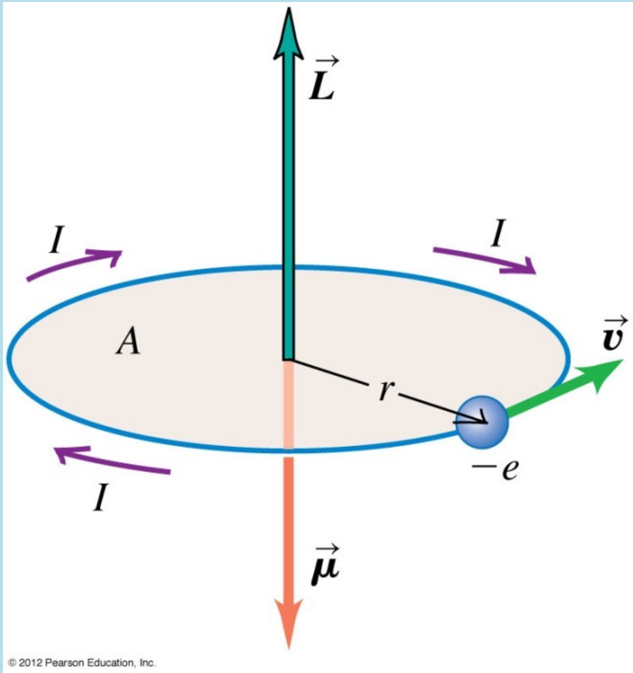
Angular momentum operators 角動量算子



180 W. Heisenberg,

ermöglichen, als es der Gleichung (1) entspricht, so wäre die Quantenmechanik unmöglich. Diese Ungenauigkeit, die durch Gleichung (1) festgelegt ist, schafft also erst Raum für die Gültigkeit der Beziehungen, die in den quantenmechanischen Vertauschungsrelationen

$$pq - qp = \frac{h}{2\pi i}$$

ihren prägnanten Ausdruck finden; sie ermöglicht diese Gleichung, ohne daß der physikalische Sinn der Größen p und q geändert werden müßte.

Für diejenigen physikalischen Phänomene, deren quantentheoretische Formulierung noch unbekannt ist (z. B. die Elektrodynamik), bedeutet Gleichung (1) eine Forderung, die zum Auffinden der neuen Gesetze nützlich sein mag. Für die Quantenmechanik läßt sich Gleichung (1) durch eine geringfügige Verallgemeinerung aus der Dirac-Jordanschen Formulierung herleiten. Wenn wir für den bestimmten Wert η irgend eines Parameters den Ort q des Elektrons zu q' bestimmen mit einer Genauigkeit q_1, so können wir dieses Faktum durch eine Wahrscheinlichkeitsamplitude $S(\eta, q)$ zum Ausdruck bringen, die nur in einem Gebiet der ungefähren Größe q_1 um q' von Null merklich verschieden ist. Insbesondere kann man z. B. setzen

$$S(\eta, q) \text{ prop } e^{-\frac{(q-q')^2}{2q_1^2} - \frac{2\pi i}{h}p'(q-q')}, \text{ al}$$

Dann gilt für die zu p gehörige Wahrscheinl

$$S(\eta, p) = \int S(\eta, q) S(q$$

Für $S(q, p)$ kann nach Jordan gesetzt

$$S(q, p) = e^{\frac{2\pi i p q}{h}}$$

Dann wird nach (4) $S(\eta, p)$ nur für Werte von

nicht wesentlich größer als 1 ist, merklich

Insbesondere gilt im Falle (3):

$$S(\eta, p) \text{ prop} \int e^{\frac{2\pi i(p-p')q}{h} - \frac{}{2q_1^2}} dq,$$

d. h.

$$S(\eta, p) \text{ prop } e^{-\frac{(p-p')^2}{2p_1^2} + \frac{2\pi i}{h}q'(p-p')}, \text{ also } S\bar{S} \text{ prop } e^{-\frac{(p-p')^2}{p_1^2}},$$

wo

$$p_1 q_1 = \frac{h}{2\pi}. \qquad (6)$$

電子的位置與動量不能同時確定，

海森堡的測不準原理 Uncertainty Principle。

對於電子任何狀態而言，

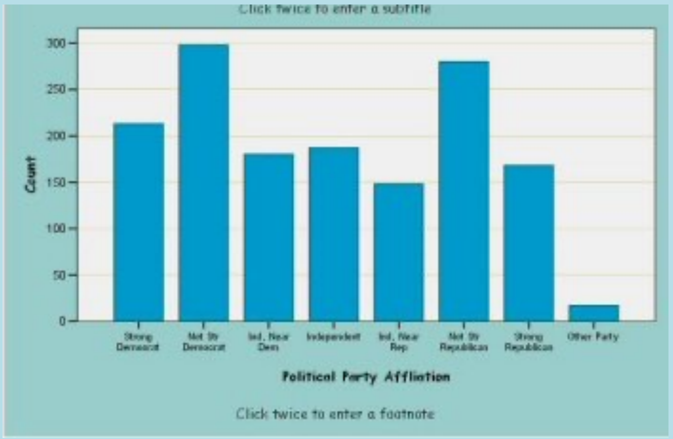
可以證明位置與動量的不確定性必須滿足：

$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

不準度的定義是植基於前述測量的不確定性

量子世界特性一：一個粒子處於完全相同的狀態下，某些物理測量的結果卻並不確定。

在一個特定狀態下，對位置或動量測量所得的結果形成一個統計分布，
計算這個分布的標準差，即是位置與動量的不確定性：



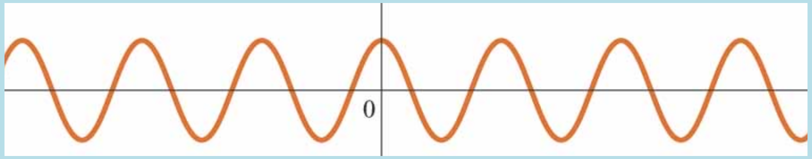
$$\Delta x \equiv \sqrt{\langle x^2 \rangle - \langle x \rangle^2}$$

$$\Delta p \equiv \sqrt{\langle p^2 \rangle - \langle p \rangle^2}$$

測不準原理有兩個極端的特例：

動量的本徵態 $\Delta p = 0$ $\Delta x = \infty$

$$u_{p_0} = \frac{1}{\sqrt{2\pi\hbar}} e^{i\frac{p_0}{\hbar}x} \rightarrow |p_0\rangle$$

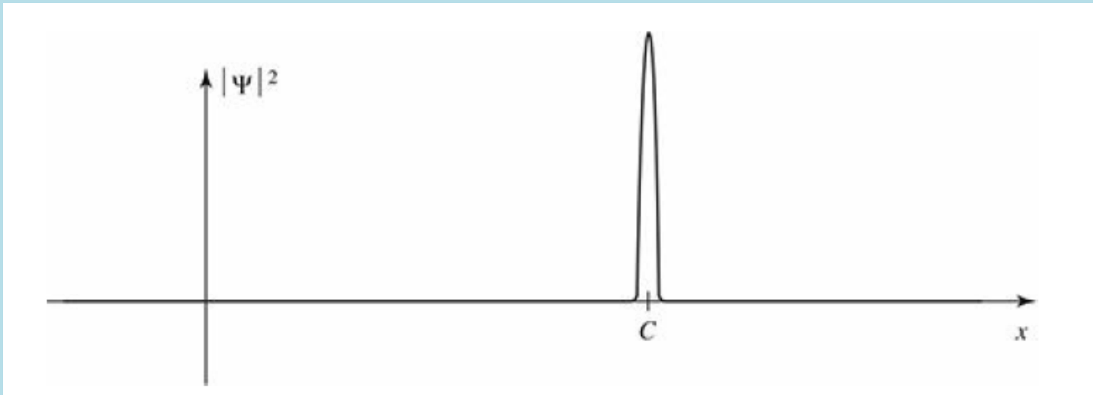


$$\hat{p}|p_0\rangle = p_0|p_0\rangle$$

位置的本徵態 $\Delta x = 0$ $\Delta p = \infty$

$$\delta(x - x_0) \rightarrow |x_0\rangle$$

$$\hat{x}|x_0\rangle = x_0|x_0\rangle$$



$$\Delta x \cdot \Delta p \geq \frac{\hbar}{2}$$

沒有任何狀態，位置與動量的測量都完全確定。

古典牛頓力學的粒子，違反測不準原理 $\Delta x = 0, \Delta p = 0$

因此，這也表示位置與動量的沒有共同的本徵態，使兩個測量都完全確定。

位置與動量不能同時精準測量，兩個量的不準度滿足測不準原理。

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

位置與動量恰好也不對易。這兩件事是否彼此相關？

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

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

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

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

For the operators p and x for which

$$[p, x] = -i\hbar \tag{5A-12}$$

this leads to

$$\Delta p \, \Delta x \geq \frac{\hbar}{2} \tag{5A-13}$$

動量與位置不能同時精準測量！

測量要得到完全確定結果，要在本徵態！

因此，這表示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！

$[A, B] \neq 0$

這兩物理量不能同時精準測量。

它們沒有共同的本徵態。

$[A, B] = 0$

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。

A與B為兩個算子

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

證明：A的本徵態$|a\rangle$滿足：

$$A|a\rangle = a|a\rangle$$

考慮狀態$B|a\rangle$，現在計算算子A對此態$B|a\rangle$的作用：

$$A(B|a\rangle) = AB|a\rangle = BA|a\rangle = Ba|a\rangle = a \cdot B|a\rangle$$

因此狀態$B|a\rangle$也是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$B|a\rangle$與$|a\rangle$都是A算子本徵值為a的本徵態，

$A|a\rangle$必須正比於$|\psi_a\rangle$，設比例常數為b，則：

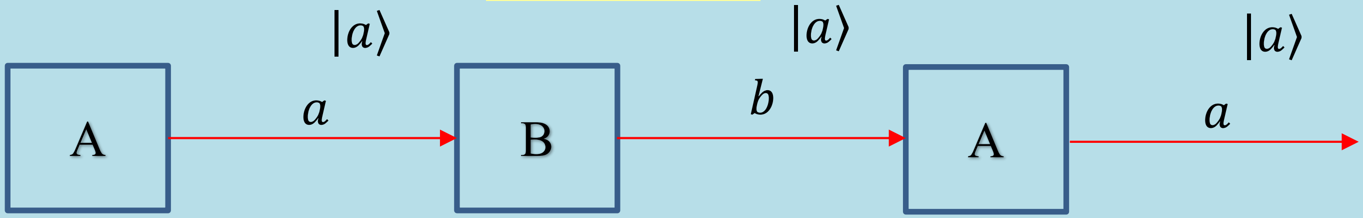
$$\hat{B}|a\rangle = b|a\rangle$$

此式顯示$|a\rangle$也是B的本徵態，本徵值為b。得證！

結論：A的本徵態也會是B的本徵態，因此A與B可以同時精準測量。

這有很重要的結果。

$[A, B] = 0$

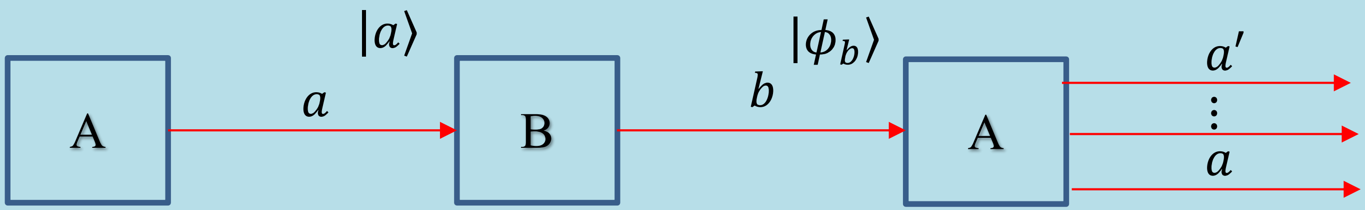


A若測得a，狀態會崩潰為本徵態$|a\rangle$。

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

$|a\rangle$如果再測一次A只能得到確定的結果：a。B測量不改變A測量結果。

$[A, B] \neq 0$



$|a\rangle$只是A的本徵態，不是B的本徵態。

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

$|\phi_b\rangle$可能包含所有A的本徵態，是一基底展開，

原則上第二個A測量所有結果都可能。所以B測量改變了A測量結果。

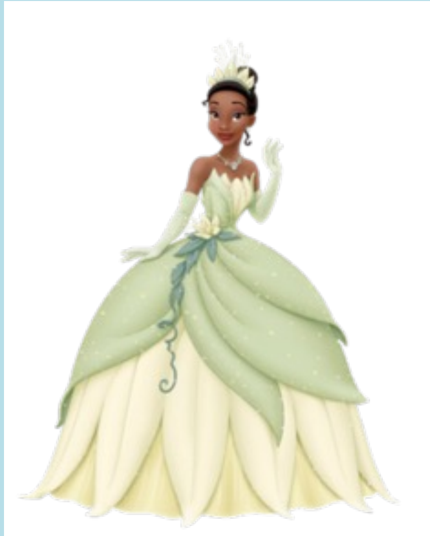
$$(\Delta A)^2(\Delta B)^2 \geq \frac{1}{4}\langle i[A, B]\rangle^2$$

