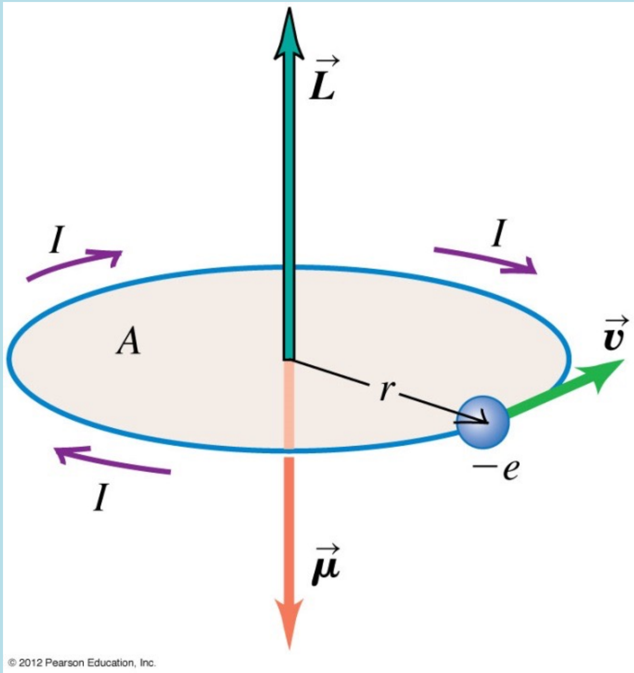
Angular momenta operators



兩物理量若不能同時精準測量，那兩個量的不準度就不能同時為零。

$$\hat{x}\cdot\hat{p}-\hat{p}\cdot\hat{x}\equiv[\hat{x},\hat{p}]=i\hbar$$

$$\Delta x\cdot\Delta p\geq\hbar$$

Supplement 5-A

Uncertainty Relations

In our discussion of wave packets in Chapter 2, we noted that there is a relationship between the *spread* of a function and its Fourier transform. When the de Broglie correspondence between wave number and momentum is made, the relationship takes the form

$$\Delta p\,\Delta x\geq\hbar$$

$$(\Delta A)^2(\Delta B)^2\geq\frac{1}{4}\langle i[A,B]\rangle^2 \qquad (5A\text{-}11)$$

For the operators p and x for which

$$[p,x]=-i\hbar \qquad (5A\text{-}12)$$

this leads to

$$\Delta p\,\Delta x\geq\frac{\hbar}{2} \qquad (5A\text{-}13)$$

兩個物理量是否對易 commute，關係重大！

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

動量與位置就不能同時精準測量！

測量要得到完全確定結果，要在本徵態！

因此，動量與位置沒有共同的本徵態！

兩個物理量能否同時精確測量，真的就由它們是否對易決定！

$$[\hat{A}, \hat{B}] \neq 0$$

這兩物理量不能同時精準測量。

它們沒有共同的本徵態。

$$[\hat{A}, \hat{B}] = 0$$

這兩物理量能同時精準測量。

它們有共同的本徵態！

$$\left[\frac{p^2}{2m}, p\right] = 0$$

動能與動量可以同時精準測量。

$$[y, p_x] = 0$$

y與x方向動量可以同時精準測量。

定理：若$[\hat{A},\hat{B}]=0$，$\hat{A}$的本徵態$|\psi_a\rangle$也會是$\hat{B}$的本徵態。

證明：$\hat{A}$的本徵態$|\psi_a\rangle$滿足： $\hat{A}|\psi_a\rangle = a|\psi_a\rangle$

考慮狀態$\hat{B}|\psi_a\rangle$，再計算算子$\hat{A}$對$\hat{B}|\psi_a\rangle$的作用：

$$\hat{A}(\hat{B}|\psi_a\rangle) = \hat{A}\hat{B}|\psi_a\rangle = \hat{B}\hat{A}|\psi_a\rangle = \hat{B}a|\psi_a\rangle = a\cdot\hat{B}|\psi_a\rangle$$

因此狀態$\hat{B}|\psi_a\rangle$也是$\hat{A}$算子的本徵態，本徵值亦為a。

一般來說，若無簡併，一個本徵值對應一個本徵態，或相差一係數乘積。

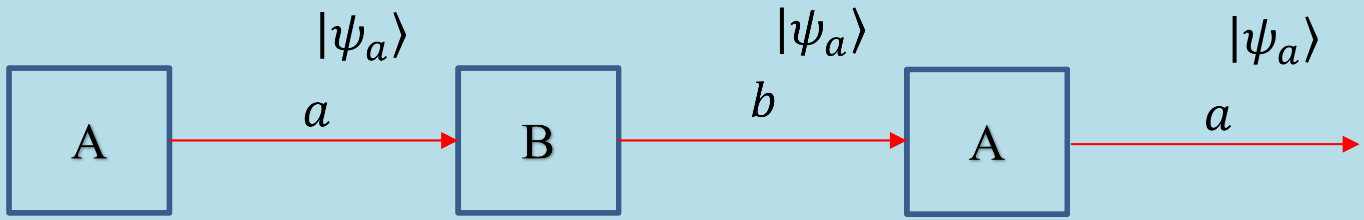
如果狀態$\hat{B}|\psi_a\rangle$與$|\psi_a\rangle$都是$\hat{A}$算子本徵值為a的本徵態，

$\hat{B}|\psi_a\rangle$必須正比於$|\psi_a\rangle$，設比例常數為b，則：

$\hat{B}|\psi_a\rangle = b|\psi_a\rangle$ 此式顯示 $|\psi_a\rangle$ 也是 $\hat{B}$ 的本徵態，本徵值為 b 。得證！

結論： $\hat{A}$的本徵態也會是$\hat{B}$的本徵態，因此$\hat{A}$與$\hat{B}$可以同時精準測量。

$$[\hat{A},\hat{B}] = 0$$

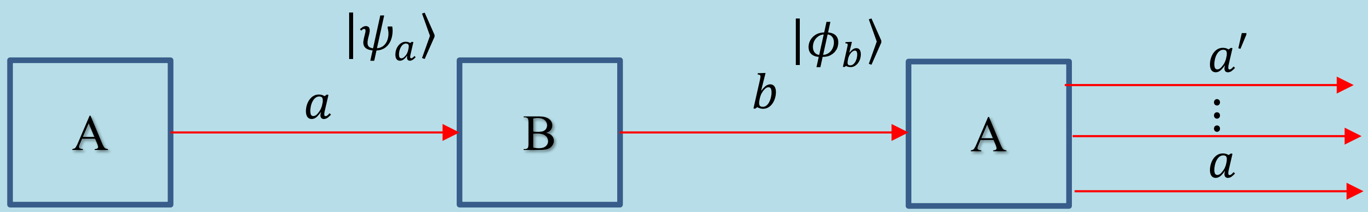


$\hat{A}$若測得a，狀態會崩潰為本徵態$|\psi_a\rangle$。

$|\psi_a\rangle$同時也是$\hat{B}$的本徵態。測時結果確定，且無崩潰，依舊還是$|\psi_a\rangle$。

$|\psi_a\rangle$再測一次$\hat{A}$只能得到a。

$$[\hat{A},\hat{B}] \neq 0$$



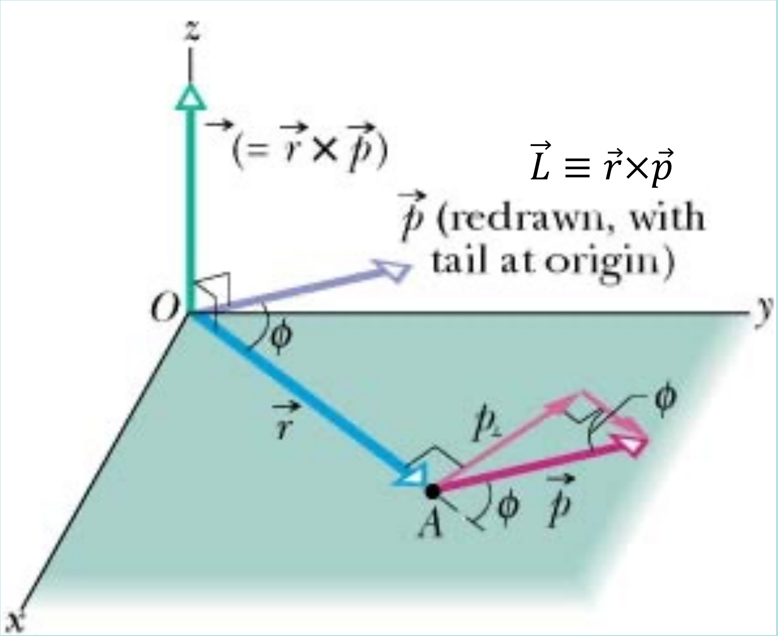
$|\psi_a\rangle$只是$\hat{A}$的本徵態，不是$\hat{B}$的本徵態。

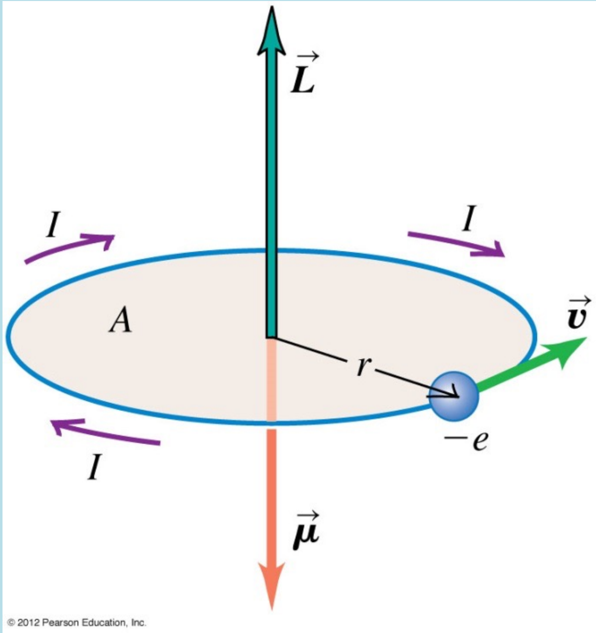
$\hat{B}$若測得b ，狀態會崩潰為$\hat{B}$本徵態$|\phi_b\rangle$。$\hat{B}$測量改變了粒子的$\hat{A}$的狀態。

