partial\theta}{\partial y} = \frac{\cos\theta \sin\varphi}{r}, \quad \frac{\partial\theta}{\partial z} = -\frac{\sin\theta}{r} \quad (6.52)$$

$$\text{而} \quad \sec^2\varphi \frac{\partial\varphi}{\partial x} = \frac{\partial}{\partial x} \tan\varphi = y \frac{\partial}{\partial x} \left( \frac{1}{x} \right) = -\frac{y}{x^2} \quad (6.53)$$

$$\text{因此} \quad \frac{\partial\varphi}{\partial x} = -\frac{y}{x^2} \cos^2\varphi \quad (6.54)$$

$$\text{同理} \quad \frac{\partial\varphi}{\partial y} = -\frac{\cos^2\varphi}{x}, \quad \frac{\partial\varphi}{\partial z} = 0 \quad (6.55)$$

利用以上的結果，可將對直角坐標  $x, y, z$  之偏導數，全部轉成對球面坐標  $r, \theta, \varphi$  之偏導數：

$$\frac{\partial}{\partial x} = \frac{\partial r}{\partial x} \frac{\partial}{\partial r} + \frac{\partial\theta}{\partial x} \frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial x} \frac{\partial}{\partial\varphi} = \frac{x}{r} \frac{\partial}{\partial r} + \frac{\cos\theta \cos\varphi}{r} \frac{\partial}{\partial\theta} - \frac{y}{x^2} \cos^2\varphi \frac{\partial}{\partial\varphi} \quad (6.56)$$

$$\frac{\partial}{\partial y} = \frac{\partial r}{\partial y} \frac{\partial}{\partial r} + \frac{\partial\theta}{\partial y} \frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial y} \frac{\partial}{\partial\varphi} = \frac{y}{r} \frac{\partial}{\partial r} + \frac{\cos\theta \sin\varphi}{r} \frac{\partial}{\partial\theta} + \frac{\cos^2\varphi}{x} \frac{\partial}{\partial\varphi} \quad (6.57)$$

$$\frac{\partial}{\partial z} = \frac{\partial r}{\partial z} \frac{\partial}{\partial r} + \frac{\partial\theta}{\partial z} \frac{\partial}{\partial\theta} + \frac{\partial\varphi}{\partial z} \frac{\partial}{\partial\varphi} = \frac{z}{r} \frac{\partial}{\partial r} - \frac{\sin\theta}{r} \frac{\partial}{\partial\theta} \quad (6.58)$$

再利用式(6.43)，遂可用  $r, \theta, \varphi$  表示出角動量在直角坐標分量之運算子形式

$$\begin{aligned}
\hat{L}_x &= -i\hbar \left( y \frac{\partial}{\partial z} - z \frac{\partial}{\partial y} \right) \\
&= -i\hbar \left( \frac{yz}{r} \frac{\partial}{\partial r} - \frac{y \sin \theta}{r} \frac{\partial}{\partial \theta} - \frac{yz}{r} \frac{\partial}{\partial r} - \frac{z \cos \theta \sin \varphi}{r} \frac{\partial}{\partial \theta} - \frac{z \cos^2 \varphi}{x} \frac{\partial}{\partial \varphi} \right) \\
&= i\hbar \left( \sin \varphi \frac{\partial}{\partial \theta} + \frac{\cos \varphi}{\tan \theta} \frac{\partial}{\partial \varphi} \right) \tag{6.59}
\end{aligned}$$

$$\begin{aligned}
\hat{L}_y &= -i\hbar \left( z \frac{\partial}{\partial x} - x \frac{\partial}{\partial z} \right) \\
&= -i\hbar \left( \frac{xz}{r} \frac{\partial}{\partial r} - \frac{z \cos \theta \cos \varphi}{r} \frac{\partial}{\partial \theta} - \frac{yz}{x^2} \cos^2 \varphi \frac{\partial}{\partial \varphi} - \frac{xz}{r} \frac{\partial}{\partial r} + \frac{x \sin \theta}{r} \frac{\partial}{\partial \theta} \right) \\
&= i\hbar \left( -\cos \varphi \frac{\partial}{\partial \theta} + \frac{\sin \varphi}{\tan \theta} \frac{\partial}{\partial \varphi} \right) \tag{6.60}
\end{aligned}$$

$$\begin{aligned}
\hat{L}_z &= -i\hbar \left( x \frac{\partial}{\partial y} - y \frac{\partial}{\partial x} \right) \\
&= -i\hbar \left( \frac{xy}{r} \frac{\partial}{\partial r} + \frac{x \cos \theta \sin \varphi}{r} \frac{\partial}{\partial \theta} \right. \\
&\quad \left. + \frac{x \cos^2 \varphi}{x} \frac{\partial}{\partial \varphi} - \frac{xy}{r} \frac{\partial}{\partial r} - \frac{y \cos \theta \cos \varphi}{r} \frac{\partial}{\partial \theta} + \frac{y^2}{x^2} \cos^2 \varphi \frac{\partial}{\partial \varphi} \right) \\
&= -i\hbar \frac{\partial}{\partial \varphi} \tag{6.61}
\end{aligned}$$

因此得到

$$\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2 = -\hbar^2 \left( \frac{\partial^2}{\partial \theta^2} + \frac{1}{\tan \theta} \frac{\partial}{\partial \theta} + \frac{1}{\sin^2 \theta} \frac{\partial^2}{\partial \varphi^2} \right) \tag{6.62}$$

$$\hat{L}_+ = \hat{L}_x + i\hat{L}_y = \hbar e^{i\varphi} \left( \frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \varphi} \right) \tag{6.63}$$

$$\hat{L}_- = \hat{L}_x - i\hat{L}_y = \hbar e^{-i\varphi} \left( -\frac{\partial}{\partial \theta} + i \cot \theta \frac{\partial}{\partial \varphi} \right) \tag{6.64}$$

已知  $\hat{L}$  滿足角動量的定義(6.4)~(6.5)，故由角動量量子化定理 6.1，所作用的狀態空間裡， $\hat{L}^2$  和  $\hat{L}_z$  享有共同之固有狀態  $|\ell, m\rangle$ ，並可給出對應之固有值  $\ell(\ell+1)\hbar^2$  與  $m\hbar$ 。