$$[A, B] = 0$$

$$A(B|a\rangle) = AB|a\rangle = BA|a\rangle = Ba|a\rangle = a \cdot B|a\rangle$$

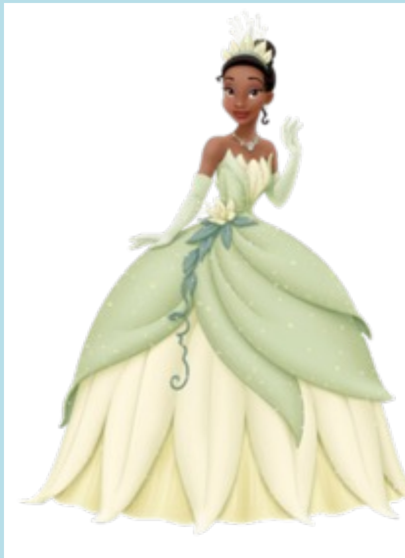
A

B

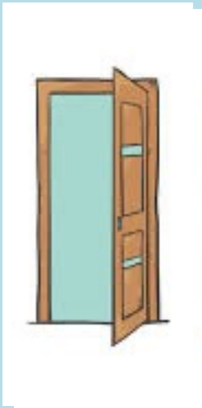


A

$|a\rangle$



B

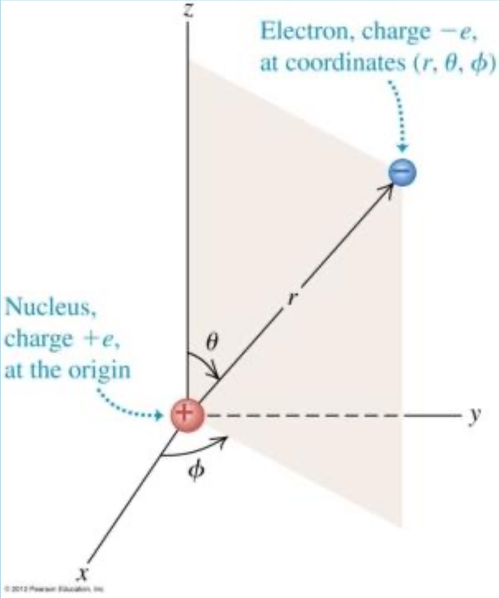


現在我們正式由一維空間進入三維空間：

狀態函數是三個空間座標的函數！

$$\psi(x) \rightarrow \psi(\vec{r}) = \psi(x, y, z) = \psi(r, \theta, \phi)$$

在許多球對稱的情況下，用極座標更方便！



三個動量分量分別是三個空間座標的微分：

動量向量就是梯度向量。

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

很明顯，不同方向的位置可以同時測量，因此彼此對易。

$$[x,y]=[x,z]=[z,y]=0$$

動量算子依舊可以以空間座標微分代表！

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

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

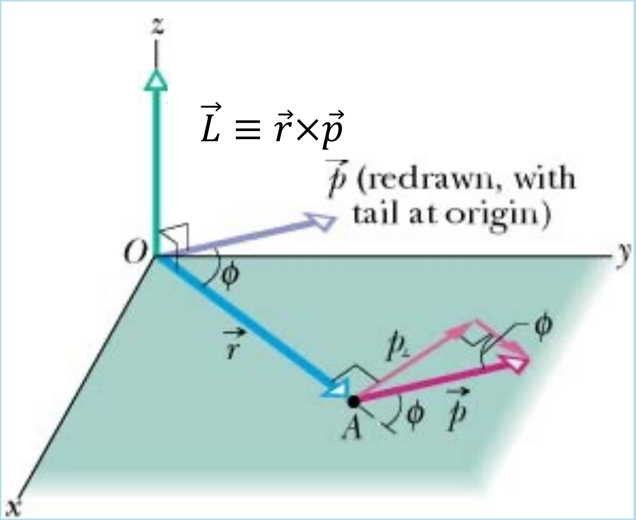
$$\left[p_x,p_y\right]=[p_x,p_z]=\left[p_z,p_y\right]=0$$ 不同方向位置微分彼此對易！

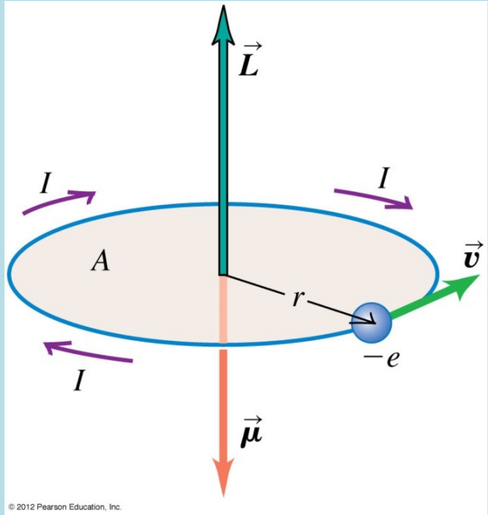
那麼不同方向的位置與動量也彼此對易了。例如：

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

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

三度空間中粒子可以旋轉。





$\vec{\tau} = \frac{d\vec{L}}{dt}$ 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

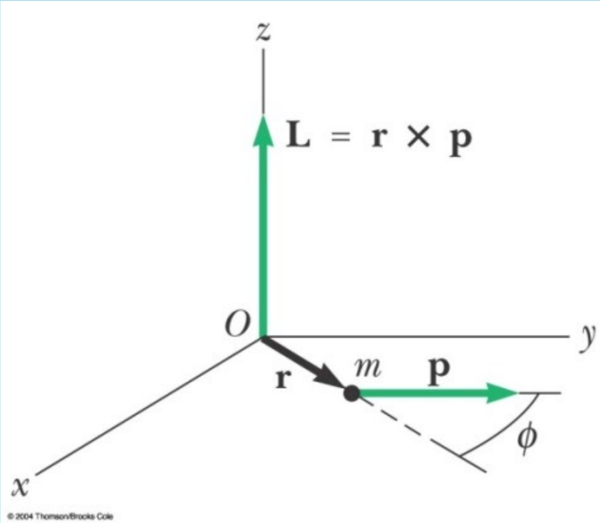
若$\vec{\tau} = 0$，則角動量$\vec{L}$守恆。

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！非常容易！

角動量算子有三個分量：

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



$L_z = xp_y - yp_x$

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

量子角動量的定義非常清楚！

$L_x = yp_z - zp_y$

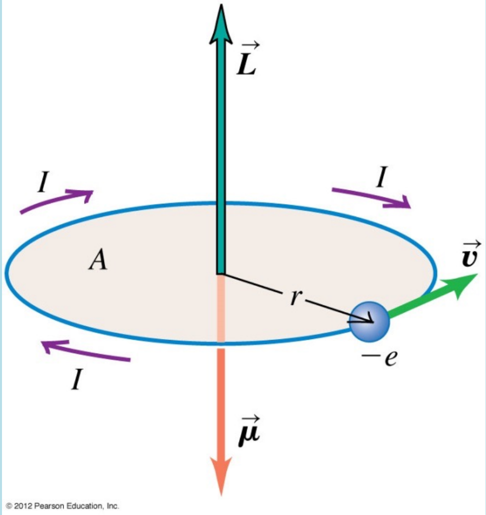
$L_y = zp_x - xp_z$

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

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

此三個算子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 $\vec{L} = \vec{r}\times\vec{p}$



$$L_x = yp_z - zp_y$$

$$L_y = zp_x - xp_z$$

$$L_z = xp_y - yp_x$$

比較規矩的推導：

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！

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

$$= [zp_x, x]p_y + x[zp_x, p_y] + y[xp_z, p_x] + [xp_z, y]p_x$$

$$= z[p_x, x]p_y + [z, x]p_xp_y + y[x, p_x]p_z + yx[p_z, p_x]$$

$$= i\hbar(-zp_y + yp_z) = i\hbar L_x$$

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

這兩物理量L_y,L_z不能同時測量。

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

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

比較簡易的推導：

$L_x = yp_z - zp_y$ $L_y = zp_x - xp_z$ $L_z = xp_y - yp_x$

計算角動量分量彼此的對易子：

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

$$= [zp_x, xp_y] + [xp_z, yp_x] + [zp_x, yp_x] + [xp_z, xp_y]$$ 後兩項所有算子都彼此對易！

前兩項中只有$[x, p_x] = i\hbar$，

第一項中z, p_y與對易子內其他算子都對易，可視為常數，

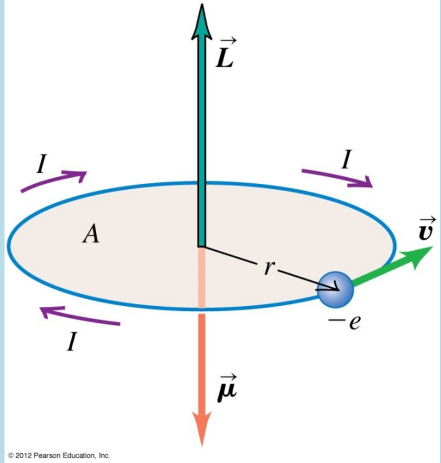
第二項中y, p_z與其他算子都對易，也可視為常數，可以從對易子中提出來！

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

$[L_y, L_z] = i\hbar L_x$ 這兩物理量L_y, L_z不能同時測量。

計算角動量分量彼此的對易子：

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



同時：

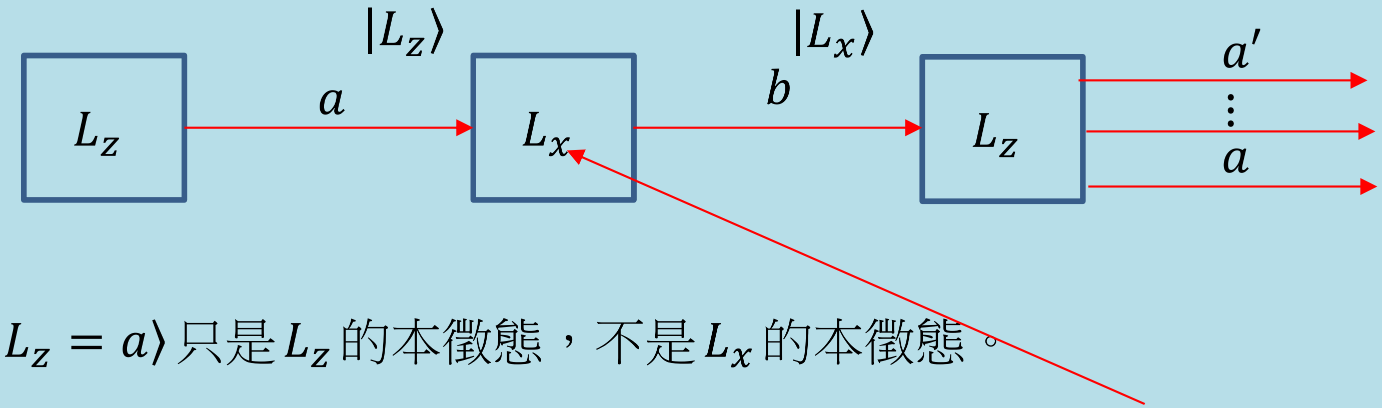
$$[L_z, L_x] = i\hbar L_y$$

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

角動量任兩個分量都不能同時測量。

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

適用剛才的：$[\hat{A}, \hat{B}] \neq 0$



$|L_z = a\rangle$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$|L_x = b\rangle$。L_x測量改變了粒子的L_z狀態。