$|\phi_b\rangle$可能包含所有$\hat{A}$的本徵態，是一基底展開，

原則上第二個$\hat{A}$測量所有結果都可能。

現在我們正式由一維進入三維：





$\vec{\tau} = \dfrac{d\vec{L}}{dt}$ 力矩等於角動量的變化率。

$\vec{L} \equiv \vec{r}\times\vec{p}$ 一個粒子的角動量

若$\vec{\tau} = 0$，則角動量$\vec{L}$守恆。

若是帶電粒子，其磁偶極矩會與角動量成正比

量磁偶極矩就是量角動量！

假設三度空間，動量算子依舊可以以空間座標微分代表！

$$\vec{p} = (p_x, p_y, p_z) = \left(-i\hbar\frac{\partial}{\partial x}, -i\hbar\frac{\partial}{\partial y}, -i\hbar\frac{\partial}{\partial z}\right)$$

那麼不同方向位置與動量就是對易的了。例如：

$$(\hat{x}\cdot\hat{p}_y - \hat{p}_y\cdot\hat{x})\psi(x) = -i\hbar x\frac{d\psi}{dy} - \left(-i\hbar\frac{\partial}{\partial y}\right)[x\cdot\psi(x)] = 0$$

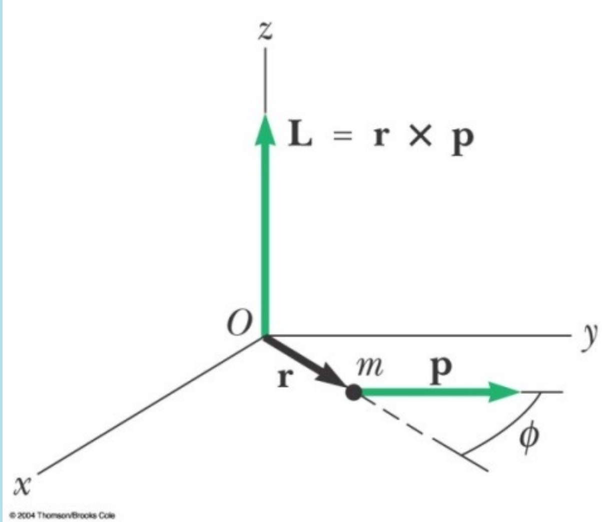
$$[x, p_y] = \cdots = 0$$

$$[x, y] = \cdots = 0$$

$$[p_x, p_y] = \cdots = 0$$

角動量算子

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



$$L_z = xp_y - yp_x$$

$$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$$

量子角動量的定義非常清楚！

$$L_x = yp_z - zp_y$$

$$L_y = zp_x - xp_z$$

$$L_x = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

$$L_y = -i\hbar\left(z\frac{\partial}{\partial x} - x\frac{\partial}{\partial z}\right)$$

此量與粒子的位置變化相關，將稱為Orbital 軌道角動量算子。

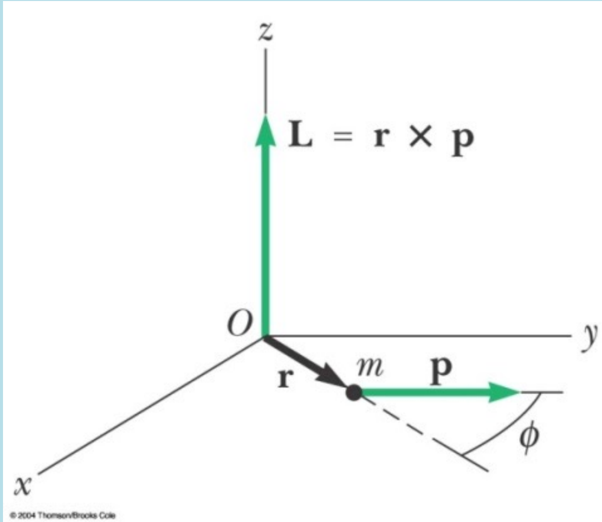
角動量算子

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

$L_x = yp_z - zp_y$

$L_y = zp_x - xp_z$

$L_z = xp_y - yp_x$



$[x, p_x] = [y, p_y] = [z, p_z] = i\hbar$

其餘都對易！

計算角動量分量彼此的對易子：　　　只有$[x, p_x] = i\hbar$，其餘都對易！

$$[L_y, L_z] = [(zp_x - xp_z), (xp_y - yp_x)] = [zp_x, xp_y] + [xp_z, yp_x]$$

$$= [zp_x, x]p_y + y[xp_z, p_x] = z[p_x, x]p_y + y[x, p_x]p_z = i\hbar(-zp_y + yp_z) = i\hbar L_x$$

$[L_y, L_z] = i\hbar L_x$

這兩物理量L_y,L_z不能同時測量。

$[A, BC] = [A, B]C + B[A, C]$

$[AB, C] = A[B, C] + [A, C]B$

同時：

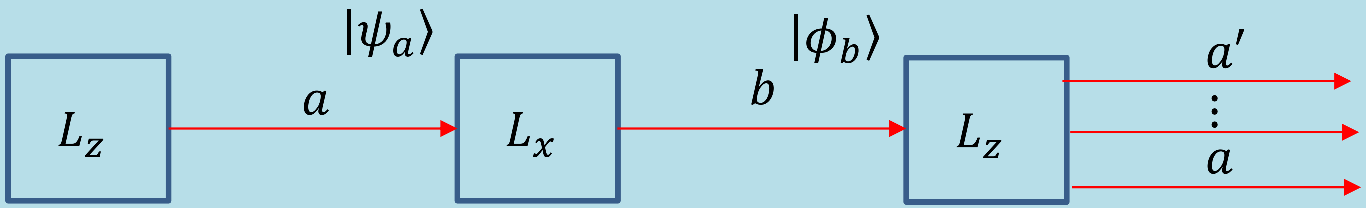
$[L_z, L_x] = i\hbar L_y$

$[L_x, L_y] = i\hbar L_z$

角動量任兩個分量都不能同時測量。

$$[L_z, L_x] = i\hbar L_y \neq 0$$

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



$|\psi_a\rangle$只是L_z的本徵態，不是L_x的本徵態。

L_x若測得b ，狀態會崩潰為L_x本徵態$|\phi_b\rangle$。L_x測量改變了粒子的L_z狀態。

$|\phi_b\rangle$可能包含所有L_z的本徵態，是一基底展開，。

原則上第二個L_z測量所有結果都可能

角動量任兩個分量都不對易。

但沒想到角動量任一個分量都與角動量大小L^2對易。

$[L_y, L_z] = i\hbar L_x$ $[L_z, L_x] = i\hbar L_y$ $[L_x, L_y] = i\hbar L_z$

$$[L^2, L_z] = [L_x^2 + L_y^2 + L_z^2, L_z] = 0$$

$$[AB, C] = A[B, C] + [A, C]B$$

$$[L_x^2 + L_y^2 + L_z^2, L_z] = [L_x^2, L_z] + [L_y^2, \hat{L}_z]$$

$$= L_x[L_x, L_z] + [L_x, L_z]L_x + L_y[L_y, L_z] + [L_y, L_z]L_y$$

$$= -i\hbar L_x L_y - i\hbar L_y L_x + i\hbar L_y L_x + i\hbar L_x L_y = 0$$

$$[L^2, L_z] = 0 = [L^2, L_x] = [L^2, L_y]$$

因此L^2 可以與任一分量、但僅一個分量有共同的本徵函數。

選擇L^2及L_z共同的本徵態，記為：$|a, m\rangle$， $a\hbar^2$及$m\hbar$為其本徵值。

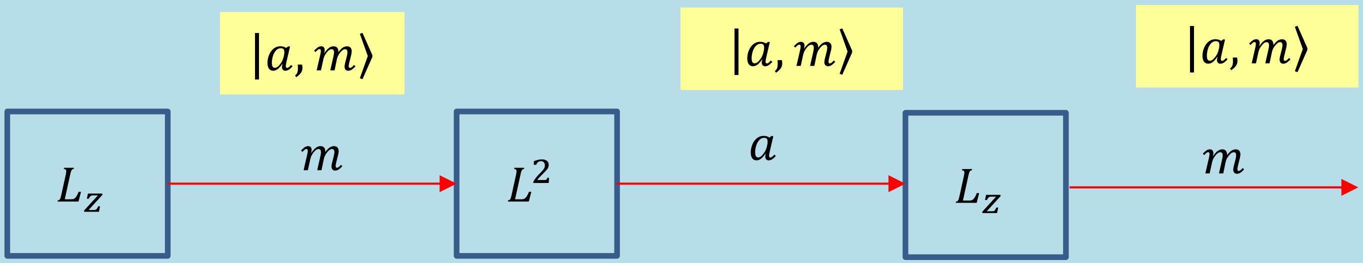
$$L^2|a, m\rangle = a\hbar^2 \cdot |a, m\rangle$$

$$L_z|a, m\rangle = m\hbar \cdot |a, m\rangle$$

Spherical Harmonics $|a, m\rangle \sim Y_{am}(\theta, \phi)$

別忘了$|a, m\rangle$就是一個位置波函數，最好以極座標 θ, ϕ 表示。記為Y_{am}。

$$[L^2, L_z] = 0$$



L_z若測得m，狀態會崩潰為本徵態$|a, m\rangle$。

$|a, m\rangle$同時也是L^2的本徵態。測時結果確定為a，

且無崩潰，依舊還是$|a, m\rangle$。

$|a, m\rangle$再測一次L_z只能得到m。

以上角動量分量與大小的對易關係竟然可以讓我們決定可能的本徵值！

$[L_z, L_x] = i\hbar L_y$ $+$ $[L_z, L_y] = -i\hbar L_x$ $\times i$

$$[L_z, L_x + iL_y] = \hbar(L_x + iL_y)$$

$$[L_z, L_x - iL_y] = -\hbar(L_x - iL_y)$$

定義算子：$L_+ \equiv L_x + iL_y$ $L_- \equiv L_+^\dagger = L_x - iL_y$

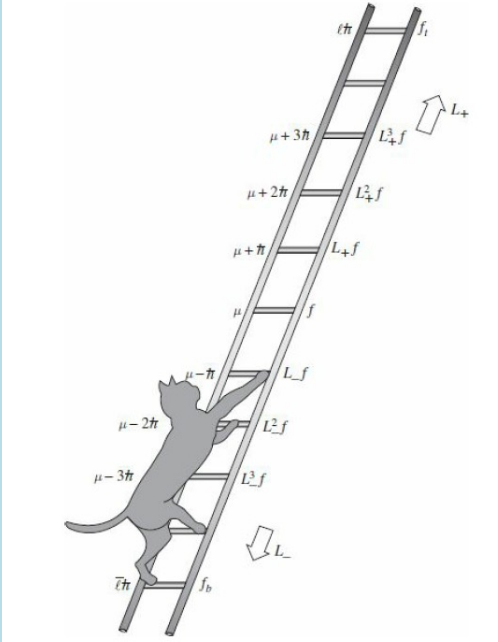


Figure 4.11: The "ladder" of angular momentum states.