$|L_x = b\rangle$可能包含所有L_z的本徵態。

原則上第二個L_z測量所有結果都可能

角動量任兩個分量彼此都不對易。

但沒想到角動量任一個分量與角動量的大小L^2都對易。

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

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

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

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

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

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

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

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。

這幾頁的結果是量子力學的里程碑！與古典物理完全迥異。

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

因此L^2可以與任一分量、但僅一個分量可同時測量，有共同的本徵函數。

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

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

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

別忘了$|a, m\rangle$就是一個位置的狀態波函數，記為Y_{am}，一般以極座標θ, ϕ表示位置。

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

氫原子能階：

$$E_n = (-13.6\text{eV})\left(\frac{1}{n^2}\right)$$

能量只與n有關

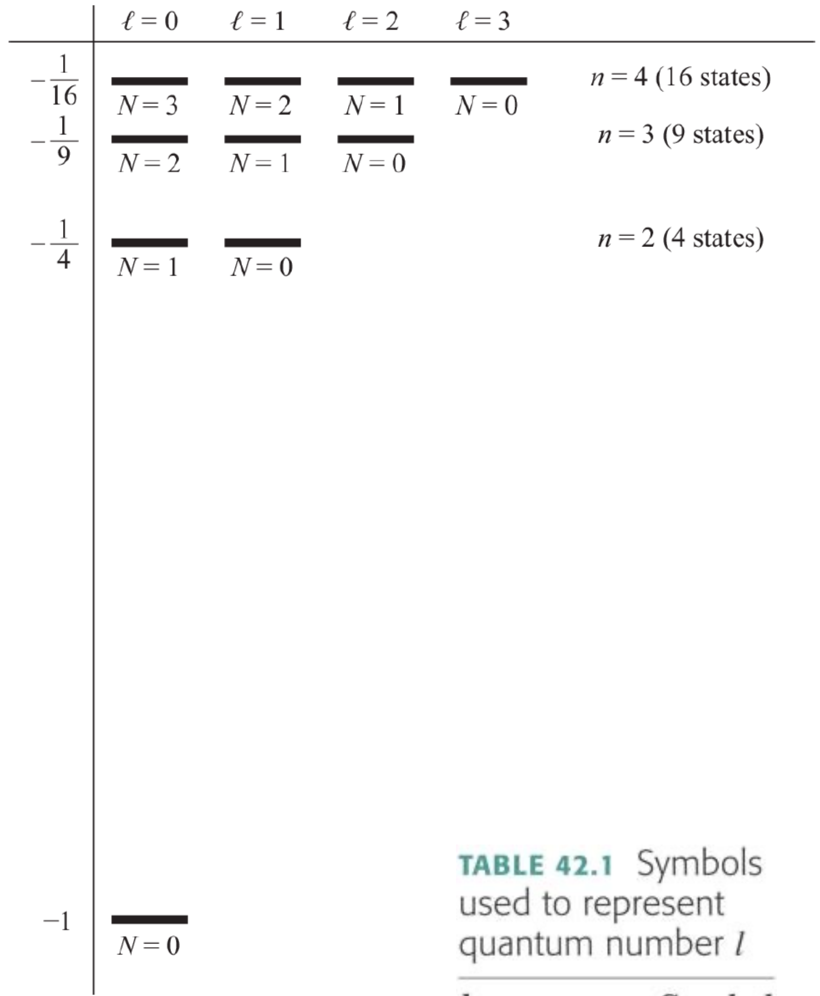


TABLE 42.1 Symbols used to represent quantum number l

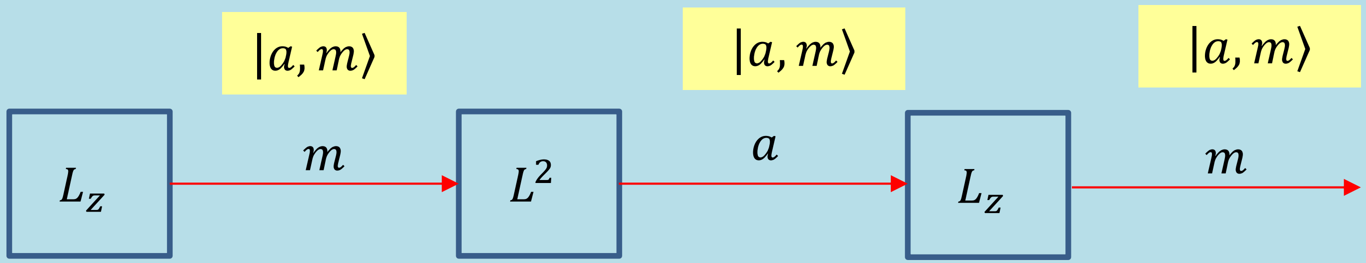
l	Symbol
0	s
1	p
2	d
3	f

主量子數 $n = \text{positive integer}$

軌道量子數 $l = 0,1,2 \cdots n-1$

軌道磁量子數 $m = -l, -l+1 \cdots 0,1, \cdots l-1, l$

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



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，

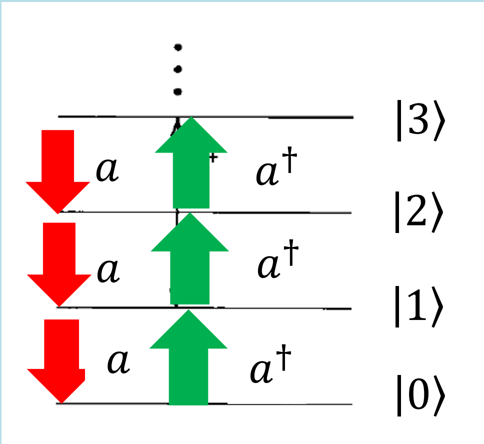
且無崩潰，依舊還是$|a,m\rangle$。

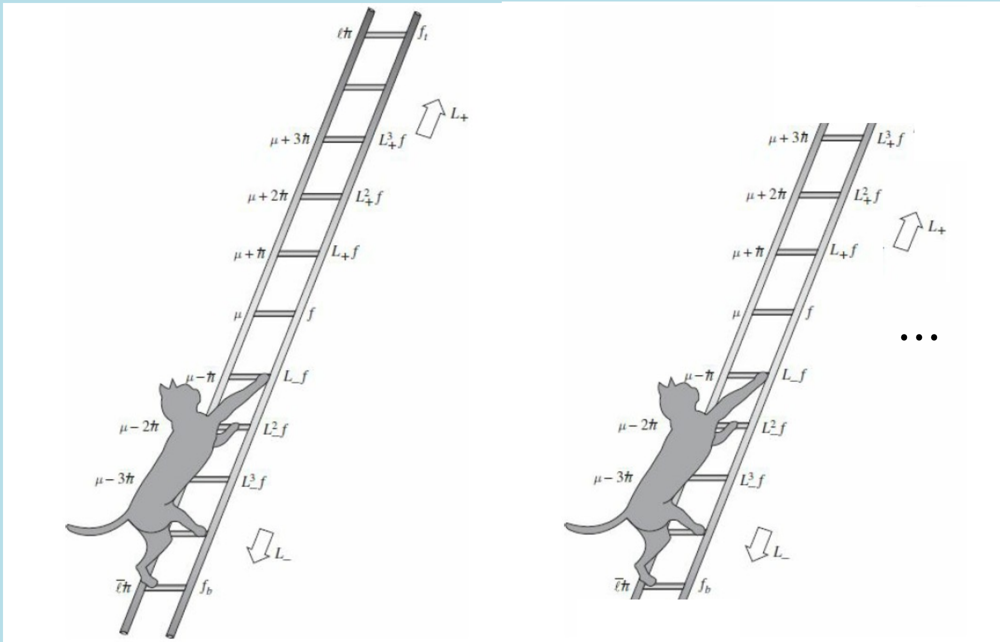
$|a,m\rangle$再測一次L_z只能得到m。

更令人驚訝的：如同在簡諧振盪器中，x, p, H的對易關係可給出H本徵值，

角動量分量L_x, L_y, L_z的對易關係，竟也可讓我們決定L^2, L_z的本徵值a, m！

更更令人驚訝的：





簡諧振盪器的能量本徵值神似角動量分量L_z的本徵值！

角動量分量定態有不同長度的階梯！

作一點代數運算：

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

$[L_z, L_x + iL_y] = \hbar(L_x + iL_y)$ 兩式相加

定義算子：$L_+ \equiv L_x + iL_y$ 上式可以簡化為：

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

這式與簡諧振盪中H與$a^\dagger$的對易關係完全相同！ $[H, a^\dagger] = \hbar\omega \cdot a^\dagger$

$[L_z, L_x - iL_y] = -\hbar(L_x - iL_y)$ 兩式相減，並定義：

$L_- \equiv L_+^\dagger = L_x - iL_y$ 因為$L_{x,y}$是Hermitian，所以$L_-^\dagger$是L_+的adjoint。