上式可以簡化為：

$[L_z, L_+] = \hbar \cdot L_+$ $[L_z, L_-] = -\hbar \cdot L_-$

$[H, a^\dagger] = \hbar\omega \cdot a^\dagger$

$[H, a] = -\hbar\omega \cdot a$

這兩式與量子彈簧中H與$a^\dagger$的對易關係完全相同！

$a^\dagger$ a H

$\Updownarrow$

L_+ L_- L_z

$a^\dagger$ a H

$\Updownarrow$

L_+ L_- L_z

$[L_z, L_+] = \hbar L_+$ $[L_z, L_-] = -\hbar L_-$

將L_+作用於任一L_z的本徵態$|a, m\rangle$：$L_+|a, m\rangle$竟又是一L_z本徵態：

$$L_z L_+|a, m\rangle = (L_+ L_z + \hbar L_+)|a, m\rangle$$

$$= m\hbar \cdot L_+|a, m\rangle + \hbar L_+|a, m\rangle = (m+1)\hbar \cdot L_+|a, m\rangle$$

$$L_z \cdot L_+|a, m\rangle = (m+1)\hbar \cdot L_+|a, m\rangle$$

$$L_z \cdot L_-|a, m\rangle = (m-1)\hbar \cdot L_-|a, m\rangle$$

$L_\pm$可以增加及減少L_z的本徵值一個量子$\hbar$。

本徵態$L_\pm|a, m\rangle$的本徵值為$(m \pm 1)\hbar$，但它是L^2的本徵態嗎？

$[L^2, L_x] = [L^2, L_y] = 0$

$L_\pm \equiv L_x \pm iL_y$

因此： $[L^2, L_\pm] = 0$

$L_+|a,m\rangle$，也是L^2本徵態：

$$L^2 L_+|a,m\rangle = L_+ L^2|a,m\rangle = a\hbar^2 \cdot L_+|a,m\rangle$$

本徵值不變，依舊是$a\hbar^2$。

$L_+|a,m\rangle$同時是L^2及L_z的本徵態，L_z的本徵值$m+1$，L^2本徵值$a\hbar^2$：

$$L_+|a,m\rangle \sim |a,m+1\rangle$$

同理：$L_-|a,m\rangle \sim |a,m-1\rangle$

$L_\pm$可以增加及減少L_z的本徵值一個量子$\hbar$。維持L^2本徵值不變！

L_z的本徵值是量子化的。一個量子是$\hbar$。

特定的a

$L_+|a,m\rangle \sim |a,m+1\rangle$

$L_-|a,m\rangle \sim |a,m-1\rangle$

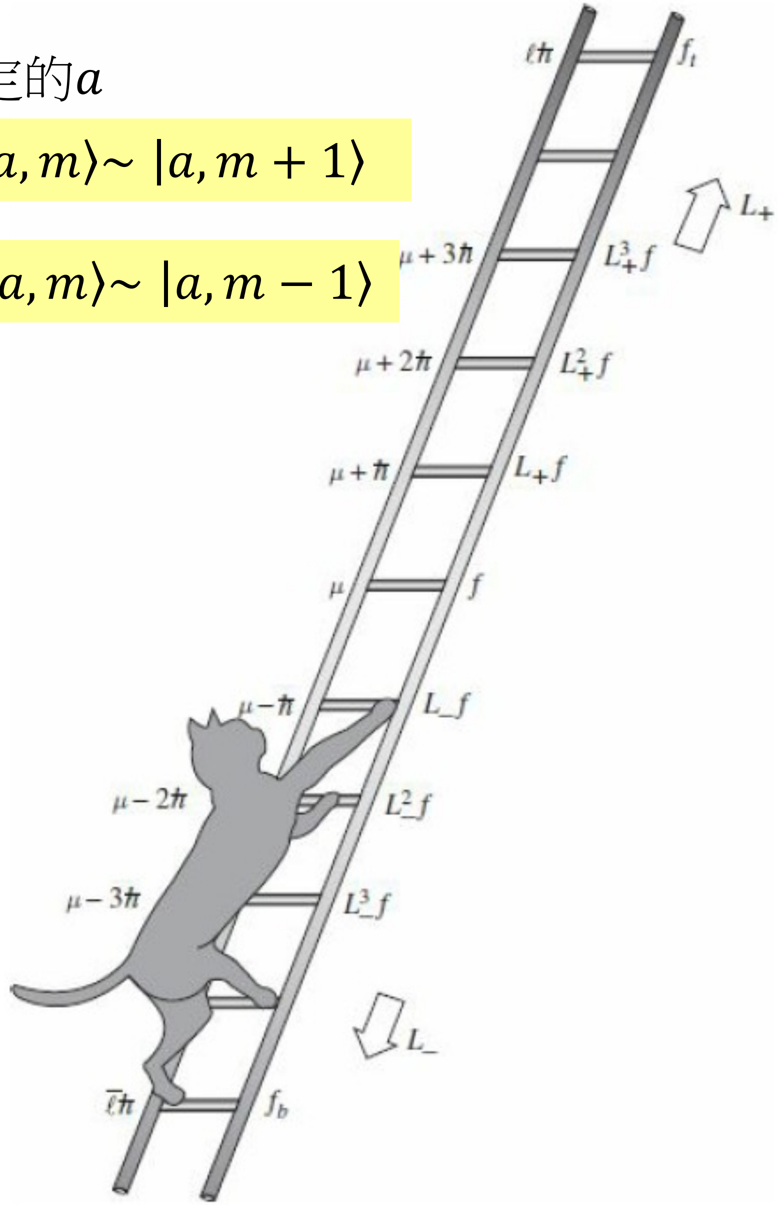


Figure 4.11: The "ladder" of angular momentum states.