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

這式與H與a的對易關係完全相同！ $[H, a] = -\hbar\omega \cdot a$

a	$a^\dagger$	H
L_-	L_+	L_z

這對應關係，暗示H與L_z的能階是一樣。

$a^\dagger$	a	H
	⇕	
L_+	L_-	L_z

這裡的對應關係，幾乎讓我們立刻猜到：可以利用幾乎一樣的推導技巧。

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

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：

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

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

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

L_+可以增加L_z的本徵值一個量子$\hbar$。

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

請自己推導！

L_-可以減少L_z的本徵值一個量子$\hbar$。

可見L_z的本徵值是量子化的，一個量子是$\hbar$。

這是本課程中第二個量子化的物理量！

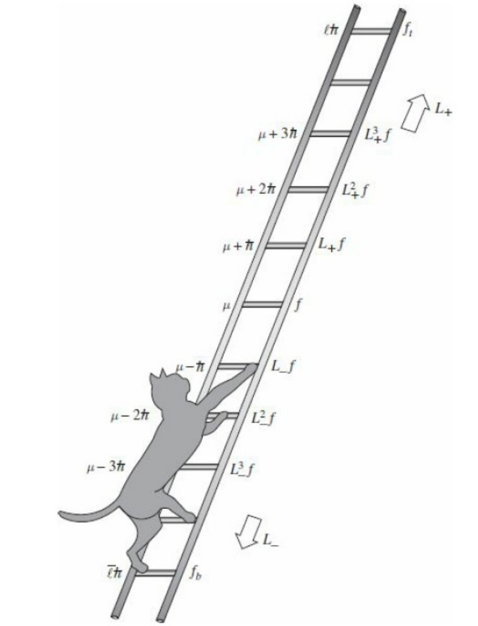
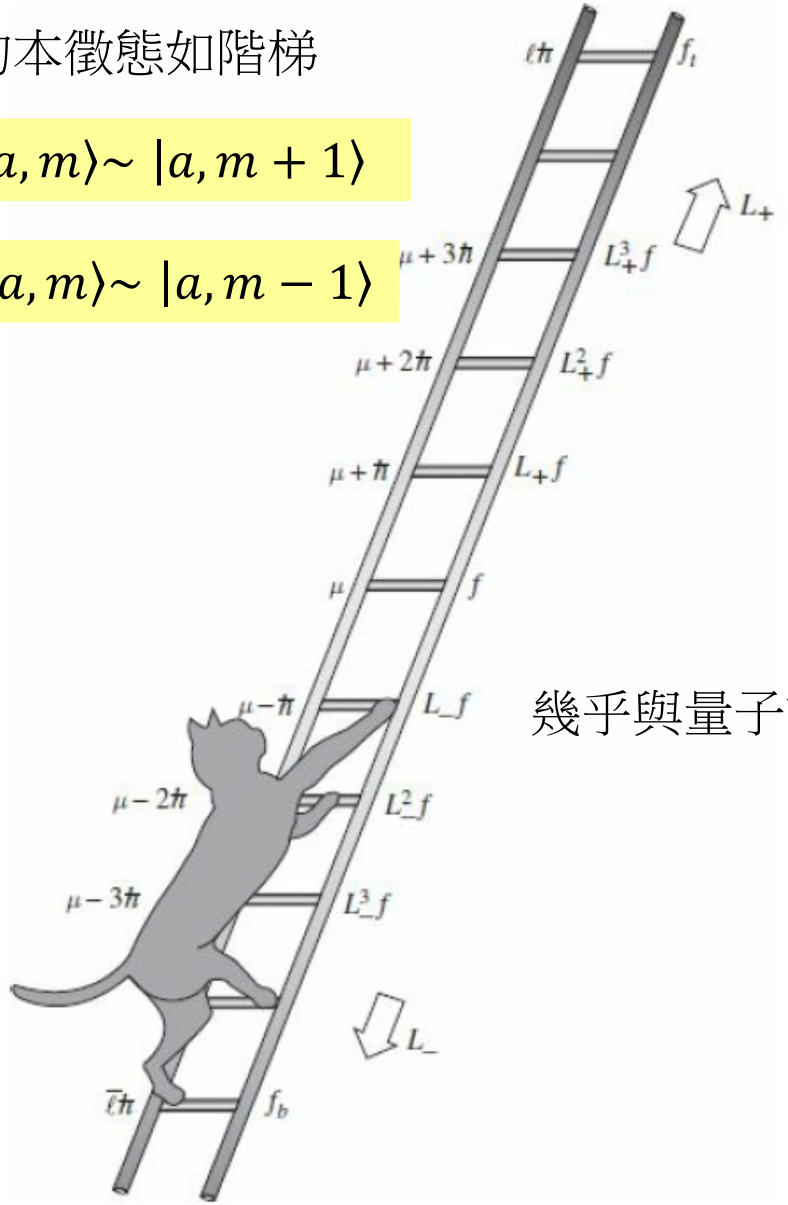


Figure 4.11: The "ladder" of angular momentum states.

L_z的本徵態如階梯

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

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



幾乎與量子簡諧振盪器一樣。

$L_\pm|a,m\rangle$是L_Z本徵態，本徵值為$(m\pm1)\hbar$，但它是L^2的本徵態嗎？

角動量任一個分量與L^2都對易，因此與$L_\pm$也對易。

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

$$L_\pm \equiv L_x \pm iL_y$$

因此： $[L^2, L_\pm] = 0$

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

$L_+|a,m\rangle$，也是L^2本徵態，本徵值依舊是$a\hbar^2$，同時是L_z的本徵態。

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

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！

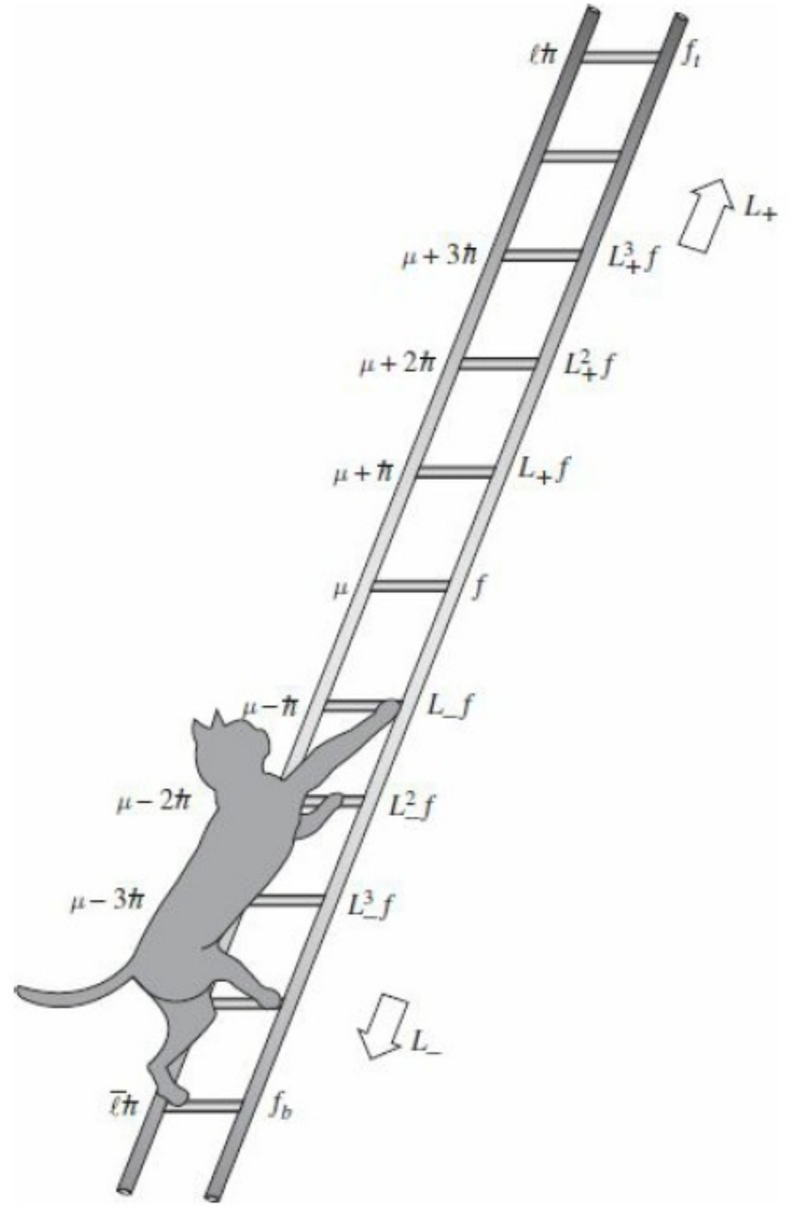


Figure 4.11: The “ladder” of angular momentum states.

特定的a的本徵態如階梯

幾乎與量子簡諧振盪器一樣。

只是量子簡諧振盪器只有一把梯子。

角動量本徵態有許多梯子對應不同的a。

L^2本徵值a有那些可能呢？

將特定的a所對應的$|a,m\rangle$（a的梯子）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（無極大值）。

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

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

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

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

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

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

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

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

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

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

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

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

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

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

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

前一頁已經得到：

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

兩式要同時成立，唯一可能是$m_{\max}$等於$-m_{\min}$：

給這個值一個新的符號：$m_{\max} = -m_{\min} \equiv l > 0$

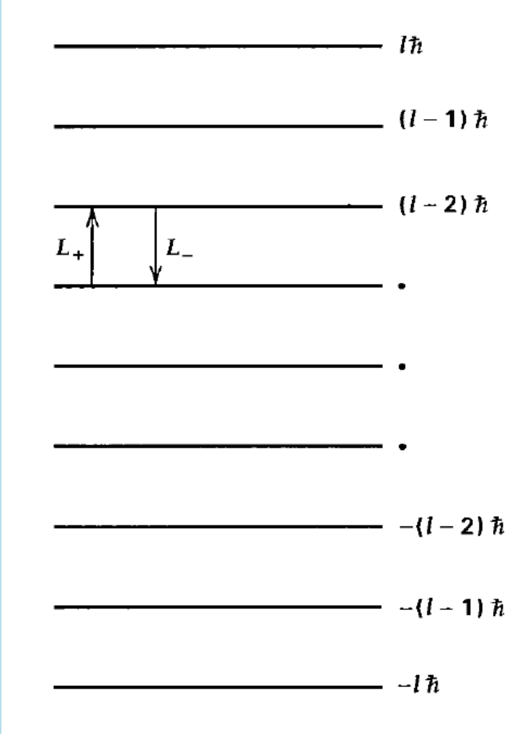
因此，m可以是介於$m_{\min}$及$m_{\max}$之間，也就是 $-l$及l之間，相差1的所有數：

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

注意：$2l$ 必須是整數！

而且：$a = l^2 + l = l(l+1)$

L^2的本徵值等於$l(l+1)$ 。



$2l$必須是整數，l可以是自然數，但也可以是半自然數，真令人驚訝！

若l是自然數，

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

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

一個l就有一個階梯！

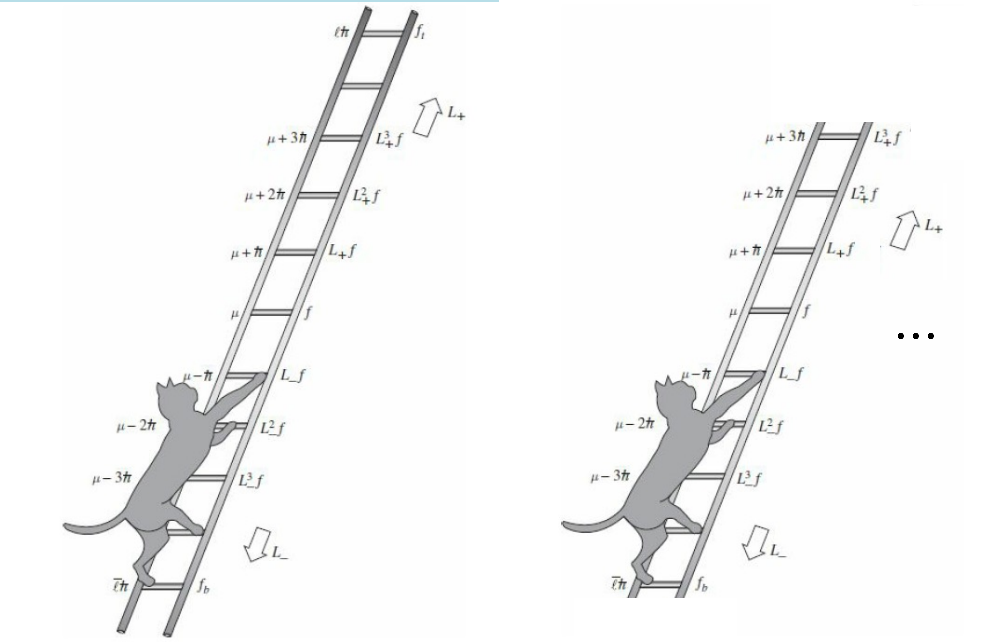
階梯有最高階、也有最低階！

階梯數目等於$2l+1$！

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！真令人驚訝！

不久會發現位置變化產生的軌道角動量$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$, 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。那就是電子的自旋。下下一章會討論。

L^2及L_z共同的本徵態，在符號上可以以量子數l取代a，並以l來歸類。

$$|a = l(l+1), m\rangle \rightarrow |l, m\rangle$$

一個l對應一系列階梯狀的本徵態，同l的階梯規則完全一樣，即使物理系統不同。

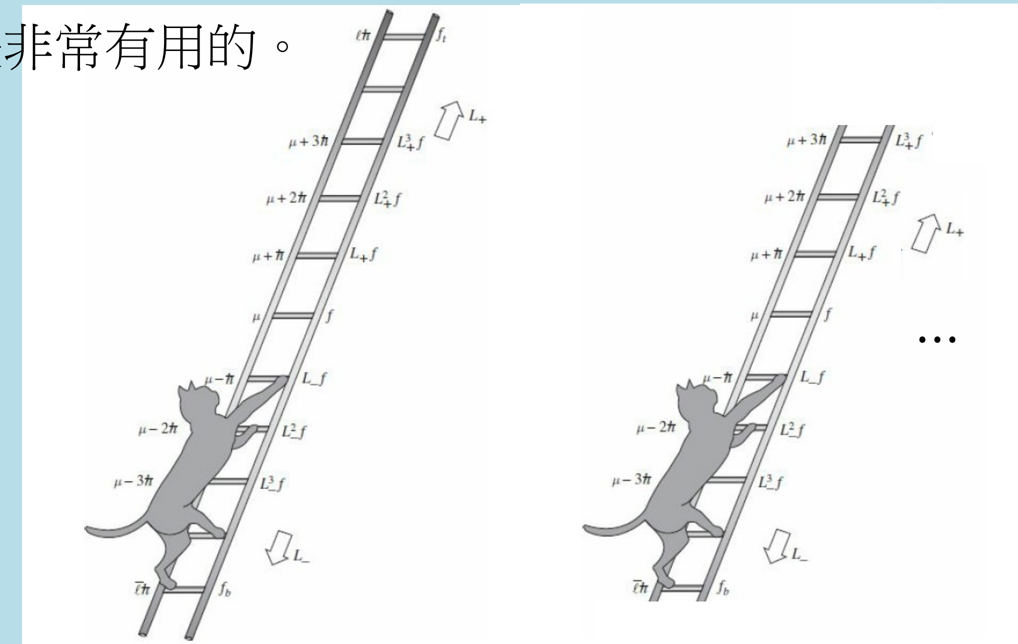
$$L^2|l, m\rangle = l(l+1)\hbar^2 \cdot |l, m\rangle$$

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

角動量大小L^2經常是守恆的，

收集特定l，即同一階梯的本徵態$|l, m\rangle$，

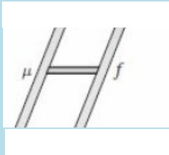
並以它們為基底組成線性空間，會是非常有用的。



特定l的這些線性空間都是有限維的，因為基底包含有限數量的態：

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

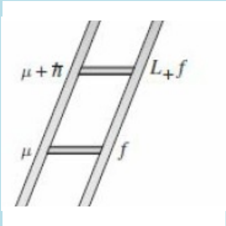
$|0,0\rangle$

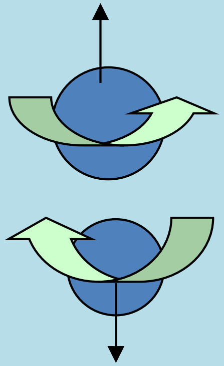


$l = 0$

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

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





$l = \frac{1}{2}$

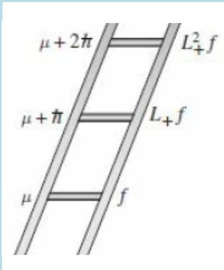
二維

對應電子自旋，注意沒有$L_Z = 0$狀態。

$|1,1\rangle$

$|1,0\rangle$

$|1,-1\rangle$



$l = 1$

三維

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。

一個粒子的狀態一般會維持在同一個空間內。

但如果角動量大小增加或減小，粒子就會在不同空間躍遷。

角動量大小是量子化的，增加或減小不會是連續的變化。$l = 0 \rightarrow 1$。

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

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

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

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

$\langle L_+Y_{l,m}|L_+Y_{l,m}\rangle =$ 　　前第五頁：

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

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

將$L_+|l,m\rangle$除以向量長度$\sqrt{(l-m)(l+m+1)}\hbar$。

就得到歸一化的$|l,m+1\rangle$：

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

倒過來：

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

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。

以上公式可以用來計算期望值。 $L_+ \equiv L_x + iL_y$ $L_- \equiv L_x - iL_y$

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

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

練習：計算 $\langle 0,0|L_x^2|0,0\rangle$

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

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

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

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

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

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

練習：計算

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

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

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

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

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

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

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

角動量大小經常守恆的，粒子通常會維持在特定l的$|l,m\rangle$為基底組成的線性空間，特定l的$|l,m\rangle$有$2l+1$個，因此這個空間為有限$2l+1$維的線性空間。

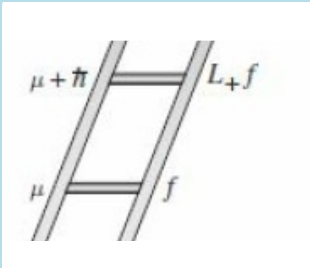
算子為此$2l+1$維線性空間的線性變換，因此可以以矩陣表示！

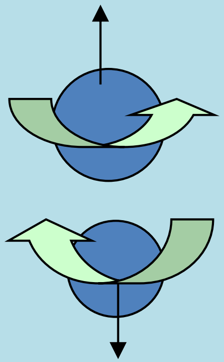
在此空間裡面，角動量的討論，可以不需要用到原來的微分算子！

現在以電子的自旋狀態為例：

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

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





$$l=\frac{1}{2}$$

$l=\frac{1}{2}$有兩個本徵態！以較為簡單的符號來代表

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

以它們為基底組成二維線性空間。

電子的自旋狀態從來沒有離開這個二維空間！

取$|\uparrow\rangle,|\downarrow\rangle$為基底，線性代數的標準符號寫成行向量：

$$|\uparrow\rangle=\begin{pmatrix}1\\0\end{pmatrix}\qquad|\downarrow\rangle=\begin{pmatrix}0\\1\end{pmatrix}$$

如何找到角動量算子對應的矩陣？

要找到算子對應的矩陣，只要算出算子對基底的作用即可，以L_+ 為例：

$L_+|\uparrow\rangle = 0$ $L_+|\downarrow\rangle = \hbar|\uparrow\rangle$

L_+算子將兩個基底向量$|\uparrow\downarrow\rangle$分別變換為兩個向量$L_+|\uparrow\downarrow\rangle$，

這兩個分量各自又可算出沿此基底$|\uparrow\downarrow\rangle$的兩個投影分量，得到四個數：

$\langle\uparrow\downarrow|L_+|\uparrow\downarrow\rangle$ 將這四個數，收集為2×2矩陣。

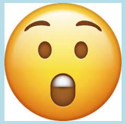
$\langle\uparrow|L_+|\uparrow\rangle = 0$ $\langle\downarrow|L_+|\uparrow\rangle = 0$ $\langle\uparrow|L_+|\downarrow\rangle = \hbar$ $\langle\downarrow|L_+|\downarrow\rangle = 0$

$L_+ \sim \hbar\begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$ $\langle j|L_+|i\rangle \equiv L_{+\,ji}$ $\langle\uparrow|L_+|\downarrow\rangle = \hbar \equiv L_{+\,12}$

同理：

$L_-|\uparrow\rangle = \hbar|\downarrow\rangle$ $L_-|\downarrow\rangle = 0$

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



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

線性空間上的一個線性變換，完全由它對基底的作用所決定。

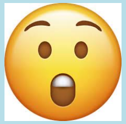
L_{-}, L_{+}對基底的變換，與上述矩陣相同，因此L_{-}, L_{+}可以使用矩陣來代表：

$$L_{+}\left|\frac{1}{2},\frac{1}{2}\right\rangle = 0 \quad \rightarrow \quad \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = 0$$

$$L_{+}\left|\frac{1}{2},-\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},\frac{1}{2}\right\rangle \quad \rightarrow \quad \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = \hbar\begin{pmatrix} 1 \\ 0 \end{pmatrix}$$

$$L_{-}\left|\frac{1}{2},\frac{1}{2}\right\rangle = \hbar\left|\frac{1}{2},-\frac{1}{2}\right\rangle \quad \rightarrow \quad \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 1 \\ 0 \end{pmatrix} = \hbar\begin{pmatrix} 0 \\ 1 \end{pmatrix}$$

$$L_{-}\left|\frac{1}{2},-\frac{1}{2}\right\rangle = 0 \quad \rightarrow \quad \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix}\begin{pmatrix} 0 \\ 1 \end{pmatrix} = 0$$



算子作用於ket就是矩陣乘行向量！ $L_{-} = \hbar \begin{pmatrix} 0 & 0 \\ 1 & 0 \end{pmatrix} \qquad L_{+} = \hbar \begin{pmatrix} 0 & 1 \\ 0 & 0 \end{pmatrix}$

角動量算子作用於ket得到另一ket，可看成矩陣乘上行向量，得到另一個行向量。

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

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

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，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。

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

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！

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。

只有整數l(不能是半整數)，角動量才能寫成空間微分：

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

不久會發現位置變化產生的軌道角動量$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$, 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。那就是電子的自旋。下下一章會討論。

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

$$\begin{pmatrix} |1,1\rangle \\ |1,0\rangle \\ |1,-1\rangle \end{pmatrix} \qquad l = 1 \qquad \text{Triplet 3}$$

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！

In general: $[L_x^2, L_y^2] \neq 0$

For $l = 1$, $[L_x^2, L_y^2] = [L_x^2, L_z^2] = [L_z^2, L_y^2] = 0$

```
In[6]:=
LX = {{0, 1, 0}, {1, 0, 1}, {0, 1, 0}}
Out[6]= {{0, 1, 0}, {1, 0, 1}, {0, 1, 0}}

In[16]:= LY = {{0, -1, 0}, {1, 0, -1}, {0, 1, 0}}
Out[16]= {{0, -1, 0}, {1, 0, -1}, {0, 1, 0}}

In[17]:= LX // MatrixForm
Out[17]//MatrixForm=
(0 1 0)
(1 0 1)
(0 1 0)

In[18]:= LY // MatrixForm
Out[18]//MatrixForm=
(0 -1  0)
(1  0 -1)
(0  1  0)

LX.LX // MatrixForm
Out[19]= {{0, -1, 0}, {1, 0, -1}, {0, 1, 0}}
Out[20]//MatrixForm=
(1 0 1)
(0 2 0)
(1 0 1)

In[21]:= LY.LY // MatrixForm
Out[21]//MatrixForm=
(-1  0  1)
( 0 -2  0)
( 1  0 -1)

In[23]:= LX.LX.LY.LY  // MatrixForm
Out[23]//MatrixForm=
(0  0 0)
(0 -4 0)
(0  0 0)

In[24]:= LY.LY.LX.LX  // MatrixForm
Out[24]//MatrixForm=
(0  0 0)
(0 -4 0)
(0  0 0)
```