將特定的a所對應的$|a, m\rangle$收集起來，

對特定的a，角動量大小是有限的，L_+增加L_z的本徵值不能無限制地繼續，

$|a, m\rangle$容許的m一定有一極大值$m_{\max}$。這不同於SHO的能量。

$$L_+|a, m_{\max}\rangle = 0 \qquad L_-L_+|a, m_{\max}\rangle = 0$$

$$L_-L_+ = (L_x - iL_y)(L_x + iL_y) = L_x^2 + L_y^2 + iL_xL_y - iL_yL_x$$

$$= L_x^2 + L_y^2 + i[L_x, L_y] = L^2 - L_z^2 - \hbar L_z$$

$$L_-L_+|a, m_{\max}\rangle = (L^2 - L_z^2 - \hbar L_z)|a, m_{\max}\rangle = 0$$

$$(a\hbar^2 - m_{\max}^2\hbar^2 - \hbar^2 m_{\max})|a, m_{\max}\rangle = 0$$

$$a = m_{\max}^2 + m_{\max}$$

特定的a，$|a,m\rangle$容許的m也一定有一極小值$m_{\min}$

$$L_-|a,m_{\min}\rangle = 0 \qquad L_+L_-|a,m_{\min}\rangle = 0$$

$$L_+L_- = (L_x + iL_y)(L_x - iL_y) = L_x^2 + L_y^2 - iL_xL_y + iL_yL_x$$

$$= L_x^2 + L_y^2 - i[L_x, L_y] = L^2 - L_z^2 + \hbar L_z$$

$$L_+L_-|a,m_{\min}\rangle = (L^2 - L_z^2 + \hbar L_z)|a,m_{\min}\rangle = 0$$

$$(a\hbar^2 - m_{\min}^2\hbar^2 + \hbar^2 m_{\min})|a,m_{\min}\rangle = 0$$

$$a = m_{\min}^2 - m_{\min}$$

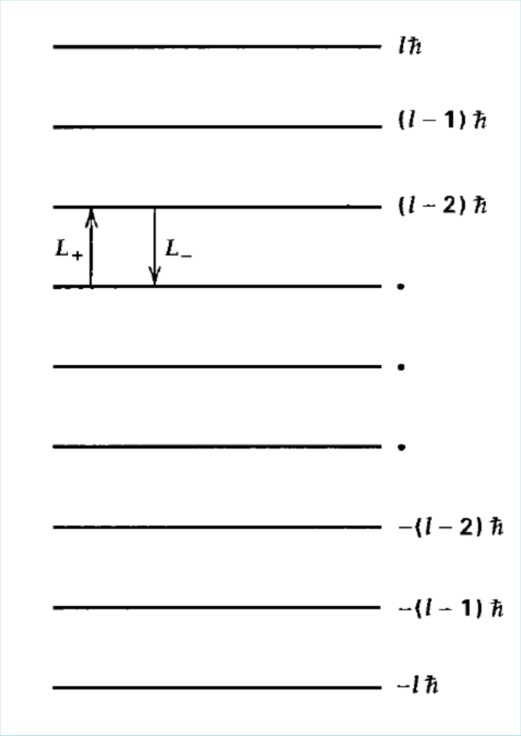
前一頁已經得到：

$$a = m_{\max}^2 + m_{\max}$$

兩式要同時成立，唯一可能： $m_{\max} = -m_{\min} \equiv l$

因此： $m = -l, -l+1, \cdots l-1, l$ $\qquad |m| \le l \qquad 2l$ 必須是整數

而且： $a = l^2 + l = l(l+1)$ $\qquad L^2$的本徵值是量子化的，等於$l(l+1)$ 。



L^2及L_z共同的本徵函數可以以量子數l來歸類：$|l(l+1),m\rangle \to |l,m\rangle$

$L^2|l,m\rangle = l(l+1)\hbar^2 \cdot |l,m\rangle$

$L_z|l,m\rangle = m\hbar \cdot |l,m\rangle$

$|l,m\rangle \sim Y_{lm}(\theta,\phi)$

一個l就有一個階梯！

階梯有最高階、也有最低階！

階梯數目等於$2l+1$！

$2l$必須是整數，因此l是自然數，

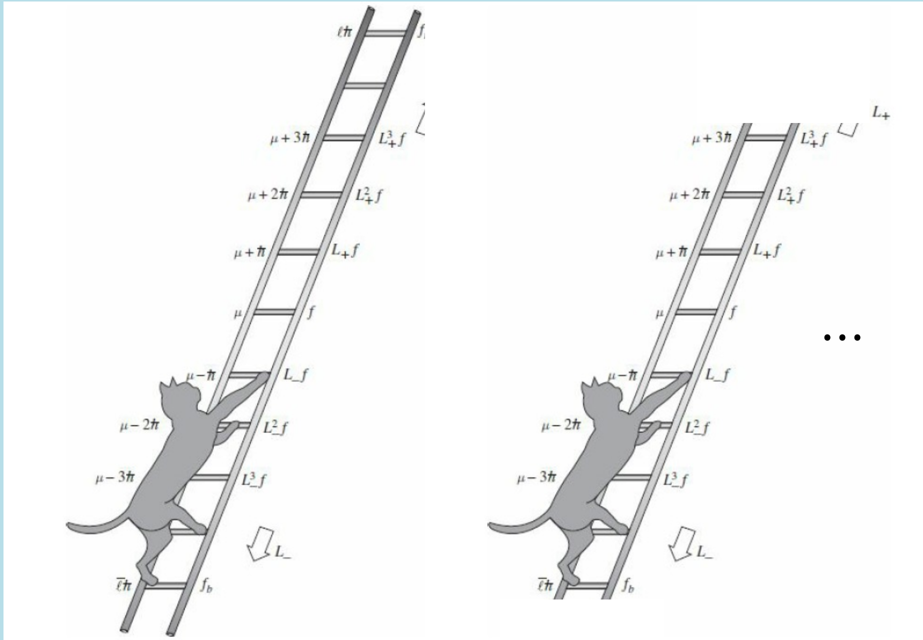
$l = 0,1,2,3\cdots$

$m = -l, -l+1, \cdots -1,0,1 \cdots l-1, l$

或l是半自然數：

$l = \frac{1}{2}, \frac{3}{2}, \frac{5}{2}, \cdots$

$m = -l, -l+1, \cdots -\frac{1}{2}, \frac{1}{2}, \cdots l-1, l$



m沒有0的可能，繞z軸不能不轉！

接下來會發現粒子位置變化產生的角動量$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$，$l$不能是半整數。

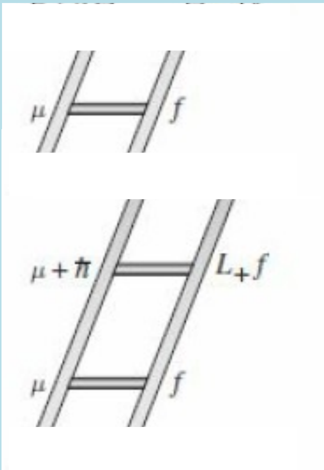
但若有其他不是位置變化產生的角動量，也滿足一樣的對易關係$[L_x, L_y] = i\hbar L_z$，l就可能是半自然數。

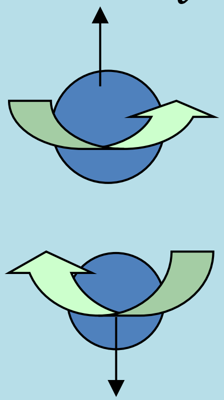
角動量大小經常是守恆的，收集特定l的角動量本徵態$|l,m\rangle$，
並以它們為基底組成線性空間，會是非常有用的。

$m=-l,-l+1,\cdots l-1,l$

$|0,0\rangle$

$l=0$

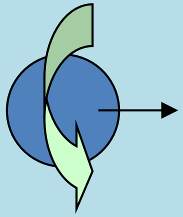




$\left|\frac{1}{2},\frac{1}{2}\right\rangle$

$\left|\frac{1}{2},-\frac{1}{2}\right\rangle$

$l=\frac{1}{2}$ 對應自旋

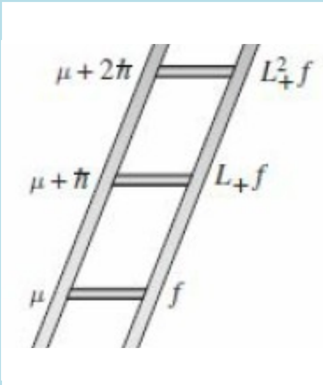


沒有$L_Z=0$這個狀態

$|1,1\rangle$

$|1,0\rangle$

$|1,-1\rangle$



$l=1$

整數l的本徵態有奇數個。

$\left|\frac{3}{2},\frac{3}{2}\right\rangle$

$\left|\frac{3}{2},\frac{1}{2}\right\rangle$

$\left|\frac{3}{2},-\frac{1}{2}\right\rangle$

$\left|\frac{3}{2},-\frac{3}{2}\right\rangle$

$l=\frac{3}{2}$

半整數l的本徵態有偶數個。

$$L_+|l,m\rangle \equiv |L_+Y_{l,m}\rangle \sim |l,m+1\rangle$$

$$\langle\phi|\hat{A}|\psi\rangle = (\langle\hat{A}^\dagger\phi|)\cdot|\psi\rangle$$

如同SHO，這個態$L_+|l,m\rangle$，不滿足歸一化條件，向量長不為一。

$$\langle L_+Y_{l,m}|L_+Y_{l,m}\rangle =$$

$$\langle\phi|\hat{A}^\dagger|\psi\rangle = (\langle\hat{A}\phi|)\cdot|\psi\rangle$$

$$\langle l,m|L_+^\dagger\cdot L_+|l,m\rangle = \langle l,m|L_-\cdot L_+|l,m\rangle = \langle l,m|(L^2 - L_z^2 - \hbar L_z)|l,m\rangle$$

$$= [l(l+1) - m^2 - m]\hbar^2\langle l,m|l,m\rangle = (l-m)(l+m+1)\hbar^2$$

若要得歸一化的$|a,m+1\rangle$，必須將$L_+|l,m\rangle$除以向量長$\sqrt{(l-m)(l+m+1)}\hbar$。

因此：

$$|l,m+1\rangle = \frac{1}{\sqrt{(l-m)(l+m+1)}\hbar}L_+|l,m\rangle$$

$$L_+|l,m\rangle = \sqrt{(l-m)(l+m+1)}\hbar|l,m+1\rangle$$

同理：

$$|l,m-1\rangle = \frac{1}{\sqrt{(l+m)(l-m+1)}\hbar}L_-|l,m\rangle$$

$$L_-|l,m\rangle = \sqrt{(l+m)(l-m+1)}\hbar|l,m-1\rangle$$

這兩個公式雖然複雜，卻非常有用。

可以計算期望值。

$$L_+ \equiv L_x + iL_y$$

$$L_- \equiv L_x - iL_y$$

$$L_+|l,m\rangle = \sqrt{(l-m)(l+m+1)}\hbar|l,m+1\rangle$$

$$L_-|l,m\rangle = \sqrt{(l+m)(l-m+1)}\hbar|l,m-1\rangle$$

練習：計算

$$\langle 0,0|L_x^2|0,0\rangle$$

$$L_x^2 = \left(\frac{L_- + L_+}{2}\right)\left(\frac{L_- + L_+}{2}\right)$$

$$\langle 0,0|L_x^2|0,0\rangle = \frac{1}{4}\langle 0,0|(L_-L_- + L_+L_+ + L_-L_+ + L_+L_-)|0,0\rangle$$

$$L_{+,-}|0,0\rangle = 0$$

練習：計算

$$\left\langle \frac{1}{2},\frac{1}{2}\middle| L_x^2 \middle| \frac{1}{2},\frac{1}{2}\right\rangle$$

$$L_+|l,m\rangle = \sqrt{(l-m)(l+m+1)}\hbar|l,m+1\rangle$$

$$L_-|l,m\rangle = \sqrt{(l+m)(l-m+1)}\hbar|l,m-1\rangle$$

$$L_x^2 = \left(\frac{L_- + L_+}{2}\right)\left(\frac{L_- + L_+}{2}\right)$$

$$\left\langle \frac{1}{2},\frac{1}{2}\middle| L_x^2 \middle| \frac{1}{2},\frac{1}{2}\right\rangle = \frac{1}{4}\left\langle \frac{1}{2},\frac{1}{2}\middle| (\cancel{L_-L_-} + \cancel{L_+L_+} + \cancel{L_-L_+} + L_+L_-) \middle| \frac{1}{2},\frac{1}{2}\right\rangle$$

$$L_-\left|\frac{1}{2},\frac{1}{2}\right\rangle = \sqrt{\left(\frac{1}{2}+\frac{1}{2}\right)\left(\frac{1}{2}-\frac{1}{2}+1\right)}\hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle$$

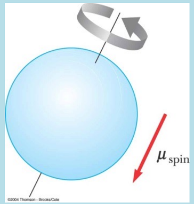
$$L_-\left|\frac{1}{2},\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle$$

$$L_+\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \sqrt{\left(\frac{1}{2}-\frac{-1}{2}\right)\left(\frac{1}{2}+\frac{-1}{2}+1\right)}\hbar\left|\frac{1}{2},\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},\frac{1}{2}\right\rangle$$

$$L_+\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},\frac{1}{2}\right\rangle$$

$$\left\langle \frac{1}{2},\frac{1}{2}\middle| L_x^2 \middle| \frac{1}{2},\frac{1}{2}\right\rangle = \frac{1}{4}\left\langle \frac{1}{2},\frac{1}{2}\middle| L_+L_- \middle| \frac{1}{2},\frac{1}{2}\right\rangle = \frac{\hbar^2}{4}\left\langle \frac{1}{2},\frac{1}{2}\middle| \frac{1}{2},\frac{1}{2}\right\rangle = \frac{\hbar^2}{4}$$

$l=\frac{1}{2}$有兩個本徵態！算子的作用如下：　$\left|\frac{1}{2},\frac{1}{2}\right\rangle, \left|\frac{1}{2},-\frac{1}{2}\right\rangle$



$$L_+\left|\frac{1}{2},\frac{1}{2}\right\rangle = 0 \qquad L_+\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},\frac{1}{2}\right\rangle$$

$$L_-\left|\frac{1}{2},\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle \qquad L_-\left|\frac{1}{2},-\frac{1}{2}\right\rangle = 0$$

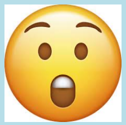
取為基底，算子的作用將基底變換為另一基底或零。這是二維空間的線性變換。若以兩個基底行向量代表此兩個本徵態，算子應該可以視為矩陣：

$$\left|\frac{1}{2},\frac{1}{2}\right\rangle = \begin{pmatrix}1\\0\end{pmatrix} \qquad \left|\frac{1}{2},-\frac{1}{2}\right\rangle = \begin{pmatrix}0\\1\end{pmatrix}$$

$$L_+ = \hbar\begin{pmatrix}0&1\\0&0\end{pmatrix} \qquad \hbar\begin{pmatrix}0&1\\0&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = 0 \qquad \hbar\begin{pmatrix}0&1\\0&0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = \hbar\begin{pmatrix}1\\0\end{pmatrix}$$

角動量算子運作於ket得到一ket，可看成矩陣乘上行向量，得到一個行向量。

$$L_- = \hbar\begin{pmatrix}0&0\\1&0\end{pmatrix} \qquad \hbar\begin{pmatrix}0&0\\1&0\end{pmatrix}\begin{pmatrix}1\\0\end{pmatrix} = \hbar\begin{pmatrix}0\\1\end{pmatrix} \qquad \hbar\begin{pmatrix}0&0\\1&0\end{pmatrix}\begin{pmatrix}0\\1\end{pmatrix} = 0$$

算子在這裡其實就是矩陣！ 

$$L_+\left|\frac{1}{2},\frac{1}{2}\right\rangle = 0$$

$$L_+\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},\frac{1}{2}\right\rangle$$

$$L_-\left|\frac{1}{2},\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle$$

$$L_-\left|\frac{1}{2},-\frac{1}{2}\right\rangle = 0$$

$$\hbar\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = 0$$

$$\hbar\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}\begin{pmatrix}0\\ 1\end{pmatrix} = \hbar\begin{pmatrix}1\\ 0\end{pmatrix}$$

$$\hbar\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = \hbar\begin{pmatrix}0\\ 1\end{pmatrix}$$

$$\hbar\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}\begin{pmatrix}0\\ 1\end{pmatrix} = 0$$

量子算子operator對狀態state的運算operation，就可以以矩陣乘法來理解！

角動量算子運作於ket得到一ket，可看成矩陣乘上行向量，得到一個行向量。

$$L_+ = L_x + iL_y = \hbar\begin{pmatrix}0 & 1\\ 0 & 0\end{pmatrix}$$

$$L_- = L_x - iL_y = \hbar\begin{pmatrix}0 & 0\\ 1 & 0\end{pmatrix}$$

L_x與L_y也自然可以以矩陣代表！

$$L_x = \frac{L_+ + L_-}{2} = \frac{\hbar}{2}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}$$

$$L_y = \frac{L_+ - L_-}{2i} = \frac{\hbar}{2}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}$$

$$[L_x, L_y] = i\hbar L_z$$

根據此對易關係，L_z也必須可以以矩陣代表！

$$[L_x, L_y] = \left(\frac{\hbar}{2}\right)^2\left[\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\begin{pmatrix}0 & -i\\ i & 0\end{pmatrix} - \begin{pmatrix}0 & -i\\ i & 0\end{pmatrix}\begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}\right]$$

$$= \left(\frac{\hbar}{2}\right)^2\left[\begin{pmatrix}i & 0\\ 0 & -i\end{pmatrix} - \begin{pmatrix}-i & 0\\ 0 & i\end{pmatrix}\right] = i\hbar\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix} = i\hbar L_z$$

$$L_z = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}$$

$$\left|\frac{1}{2},\frac{1}{2}\right\rangle = \begin{pmatrix}1\\ 0\end{pmatrix} \qquad \left|\frac{1}{2},-\frac{1}{2}\right\rangle = \begin{pmatrix}0\\ 1\end{pmatrix}$$

是L_z本徵態。

$$L_z\begin{pmatrix}1\\ 0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}1\\ 0\end{pmatrix} = \frac{\hbar}{2}\begin{pmatrix}1\\ 0\end{pmatrix}$$

$$\frac{\hbar}{2}\begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}\begin{pmatrix}0\\ 1\end{pmatrix} = -\frac{\hbar}{2}\begin{pmatrix}0\\ 1\end{pmatrix}$$

驗證完全正確！所以取特定l的本徵態為基底，算子可以視為矩陣。

量子算子operator對狀態state的運算，似乎可以完全以矩陣乘法來理解！

我們可以用矩陣來算期望值！

$$\left\langle \frac{1}{2},\frac{1}{2}\middle| L_x^2 \middle| \frac{1}{2},\frac{1}{2}\right\rangle$$

角動量算子運作於ket得到一ket，就是矩陣乘上行向量，得到一個行向量。

一個ket與bra的內積，行向量transpose轉置的列向量，乘上行向量。

這是線性代數內積的標準寫法。

$$\left\langle \frac{1}{2},\frac{1}{2}\middle| L_x^2 \middle| \frac{1}{2},\frac{1}{2}\right\rangle \sim \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} =$$

$$= \left(\frac{\hbar}{2}\right)^2 \begin{pmatrix} 1 & 0 \end{pmatrix} \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \frac{\hbar^2}{4}$$

這與之前的結果完全吻合。

$$L_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix} \quad L_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix} \quad L_z = \frac{\hbar}{2}\begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix}$$

這三個2×2矩陣滿足角動量的對易關係！可以代表$l = \frac{1}{2}$的態的角動量。

同樣的辦法可以推廣到任意的l，

可以找到三個$(2l+1)\times(2l+1)$矩陣滿足角動量的對易關係！

在l的空間裡面，角動量的討論，可以不需要用到原來的微分算子！

這在整數l的情況，是一個方便。

但在半整數l的情況，卻是必要。

對於軌道角動量：

$$L_x = yp_z - zp_y = -i\hbar\left(y\frac{\partial}{\partial z} - z\frac{\partial}{\partial y}\right)$$

可以證明 l 只能是整數，不能是半整數。

Chapter 9

Matrix Representation of Operators

The original discovery of quantum mechanics is due to W. Heisenberg. He associated physical quantities like x and p with square *arrays* of numbers for which he proposed

$$\begin{pmatrix} |1,1\rangle \\ |1,0\rangle \\ |1,-1\rangle \end{pmatrix}$$

$l = 1$

Triplet 3

這三個態構成一個三維線性空間的基底。

一般狀態會是基底的線性疊加。

$$c_+|1,1\rangle + c_0|1,0\rangle + c_-|1,-1\rangle = \begin{pmatrix} c_+ \\ c_0 \\ c_- \end{pmatrix}$$

$$L_z = \hbar\begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 0 \\ 0 & 0 & -1 \end{pmatrix}$$

$$L_+|l,m\,\rangle = \hbar\sqrt{(l-m)(l+m+1)}\,|l,m+1\,\rangle$$

$$L_+|1,-1\,\rangle = \hbar\sqrt{2}|1,0\,\rangle \qquad L_+|1,0\,\rangle = \hbar\sqrt{2}|1,1\,\rangle$$

$$L_+\begin{pmatrix} 0 \\ 0 \\ 1 \end{pmatrix} = \hbar\sqrt{2}\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} \qquad L_+\begin{pmatrix} 0 \\ 1 \\ 0 \end{pmatrix} = \hbar\sqrt{2}\begin{pmatrix} 1 \\ 0 \\ 0 \end{pmatrix}$$

可以猜得到：

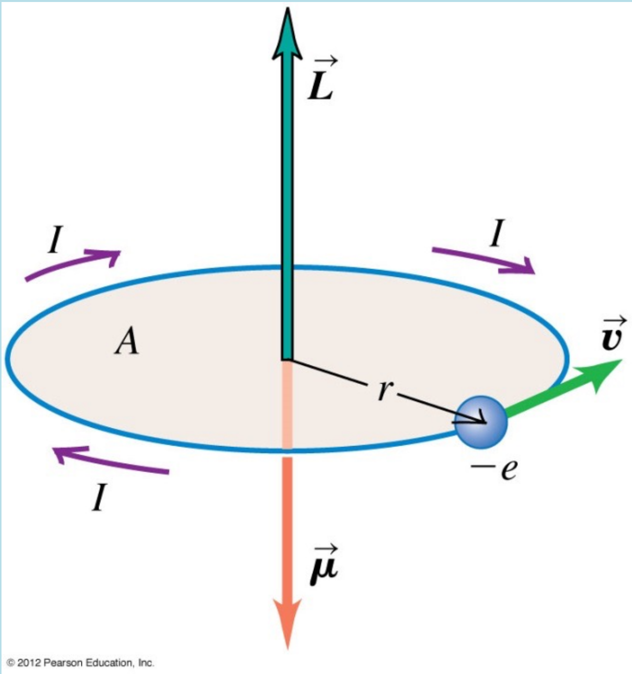
$$L_+ = \hbar\begin{pmatrix} 0 & \sqrt{2} & 0 \\ 0 & 0 & \sqrt{2} \\ 0 & 0 & 0 \end{pmatrix} \qquad L_- = \hbar\begin{pmatrix} 0 & 0 & 0 \\ \sqrt{2} & 0 & 0 \\ 0 & \sqrt{2} & 0 \end{pmatrix}$$

$L_{x,y}$就是L_{+-}的組合，因此可以得到$L_{x,y}$的矩陣表示：

$$L_x = \frac{L_+ + L_-}{2} = \frac{1}{2}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ \sqrt{2} & 0 & \sqrt{2} \\ 0 & \sqrt{2} & 0 \end{pmatrix} \qquad L_y = \frac{L_+ - L}{2i} = \frac{-i}{2}\begin{pmatrix} 0 & \sqrt{2} & 0 \\ -\sqrt{2} & 0 & \sqrt{2} \\ 0 & -\sqrt{2} & 0 \end{pmatrix}$$

可以用這三個3×3矩陣來代表角動量，它們滿足角動量的對易關係！

古典旋轉的帶電粒子就是一個磁偶極$\vec{\mu}$ 。



$$\mu = iA = i\pi r^2 = \frac{e}{\frac{2\pi r}{v}} \cdot \pi r^2 = \frac{erv}{2} = \frac{e}{2m} rp = \frac{e}{2m} L$$