In[25]:=

```
LX = {{0, Sqrt[3], 0, 0}, {Sqrt[3], 0, 2, 0}, {0, 2, 0, Sqrt[3]}, {0, 0, Sqrt[3], 0}}
```

Out[25]= $\{\{0, \sqrt{3}, 0, 0\}, \{\sqrt{3}, 0, 2, 0\}, \{0, 2, 0, \sqrt{3}\}, \{0, 0, \sqrt{3}, 0\}\}$

In[27]:=

```
LY = {{0, -Sqrt[3], 0, 0},
  {Sqrt[3], 0, -2, 0}, {0, 2, 0, -Sqrt[3]}, {0, 0, Sqrt[3], 0}}
```

Out[27]= $\{\{0, -\sqrt{3}, 0, 0\}, \{\sqrt{3}, 0, -2, 0\}, \{0, 2, 0, -\sqrt{3}\}, \{0, 0, \sqrt{3}, 0\}\}$

In[26]:=

```
LX // MatrixForm
```

Out[26]//MatrixForm=

$$\begin{pmatrix} 0 & \sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & 2 & 0 \\ 0 & 2 & 0 & \sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

In[28]:=

```
LY // MatrixForm
```

Out[28]//MatrixForm=

$$\begin{pmatrix} 0 & -\sqrt{3} & 0 & 0 \\ \sqrt{3} & 0 & -2 & 0 \\ 0 & 2 & 0 & -\sqrt{3} \\ 0 & 0 & \sqrt{3} & 0 \end{pmatrix}$$

```
LX.LX // MatrixForm
```

Out[29]= $\{\{0, -1, 0\}, \{1, 0, -1\}, \{0, 1, 0\}\}$

Out[30]//MatrixForm=

$$\begin{pmatrix} 3 & 0 & 2\sqrt{3} & 0 \\ 0 & 7 & 0 & 2\sqrt{3} \\ 2\sqrt{3} & 0 & 7 & 0 \\ 0 & 2\sqrt{3} & 0 & 3 \end{pmatrix}$$

In[31]:=

```
LY.LY // MatrixForm
```

Out[31]//MatrixForm=

$$\begin{pmatrix} -3 & 0 & 2\sqrt{3} & 0 \\ 0 & -7 & 0 & 2\sqrt{3} \\ 2\sqrt{3} & 0 & -7 & 0 \\ 0 & 2\sqrt{3} & 0 & -3 \end{pmatrix}$$

In[32]:=

```
LX.LX.LY.LY  // MatrixForm
```

Out[32]//MatrixForm=

$$\begin{pmatrix} 3 & 0 & -8\sqrt{3} & 0 \\ 0 & -37 & 0 & 8\sqrt{3} \\ 8\sqrt{3} & 0 & -37 & 0 \\ 0 & -8\sqrt{3} & 0 & 3 \end{pmatrix}$$

In[33]:=

```
LY.LY.LX.LX  // MatrixForm
```

Out[33]//MatrixForm=

$$\begin{pmatrix} 3 & 0 & 8\sqrt{3} & 0 \\ 0 & -37 & 0 & -8\sqrt{3} \\ -8\sqrt{3} & 0 & -37 & 0 \\ 0 & 8\sqrt{3} & 0 & 3 \end{pmatrix}$$

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

$$[L_x^2, L_y^2] \neq 0$$

L^2及L_z共同的本徵態$|l,m\rangle$對應的狀態函數$\psi_{lm}(r,\theta,\phi)$可以解出嗎？

$$L^2\psi_{lm}(r,\theta,\phi) = l(l+1)\psi_{lm}(r,\theta,\phi)$$

$$L_z\psi_{lm}(r,\theta,\phi) = m\hbar\psi_{lm}(r,\theta,\phi)$$

首先要將 L^2, L_z表示為極座標的微分$\frac{\partial}{\partial r},\frac{\partial}{\partial \theta},\frac{\partial}{\partial \phi}$ ！

我們將推導：L^2, L_z與$r, \frac{\partial}{\partial r}$都無關，只包含$\theta, \phi, \frac{\partial}{\partial \theta}, \frac{\partial}{\partial \phi}$！

這暗示ψ_{lm}可以分解為r的函數與θ, ϕ的函數之乘積。

$$\psi_{lm}(r,\theta,\phi) = R(r)\cdot Y_{lm}(\theta,\phi)$$

對L^2及L_z來說r如同常數，$R(r)$可以提出來，兩邊抵消：

$$L_z R(r)\cdot Y_{lm}(\theta,\phi) = R\cdot L_z Y_{lm} = m\hbar R\cdot Y$$

⇓

$$L_z Y_{lm}(\theta,\phi) = m\hbar Y_{lm}(\theta,\phi)$$

同理：

$$L^2 Y_{lm}(\theta,\phi) = l(l+1) Y_{lm}(\theta,\phi)$$

$Y_{lm}(\theta,\phi)$稱為Spherical Harmonics

換句話說，Y_{lm}的決定與$R(r)$無關，有時就直接說Y_{lm}是L^2及L_z的本徵函數。

如何解出$Y_{lm}(\theta,\phi)$？

回憶簡諧振盪的定態狀態函數的求解，我們從基態出發。

連續使用a降低能量，必須有停止之處$|0\rangle$，基態滿足以下條件：

$$a|0\rangle = 0$$

$$m\omega \cdot x u_0(x) + \hbar \frac{d}{dx} u_0(x) = 0$$

由基態可以$a^\dagger$作用得出所有本徵態。

$$\psi_n(x) = \frac{1}{\sqrt{n!}}\left(a^\dagger\right)^n|0\rangle$$

我們可以套用相同的策略：

角動量則有最大m值的本徵態$|l, m = m_{\max} = l\rangle$，它滿足：

$$L_+|l,l\rangle = 0$$

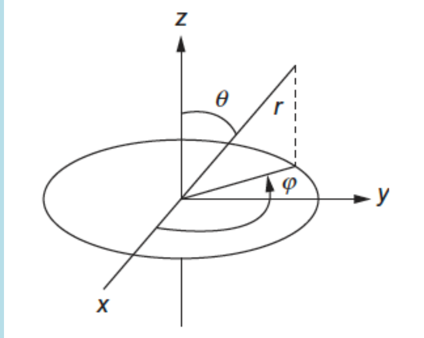
$$L_+Y_{ll}(\theta,\phi) = 0$$

由$|l,l\rangle$可以L_-作用得出其他L^2, L_z本徵態。

$$Y_{lm}(\theta,\phi) \propto (L_-)^{l-m}Y_{ll}(\theta,\phi)$$

首先必須將$L^2, L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right), L_\pm$表示為極座標的微分$\frac{\partial}{\partial r}, \frac{\partial}{\partial \theta}, \frac{\partial}{\partial \phi}$ ！

直接但繁瑣的做法



角動量算子$-i\hbar\left(x\frac{\partial}{\partial y}-y\frac{\partial}{\partial x}\right)$可以表示為極座標的微分！

$$r=\sqrt{x^2+y^2+z^2}\qquad \theta=\cos^{-1}\frac{z}{r}\qquad \phi=\tan^{-1}\frac{y}{x}$$

首先要將座標微分，先表示為極座標的微分，例如：

$$\frac{\partial}{\partial y}=\frac{\partial r}{\partial y}\frac{\partial}{\partial r}+\frac{\partial \theta}{\partial y}\frac{\partial}{\partial \theta}+\frac{\partial \phi}{\partial y}\frac{\partial}{\partial \phi}$$

需要九個偏微分為係數。

式中的偏微分保留一般座標的形式會使式子簡單。

$$\frac{\partial r}{\partial y}=\frac{y}{r}\qquad \frac{\partial r}{\partial x}=\frac{x}{r}\qquad \frac{\partial r}{\partial z}=\frac{z}{r}$$

$$\frac{\partial \theta}{\partial y}=\frac{1}{\sqrt{1-\frac{z^2}{r^2}}}\frac{z}{r^2}\frac{y}{r}=\frac{z}{r^2\sqrt{r^2-z^2}}y=\frac{\cos\theta}{r^2\sin\theta}y$$

$$\frac{\partial \theta}{\partial x}=\frac{z}{r^2\sqrt{r^2-z^2}}x=\frac{\cos\theta}{r^2\sin\theta}x$$

$$\frac{\partial \theta}{\partial z}=\frac{1}{\sqrt{1-\frac{z^2}{r^2}}}\left[\frac{z}{r^2}\left(\frac{z}{r}\right)-\frac{1}{r}\right]=-\frac{\sqrt{r^2-z^2}}{r^2}=-\frac{\sin\theta}{r}$$

$$\frac{\partial \phi}{\partial z}=0$$

$$\frac{\partial \phi}{\partial x}=-\frac{1}{1+\frac{y^2}{x^2}}\frac{y}{x^2}=-\frac{y}{x^2+y^2}=-\frac{1}{r}\frac{\sin\phi}{\sin\theta}$$

$$\frac{\partial \phi}{\partial y}=-\frac{1}{1+\frac{y^2}{x^2}}\frac{1}{x}=\frac{x}{x^2+y^2}=\frac{1}{r}\frac{\cos\phi}{\sin\theta}$$

將相關的極座標微分代入以下一般微分的式子：

$$\frac{\partial}{\partial y}=\frac{\partial r}{\partial y}\frac{\partial}{\partial r}+\frac{\partial \theta}{\partial y}\frac{\partial}{\partial \theta}+\frac{\partial \phi}{\partial y}\frac{\partial}{\partial \phi}$$

$$\frac{\partial r}{\partial y}=\frac{y}{r}\qquad \frac{\partial \theta}{\partial y}=\frac{z}{r^2\sqrt{r^2-z^2}}y\qquad \frac{\partial \phi}{\partial y}=\frac{x}{x^2+y^2}$$

再將一般微分代入角動量算子的定義，得到以極座標微分表示的定義：

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

$$=-i\hbar\left(x\cdot\frac{y}{r}\frac{\partial}{\partial r}+x\frac{zy}{r^2\sqrt{r^2-z^2}}\frac{\partial}{\partial \theta}+x\cdot\frac{x}{x^2+y^2}\frac{\partial}{\partial \phi}\right)$$

$$+i\hbar\left(y\cdot\frac{x}{r}\frac{\partial}{\partial r}+y\frac{zx}{r^2\sqrt{r^2-z^2}}\frac{\partial}{\partial \theta}-y\cdot\frac{y}{x^2+y^2}\frac{\partial}{\partial \phi}\right)$$

括號內的第一項對r的偏微分正好彼此抵消，角動量只與角度座標有關。

括號內的第二項對θ的偏微分也正好彼此抵消，角動量只與角度座標ϕ有關。

繞z軸旋轉正好對應ϕ的變化：

$$L_z=-i\hbar\frac{\partial}{\partial \phi}$$

L_x也可以以同樣手續得到：

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

$$= -i\hbar\left(y\cdot\frac{z}{r}\frac{\partial}{\partial r} - y\frac{\sqrt{r^2-z^2}}{r^2}\frac{\partial}{\partial\theta}\right)$$

$$+i\hbar\left(z\cdot\frac{y}{r}\frac{\partial}{\partial r} + z\frac{zy}{r^2\sqrt{r^2-z^2}}\frac{\partial}{\partial\theta} + z\cdot\frac{y}{x^2+y^2}\frac{\partial}{\partial\phi}\right)$$

$$\frac{\partial\theta}{\partial z} = - -\frac{\sqrt{r^2-z^2}}{r^2}$$

$$\frac{\partial\phi}{\partial z} = 0$$

如預料的對r的偏微分消掉了。

$$= -i\hbar\left(-y\frac{\sqrt{r^2-z^2}}{r^2}\frac{\partial}{\partial\theta} - y\frac{z^2}{r^2\sqrt{r^2-z^2}}\frac{\partial}{\partial\theta} - z\cdot\frac{y}{x^2+y^2}\frac{\partial}{\partial\phi}\right)$$

$$= -i\hbar\left(-\frac{y}{\sqrt{r^2-z^2}}\frac{\partial}{\partial\theta} - z\cdot\frac{y}{x^2+y^2}\frac{\partial}{\partial\phi}\right)$$