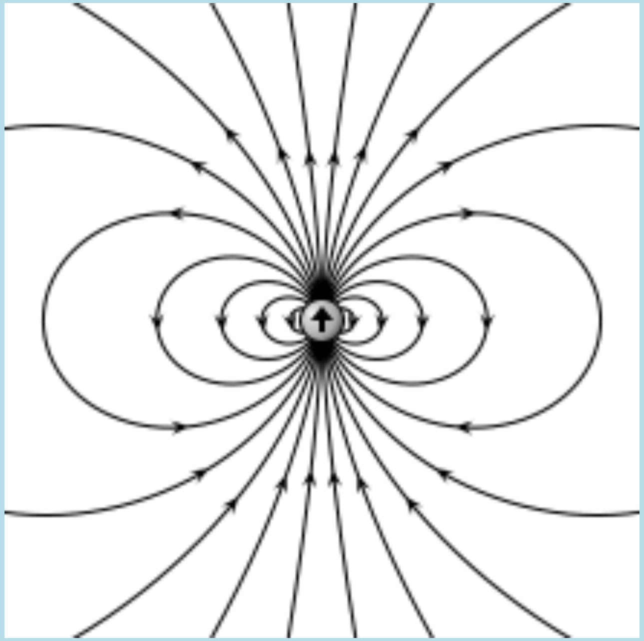
$$\vec{\mu} = -\frac{e}{2m}\vec{L}$$

磁偶極矩與角動量成正比

假設此古典的公式對量子力學電子也成立！

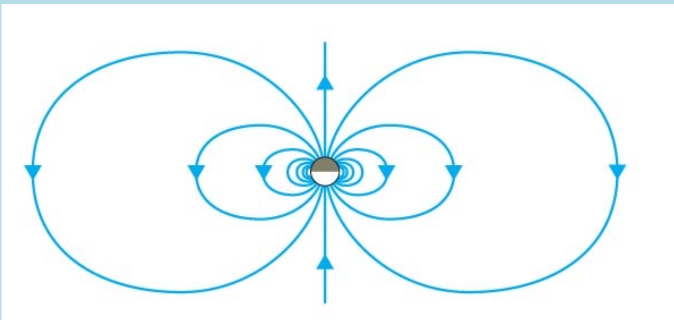
有角動量的帶電粒子是一個磁偶極！

量測磁偶極矩就是量測角動量！



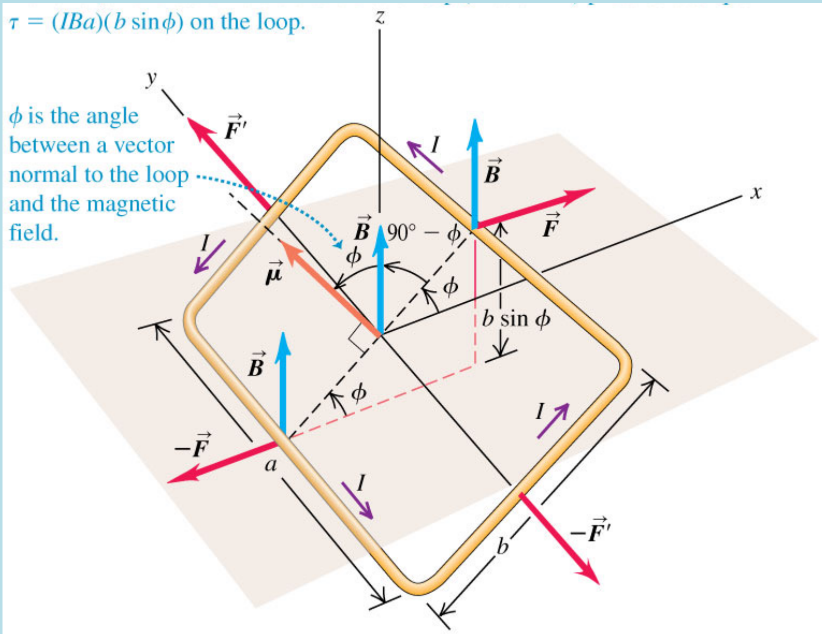
電偶極周圍的電場

$$\vec{E} = \frac{1}{4\pi\varepsilon_0 r^3}[3(\vec{p}\cdot\hat{r})\hat{r} - \vec{p}]$$



$$\vec{B} = \frac{1}{4\pi\varepsilon_0 r^3}[3(\vec{\mu}\cdot\hat{r})\hat{r} - \vec{\mu}]$$

磁偶極在均勻磁場中所受的磁效應



受力為零，力矩不為零：

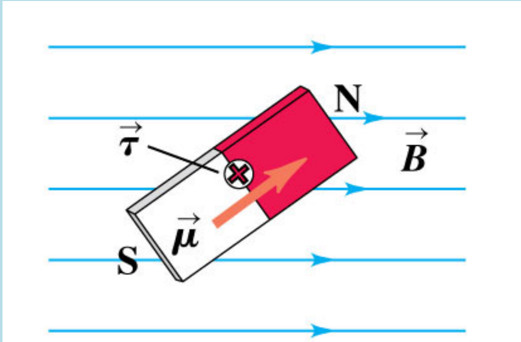
$$\tau = F \cdot \frac{b}{2} \sin\theta \cdot 2 = iaB \cdot b \sin\theta = \mu B \sin\theta = \left| \vec{\mu} \times \vec{B} \right|$$

$$\vec{\tau} = \vec{\mu} \times \vec{B}$$

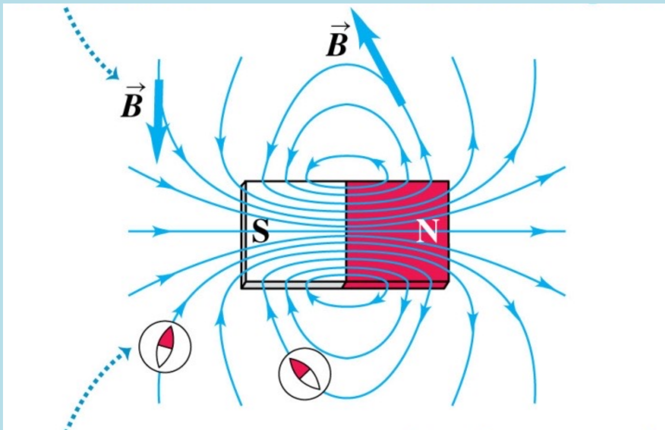
所受力矩只由磁偶極矩向量決定。

力矩會推動磁偶極至平行磁場的方向！

在磁場中，磁偶極會趨向與磁場同向！



這就是為什麼可以以磁鐵指向來定義磁場方向



角度改變時，此力矩會做功，

我們可以用位能來討論磁場中的磁偶極：

$$\Delta U = -W = -\int_{\theta_1}^{\theta_2} (-d\theta) \cdot \tau = -\int_{\theta_1}^{\theta_2} d\theta \cdot \mu B \sin\theta = -\mu B \cos\theta_2 + \mu B \cos\theta_1 = -\Delta(\vec{\mu} \cdot \vec{B})$$

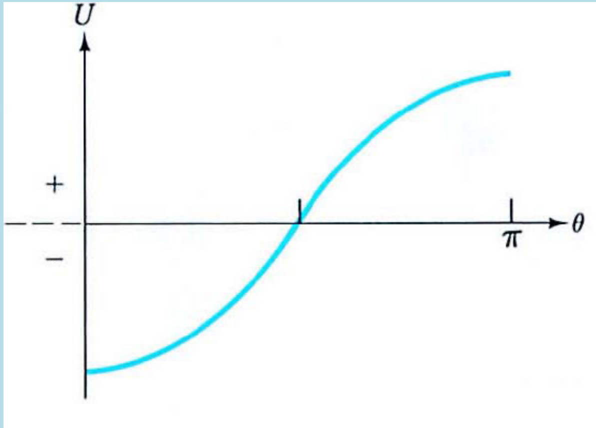


圖 23.28
電偶極的位能為其方向角度的函數

$$U = -\vec{\mu} \cdot \vec{B}$$

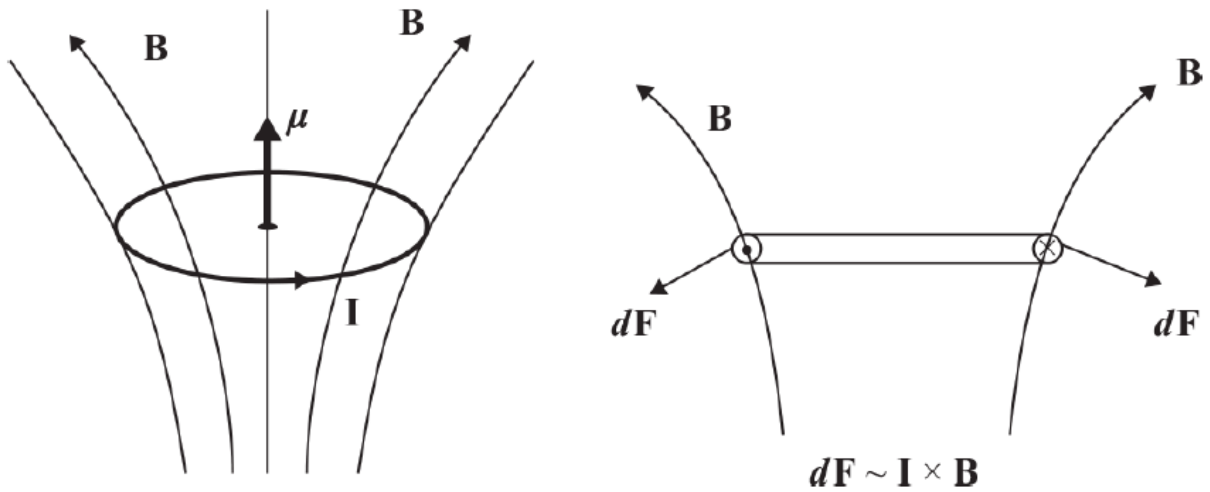


Figure 12.2
A magnetic dipole in a nonuniform magnetic field will experience a force. The force points in the direction for which $\boldsymbol{\mu} \cdot \mathbf{B}$ grows the fastest. In this case the force is downward.

$$U = -\vec{\mu} \cdot \vec{B}$$

此式在不均勻磁場中也成立。此時磁偶極會受一個力。

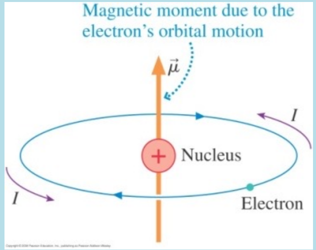
$$F = -\nabla U = \nabla(\vec{\mu} \cdot \vec{B})$$

角動量量子化，因此磁偶極矩也是量子化！

原子能量與角動量大小及z方向角動量L_z無關。完全由主量子數n決定。

但在磁場中原子能量會被磁偶極修正，就與與z方向角動量L_z有關。

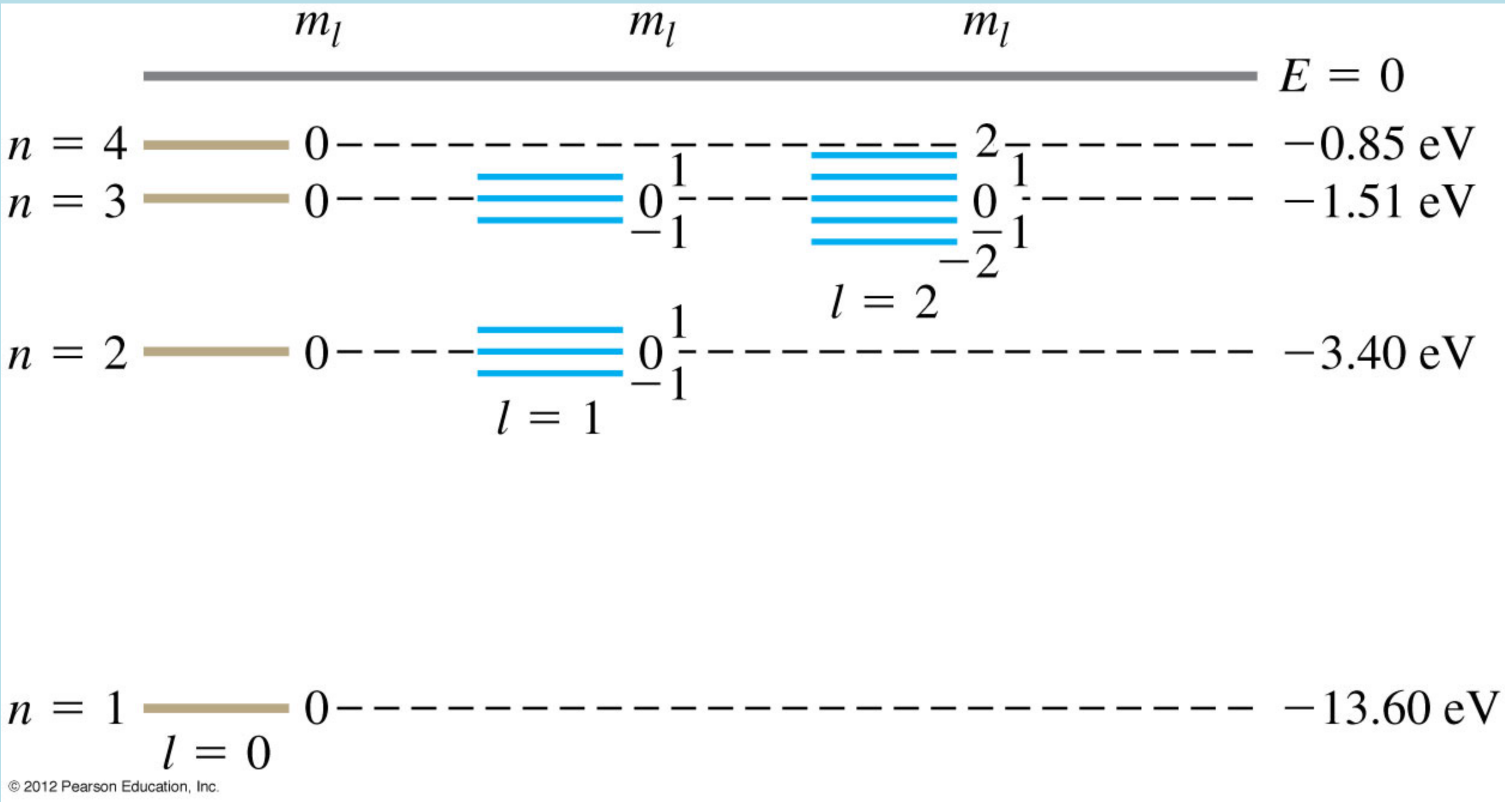
因此可加一 z方向磁場，再觀察原子光譜，即測角動量。



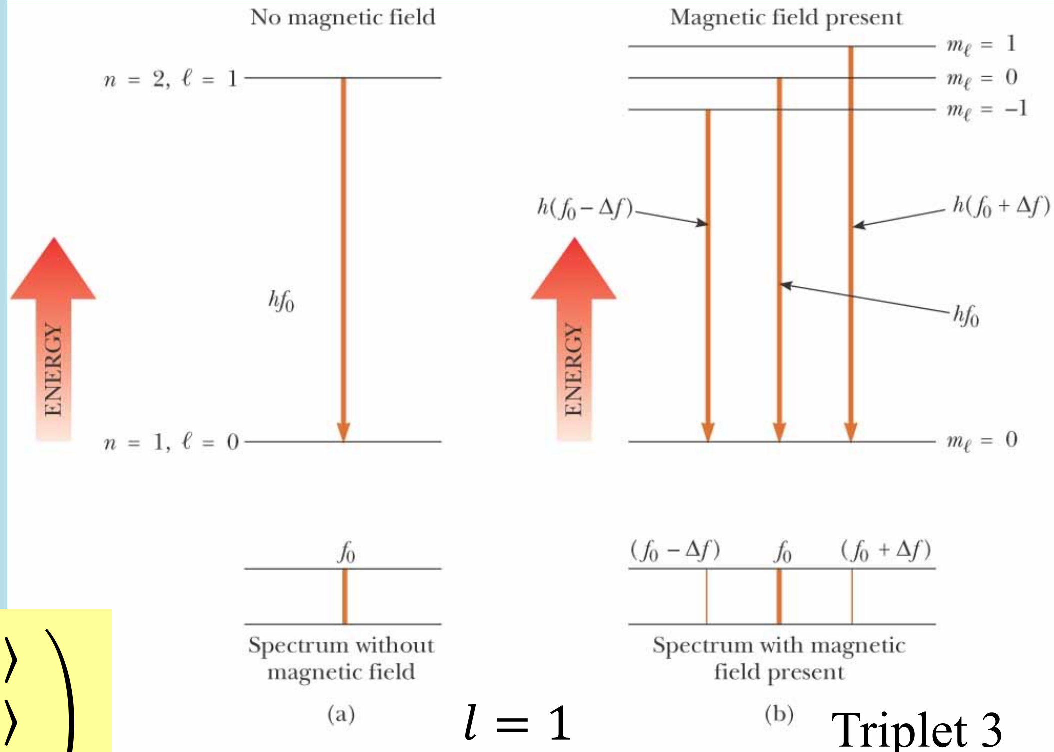
$$U = -\vec{\mu} \cdot \vec{B}$$

$$\mu_z = -\frac{e\hbar}{2m} m_z$$

$$\Delta E = \frac{Be\hbar}{2m} m_z$$



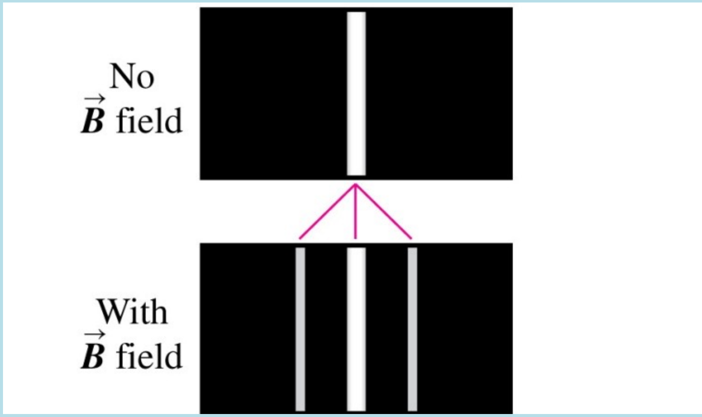
Zeeman Effect 外加磁場後原子光譜的分裂

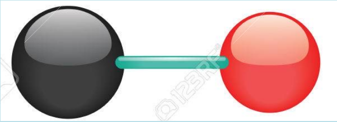


$$\begin{pmatrix} |1,1\rangle \\ |1,0\rangle \\ |1,-1\rangle \end{pmatrix}$$

$l = 1$

Triplet 3



考慮雙原子分子，例如CO：

以鍵結方向為z軸：

轉動動能可以以轉動慣量$I_{x,y,z}$及角動量表示：

$$H = \frac{L_x^2}{2I_x} + \frac{L_y^2}{2I_y} + \frac{L_z^2}{2I_z}$$

已知 $I_x = I_y = I$

$$H = \frac{L_x^2 + L_y^2}{2I} + \frac{L_z^2}{2I_z}$$

$L_x^2 + L_y^2$可以以$L^2 - L_z^2$表示：

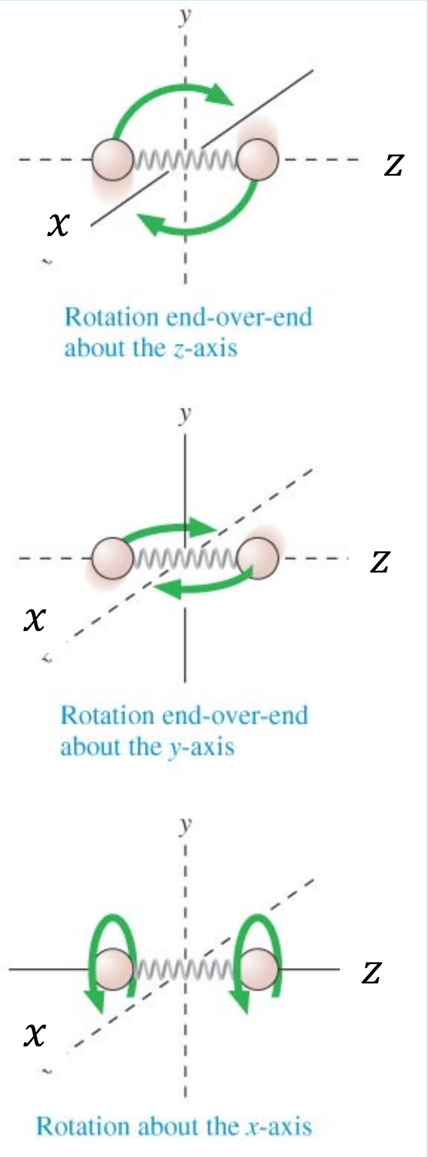
$$L_x^2 + L_y^2 = L^2 - L_z^2$$

$$H = \frac{L^2}{2I} + \left(\frac{1}{2I_z} - \frac{1}{2I}\right) L_z^2$$

因此L^2, L_z的本徵態：$|l, m\rangle$，也是能量H的本徵態，

能量H的本徵值就是將對應的L^2, L_z的本徵值代入即可：

$$E_{lm} = \hbar^2 \frac{l(l+1)}{2I} + \hbar^2 m^2 \left(\frac{1}{2I_z} - \frac{1}{2I}\right)$$



7.1.1 Rotation spectra of diatomic molecules

Knowledge of the spectrum of the angular-momentum operators enables us to understand an important part of the dynamics of a diatomic molecule such as carbon monoxide. For some purposes a CO molecule can be considered to consist of two point masses, the nuclei of the oxygen and carbon atoms, joined by a 'light rod' provided by the electrons. In this model the molecule's moment of inertia around the axis that joins the nuclei is negligible, while the same moment of inertia I applies to any perpendicular axis.