換成極座標： $y = r\sin\theta\sin\phi, z = r\cos\theta$

$$L_x = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_y = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

簡潔但較抽象的做法。

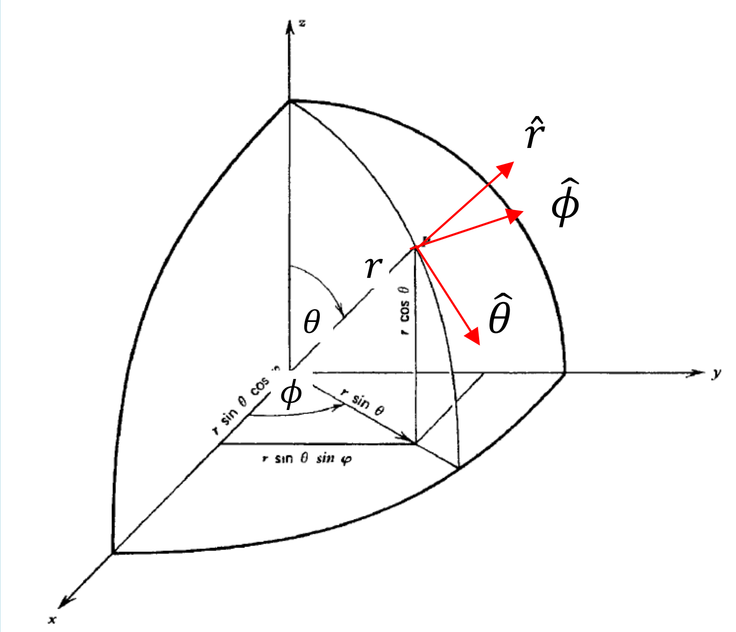
極座標的變化$dr, d\theta, d\phi$所對應的位移，方向$\hat{r}, \hat{\theta}, \hat{\phi}$在每一點都彼此垂直，可以作為一組垂直基底，只是在不同位置不互相平行！

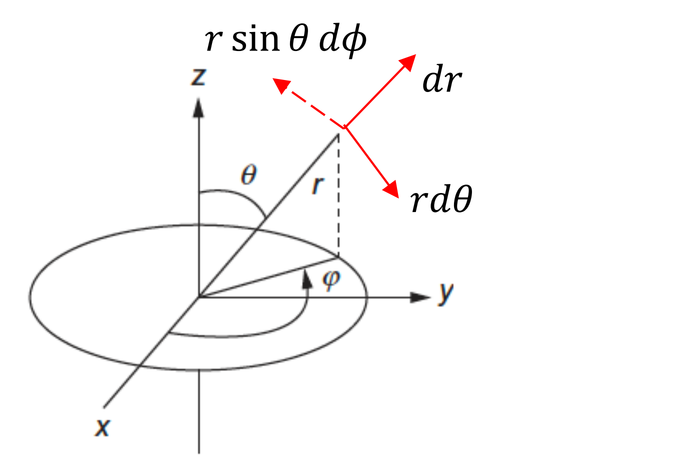
位移大小與極座標的變化成正比：

$$ds_r = dr \qquad ds_\theta = r d\theta \qquad ds_\phi = r \sin\theta \, d\phi$$

因此可以寫成位移向量：

$$d\vec{s} = \hat{r} \cdot dr + \hat{\theta} \cdot r d\theta + \hat{\phi} \cdot r \sin\theta \, d\phi$$





$\hat{r},\hat{\theta},\hat{\phi}$為一組垂直基底，各個方向的位移可以寫成：

$$ds_r = dr \qquad ds_\theta = r\,d\theta \qquad ds_\phi = r\sin\theta\, d\phi$$

梯度向量便可定義於這個垂直基底之上，分量就是沿各個方向的變化率：

$$\vec{\nabla}\psi \equiv \hat{r}\cdot\frac{\partial\psi}{\partial r} + \hat{\theta}\cdot\frac{1}{r}\frac{\partial\psi}{\partial\theta} + \hat{\phi}\cdot\frac{1}{r\sin\theta}\frac{\partial\psi}{\partial\phi}$$

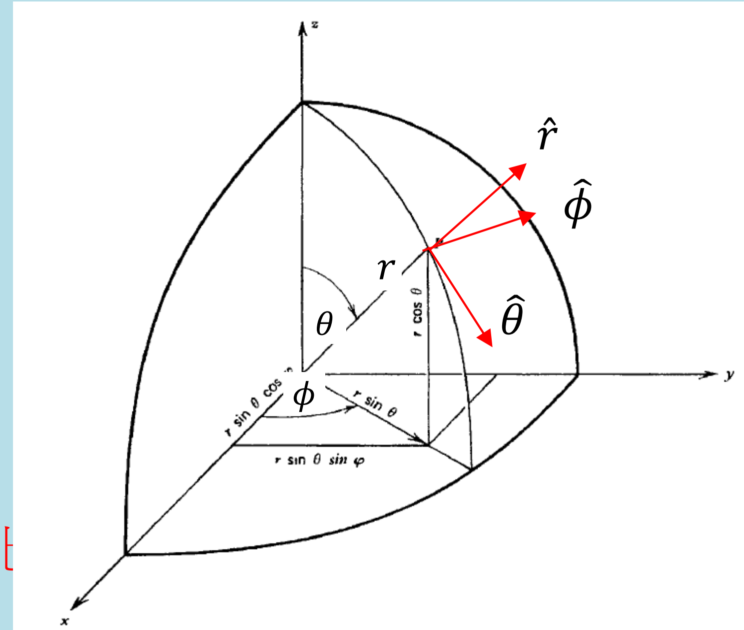
將此式代入角動量的向量定義，動量向量就是梯度向量：

$$\vec{L} = \vec{r}\times\vec{p} = -i\hbar\vec{r}\times\vec{\nabla} = -i\hbar\left[(\vec{r}\times\hat{r})\cdot\frac{\partial}{\partial r} + (\vec{r}\times\hat{\theta})\cdot\frac{1}{r}\frac{\partial}{\partial\theta} + (\vec{r}\times\hat{\phi})\cdot\frac{1}{r\sin\theta}\frac{\partial}{\partial\phi}\right]$$

利用基底的垂直特性： $\vec{r}\times\hat{\theta} = r\cdot\hat{r}\times\hat{\theta} = r\hat{\phi}$ $\quad \vec{r}\times\hat{\phi} = -r\hat{\theta}$

角動量以極座標表示的向量定義非常簡單：

$$\vec{L} = -i\hbar\left(\hat{\phi}\cdot\frac{\partial}{\partial\theta} - \hat{\theta}\cdot\frac{1}{\sin\theta}\frac{\partial}{\partial\phi}\right)$$



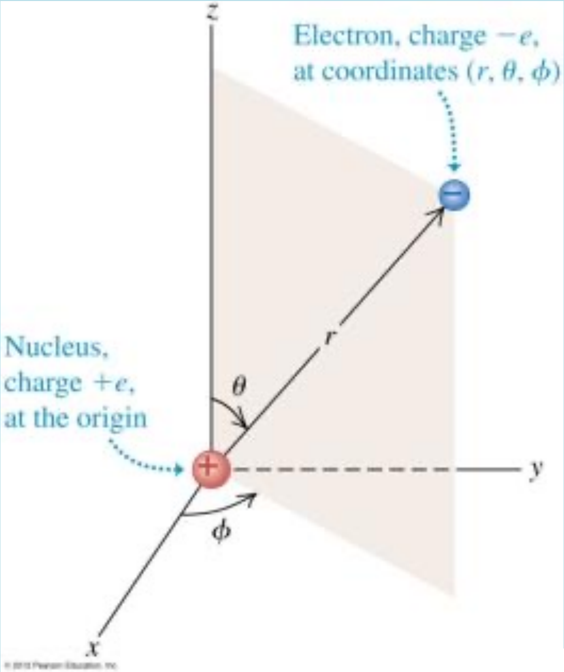
角動量分量以極座標表示也非常簡單：

利用: $\hat{e}_z\cdot\hat{\phi} = 0$ $\quad \hat{e}_z\cdot\hat{\theta} = \sin\theta$

$$L_z = \hat{e}_z\cdot\vec{L} = -i\hbar\frac{\partial}{\partial\phi}$$

L_z就是ϕ的微分，與r,θ無關。這是很重要的簡化

不意外，繞z軸的旋轉正好就是ϕ獨自的變化！



$$L_z = -i\hbar\frac{\partial}{\partial\phi}$$

L_z就是ϕ的微分，不含θ, r的微分，Y_{lm}是L_z的本徵態。

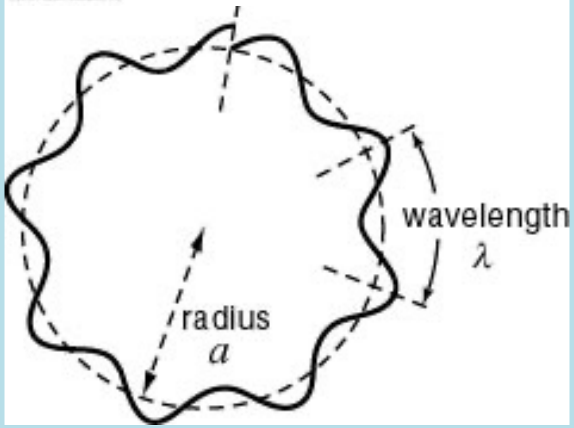
$$L_z Y_{lm}(\theta,\phi) = -i\hbar\frac{\partial Y_{lm}(\theta,\phi)}{\partial\phi} = m\hbar Y_{lm}(\theta,\phi)$$