In classical mechanics the rotational energy of a rigid body is

$$E = \tfrac{1}{2}\left(\frac{\mathcal{J}_x^2}{I_x} + \frac{\mathcal{J}_y^2}{I_y} + \frac{\mathcal{J}_z^2}{I_z}\right), \tag{7.17}$$

where the I_i are the moments of inertia about the body's three principal axes and $\boldsymbol{\mathcal{J}}$ is the angular-momentum vector due to the body's spin. We conjecture that the equivalent formula links the Hamiltonian and the angular-momentum operators in quantum mechanics:

$$H = \frac{\hbar^2}{2}\left(\frac{J_x^2}{I_x} + \frac{J_y^2}{I_y} + \frac{J_z^2}{I_z}\right). \tag{7.18}$$

The best justification for adopting this formula is that it leads us to results that are confirmed by experiments.

In the case of an axisymmetric body, we orient our body such that the symmetry axis is parallel to the z-axis. Then $I \equiv I_x = I_y$ and the Hamiltonian can be written

$$H = \frac{\hbar^2}{2}\left\{\frac{J^2}{I} + J_z^2\left(\frac{1}{I_z} - \frac{1}{I}\right)\right\}. \tag{7.19}$$

From this formula and our knowledge of the eigenvalues of J^2 and J_z, we can immediately write down the energies that form the spectrum of H:

$$E_{jm} = \frac{\hbar^2}{2}\left\{\frac{j(j+1)}{I} + m^2\left(\frac{1}{I_z} - \frac{1}{I}\right)\right\}, \tag{7.20}$$

如圖所示，$I_z \sim 0$。

若$m^2 \neq 0$，$\hbar^2 m^2 \left(\frac{1}{2I_z} - \frac{1}{2I}\right) \to \infty$

這些能階將永遠無法激發！

只有$m^2 = 0$的能階留下！能量由l決定：

$$E_l = \hbar^2 \frac{l(l+1)}{2I}$$

光譜線對應$l+1 \to l$的能差為

$$E_{l+1} - E_l = \frac{\hbar^2}{I} l$$

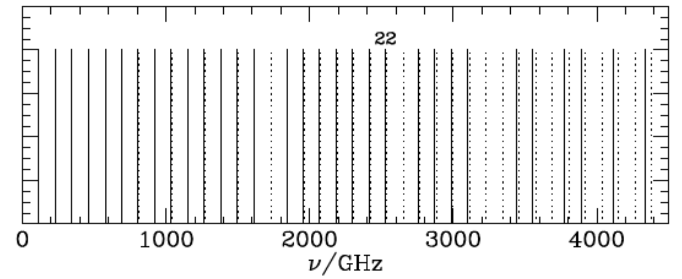
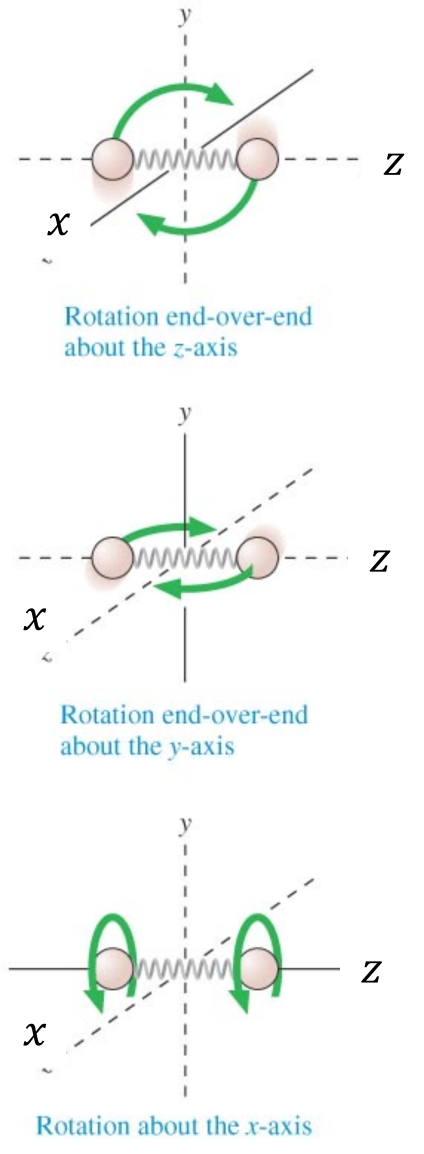


Figure 7.2 The rotation spectrum of CO. The full lines show the measured frequencies for transitions up to $j = 38 \to 37$, while the dotted lines show integer multiples of the lowest measured frequency. Up to the line for $j = 22 \to 21$ the dotted lines are obscured by the full lines except at one frequency for which measurements are not available. For $j \geq 22$ the separation between the dotted and full lines increases steadily as a consequence of the centrifugal stretching of the bond between the molecule's atoms. Measurements are lacking for several of the higher-frequency lines.



where j is the total angular-momentum quantum number and $|m| < j$. In the case of a diatomic molecule such as CO, $I_z \ll I$ so the coefficient of m^2 is very much larger than the coefficient of $j(j+1)$ and states with $|m| > 0$ will occur only far above the ground state. Consequently, the states of interest have energies of the form

$$E_l = \hbar^2 \frac{l(l+1)}{2I} \tag{7.21}$$

For reasons that will emerge in §7.2.1, only integer values of j are allowed.

CO is a significantly dipolar molecule. The carbon atom has a smaller share of the binding electrons than the oxygen atom, with the result that it is positively charged and the oxygen atom is negatively charged. A rotating electric dipole would be expected to emit electromagnetic radiation. Because we are in the quantum regime, the radiation emerges as photons which, as we shall see, can add or carry away only one unit $\hbar$ of angular momentum. It follows that the energies of the photons that can be emitted or absorbed by a rotating dipolar molecule are

$$E_p = \pm (E_j - E_{j-1}) = \pm j \frac{\hbar^2}{I}. \tag{7.22}$$

Using the relation $E = h\nu$ between the energy of a photon and the frequency ν of its radiation, the frequencies in the rotation spectrum of the molecule are

$$\nu_j = j \frac{\hbar}{2\pi I}. \tag{7.23}$$

In the case of ^{12}CO, the coefficient of j evaluates to 113.1724 GHz and spectral lines occur at multiples of this frequency (Figure 7.2).

In the classical limit of large j, $\mathcal{J} = j\hbar$ is the molecule's angular momentum, and this is related to the angular frequency ω at which the molecule rotates by $\mathcal{J} = I\omega$. When in equation (7.23) we replace $j\hbar$ by $I\omega$, we discover that the frequency of the emitted radiation ν is simply the frequency $\omega/2\pi$ at which the molecule rotates around its axis. This conclusion makes perfect sense physically. Now, because of the form of the Hamiltonian, the energy eigenstates are also the eigenstates of J_z and J^2. Therefore in any energy eigenstate, $\langle J^2 \rangle = j(j+1)$, and for low-lying states with $m = 0$ and $j \sim \mathcal{O}(1)$, $j(j+1)$ is significantly larger than j^2. Therefore ν_j in (7.23) is smaller than the frequency at which the molecule rotates when it is in the upper state of the transition. On the other hand, ν_j is larger than the rotation frequency $\sqrt{(j-1)j}\frac{\hbar}{2\pi I}$ of the lower state. Hence the frequency at which radiation emerges lies between the rotation frequencies of the upper and lower states. Again this makes sense physically. As we approach the classical regime, j becomes large so $j(j+1) \simeq j^2 \simeq (j-1)j$ and the rotation frequencies of the upper and lower states converge, from above and below, on the frequency of the emitted radiation.

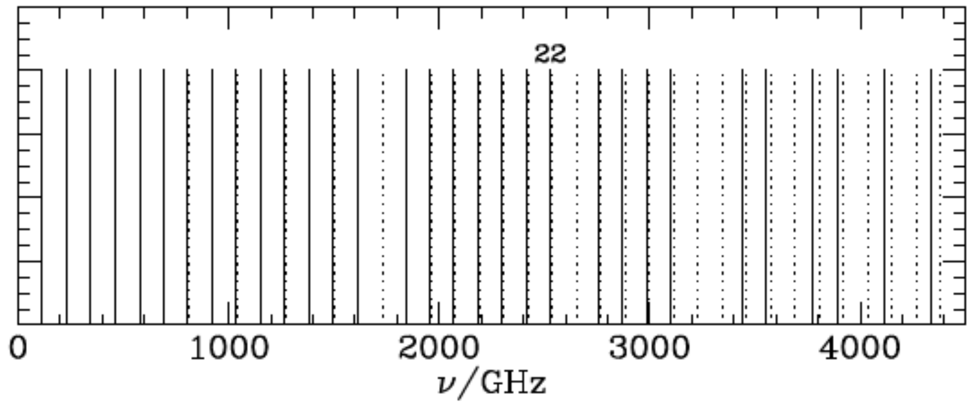


Figure 7.2 The rotation spectrum of CO. The full lines show the measured frequencies for transitions up to $j = 38 \to 37$, while the dotted lines show integer multiples of the lowest measured frequency. Up to the line for $j = 22 \to 21$ the dotted lines are obscured by the full lines except at one frequency for which measurements are not available. For $j \geq 22$ the separation between the dotted and full lines increases steadily as a consequence of the centrifugal stretching of the bond between the molecule's atoms. Measurements are lacking for several of the higher-frequency lines.

Measurements of radiation from 113 GHz and the first few multiples of this frequency provide one of the two most important probes of interstellar gas.[1] In denser, cooler regions, hydrogen atoms combine to form H_2 molecules, which are bisymmetric and do not have an electric dipole moment when they are simply rotating. Consequently, these molecules, which together with similarly uncommunicative helium atoms make up the great majority of the mass of cold interstellar gas, lack readily observable spectral lines. Hence astronomers are obliged to study the cold interstellar medium through the rotation spectrum of the few parts in 10^6 of CO that it contains.