立刻可解出Y與ϕ的關係。

$$Y_{lm}(\theta,\phi) \equiv P(\theta)\cdot e^{im\phi}$$

L_z與θ無關，前面的P可以是θ的函數。

因此波函數與三個極座標的關係分離於三個個別的函數。



要求波函數繞一圈ϕ加2π後值不變。 $e^{im\cdot 2\pi} = 1$

$m = \text{integer}$ 注意：不會是半整數。

確認L_z的本徵值為量子化$m\hbar$。這一次得到波函數了。

注意：是週期性條件確定L_z的本徵值為量子化，m是整數。

將此解運用於氫原子內的電子：

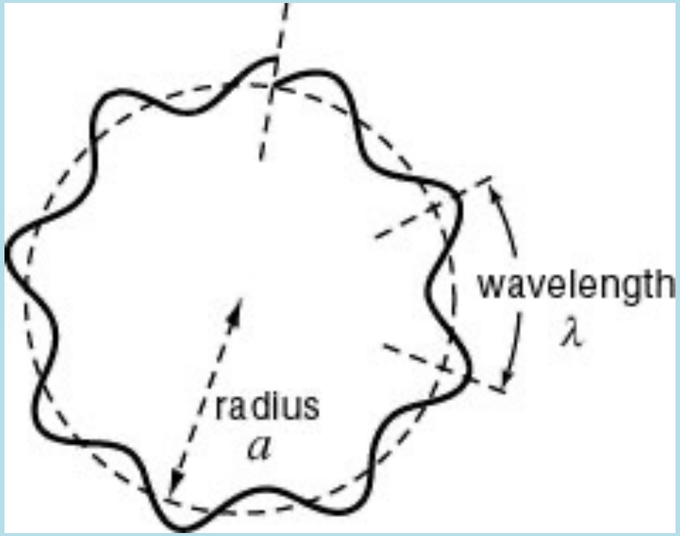
若將$e^{im\phi}$大概看成在圓形軌道一維空間上傳播的波，就類似德布羅意的想法。

$$e^{im\phi} = e^{i\left(\frac{m}{r}\right)(r\phi)} \sim e^{ikx}$$

$$p = \hbar k = \hbar\frac{m}{r}$$

$$p \cdot r = L = m\hbar$$

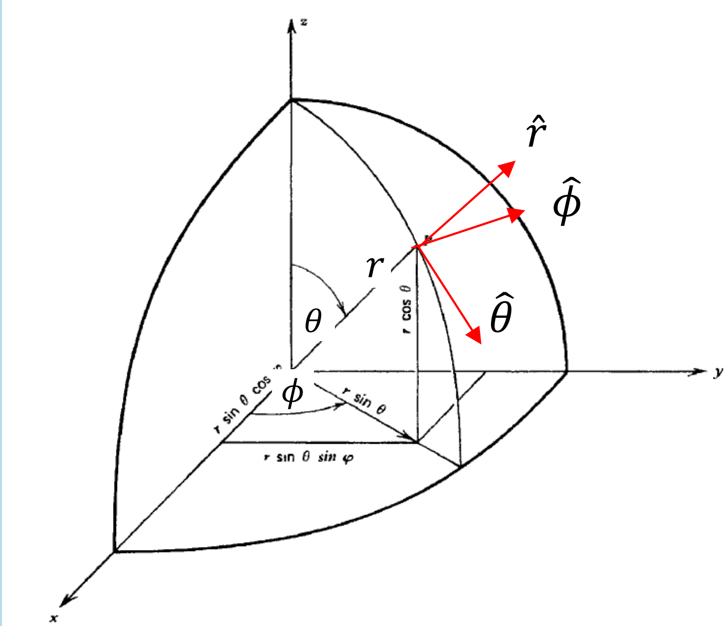
波函數在圓周上必須一致，圓周長等於波長整數倍。角動量必須量子化！



這就是為什麼當初德布羅意的推理是有一點合理性的。

Y_{lm}也是L^2的本徵態，$P(\theta)$必須由這關係得出。L^2就與$L_{x,y}$有關。

$L_{x,y}$也可以用類似方法寫成極座標微分：



$$\vec{L} = -i\hbar\left(\hat{\phi}\cdot\frac{\partial\psi}{\partial\theta} - \hat{\theta}\cdot\frac{1}{\sin\theta}\frac{\partial\psi}{\partial\phi}\right)$$

$$\hat{e}_x\cdot\hat{\phi} = -\sin\phi \qquad \hat{e}_x\cdot\hat{\theta} = \cos\phi\cos\theta$$

$$L_x = \hat{e}_x\cdot\vec{L} = -i\hbar\left(-\sin\phi\frac{\partial}{\partial\theta} - \cos\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$\hat{e}_y\cdot\hat{\phi} = -\cos\phi \qquad \hat{e}_y\cdot\hat{\theta} = \sin\phi\cos\theta$$

$$L_y = \hat{e}_y\cdot\vec{L} = -i\hbar\left(\cos\phi\frac{\partial}{\partial\theta} - \sin\phi\cot\theta\frac{\partial}{\partial\phi}\right)$$

利用$L_\pm$計算L^2比較容易：

$$L_+ = L_x + iL_y = \hbar(\cos\phi + i\sin\phi)\frac{\partial}{\partial\theta} + (\cos\phi + i\sin\phi)i\cot\theta\frac{\partial}{\partial\phi}$$

$$= \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_\pm = L_x \pm iL_y = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right)$$

$$L_{\pm} = \pm\hbar e^{\pm i\phi}\left(\frac{\partial}{\partial\theta} \pm i\cot\theta\frac{\partial}{\partial\phi}\right)$$

可以利用此式得到L^2：$L^2 = L_+L_- + L_z^2 - \hbar L_z$

$e^{-i\phi}$卡在中間，但對它有作用的就是$\frac{\partial}{\partial\phi}$，

$$L_+L_- = -\hbar^2 e^{+i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)e^{-i\phi}\left(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi}\right)$$

$e^{-i\phi}$的微分$\frac{\partial}{\partial\phi}$得$-ie^{-i\phi}$，

$$= -\hbar^2 e^{+i\phi}e^{-i\phi}\left(\frac{\partial}{\partial\theta} + \cot\theta + i\cot\theta\frac{\partial}{\partial\phi}\right)\left(\frac{\partial}{\partial\theta} - i\cot\theta\frac{\partial}{\partial\phi}\right)$$

加一項$\cot\theta$後，$e^{-i\phi}$可以提到前面。

$$= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} - i\cot^2\theta\frac{\partial}{\partial\phi} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + i\cot^2\theta\frac{\partial}{\partial\phi} + i\frac{\partial}{\partial\phi}\right)$$

$$= -\hbar^2\left(\frac{\partial^2}{\partial\theta^2} + \cot\theta\frac{\partial}{\partial\theta} + \cot^2\theta\frac{\partial^2}{\partial\phi^2} + i\frac{\partial}{\partial\phi}\right)$$

$$L^2 = L_+L_- + L_z^2 - \hbar L_z$$

$$L_z = -i\hbar\frac{\partial}{\partial\phi} \qquad L_z^2 = -\hbar^2\frac{\partial^2}{\partial\phi^2}$$

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

沒有交叉項$\frac{\partial}{\partial\theta}, \frac{\partial}{\partial\phi}$！

It is fairly straightforward to calculate 另一個推導：

$$\mathbf{L}^2 = L_x^2 + L_y^2 + L_z^2$$

$$-\hbar^2\left[\left(-\sin\varphi\frac{\partial}{\partial\theta} - \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)\left(-\sin\varphi\frac{\partial}{\partial\theta} - \cot\theta\cos\varphi\frac{\partial}{\partial\varphi}\right)\right.$$

$$\left.+\left(\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right)\left(\cos\varphi\frac{\partial}{\partial\theta} - \cot\theta\sin\varphi\frac{\partial}{\partial\varphi}\right) + \frac{\partial^2}{\partial\varphi^2}\right]$$

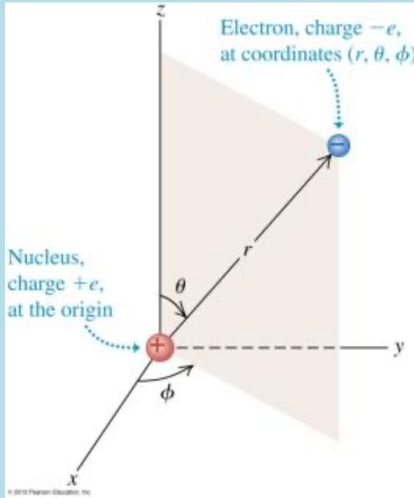
$$L^2 = -\hbar^2\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]$$

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

注意：L^2與r無關。L^2, L_z都與r無關。

這就是一開始可以寫$\psi_{lm}(r,\theta,\phi) = R(r)\cdot Y_{lm}(\theta,\phi)$的原因。

$Y_{lm}(\theta,\phi)$就是L^2的本徵態。



$$L^2 Y_{lm} = -\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y_{lm}}{\partial\theta}\right) - \frac{1}{\sin^2\theta}\frac{\partial^2 Y_{lm}}{\partial\phi^2} = l(l+1)Y_{lm}$$

代入已知的：$Y_{lm}(\theta,\phi) = P(\theta)\cdot\frac{1}{\sqrt{2\pi}}e^{im\phi}$

$$\frac{1}{\sin\theta}e^{im\phi}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial P}{\partial\theta}\right) + \frac{1}{\sin^2\theta}P\frac{\partial^2 e^{im\phi}}{\partial\phi^2} = -l(l+1)P\cdot e^{im\phi}$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right) - \frac{1}{\sin^2\theta}m^2 P + l(l+1)P = 0$$

注意偏微分可以改為常微分。

這是解$P(\theta)$的方程式。可見$P(\theta)\equiv P_l^m(\theta)$同時與兩個量子數$l,m$有關。

此式只與m^2有關，因此$P_l^m(\theta)$與$P_l^{-m}(\theta)$滿足同樣的式子：$P_l^m(\theta) = P_l^{-m}(\theta)$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP_l^m}{d\theta}\right)-\frac{1}{\sin^2\theta}m^2P_l^m+l(l+1)P_l^m=0$$

這解$P_l^m(\theta)$的方程式就是標準的Associated Legendre Equation。

它的解$P_l^m(\theta)$就是標準的Associated Legendre Function。

在特殊的情況$m=0$，方程式簡化為標準的Legendre Equation：

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP_l^0}{d\theta}\right)+l(l+1)P_l^0=0$$

它的解$P_l^0(\theta)$就是標準的Legendre Function。

$P_l^m(\theta)$可以由$P_l^0(\theta)$的微分得出。

它們都出現在古典物理以極座標表示的波動方程式(適用於球形邊界條件)，

在角度相關的波函數，古典波動方程式與薛丁格波方程式幾乎完全一致。

方法一：直接求解微分方程式Associated Legendre Equation ！

將$l(l+1)$依舊記為κ以簡化符號，同時也可以方程式求解再次確認l是整數！

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{dP(\theta)}{d\theta}\right)+\left(\kappa-\frac{m^2}{\sin^2\theta}\right)P(\theta)=0$$

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin^2\theta\frac{dP(\theta)}{\sin\theta\,d\theta}\right)+\left(\kappa-\frac{m^2}{\sin^2\theta}\right)P(\theta)=0$$

變更變數：$z\equiv\cos\theta,\ 0<z^2<1$ $\quad 1-z^2=\sin^2\theta$

$$\frac{d}{d\theta}=\frac{dz}{d\theta}\frac{d}{dz}=-\sin\theta\frac{d}{dz}$$

$$\frac{d}{dz}\left[(1-z^2)\frac{dP(z)}{dz}\right]+\left(\kappa-\frac{m^2}{1-z^2}\right)P(\theta)=0$$

$$(1-z^2)\frac{d^2P(z)}{dz^2}-2z\frac{dP(z)}{dz}+\left(\kappa-\frac{m^2}{\sin^2\theta}\right)P(z)=0$$

先考慮$m=0$的情況：Legendre E. 會有多項式解，$m\neq 0$的解可由此解得到。

$$(1-z^2)\frac{d^2P(z)}{dz^2}-2z\frac{dP(z)}{dz}+\kappa P(z)=0$$

解會是一個有限次l多項式：$P(z)=\sum_{i=0}^{l}a_i z^i$

代入微分方程式，各項取最高次項：

$$-z^2 l(l-1)a_l z^{l-2}-2zla_l z^{l-1}+\kappa a_l z^l=0$$

$$-l(l-1)a_l z^l-2la_l z^l+\kappa a_l z^l=0$$

$$\kappa=l(l+1)$$

確認角動量大小$\hat{L}^2$的本徵值λ為$l(l+1)\hbar$。

而且證實軌道角動量，l必須是正整數。半整數是不允許的！

Legendre Equation：

$$(1-z^2)\frac{d^2P(z)}{dz^2}-2z\frac{dP(z)}{dz}+\kappa P(z)=0$$

解會是一個有限次多項式：

$$P(z)=\sum_{i=0}^{l}a_i z^i$$

代入微分方程式：

$$(1-z^2)\sum_{i=2}^{l}i(i-1)a_i z^{i-2}-2z\sum_{i=2}^{l}i a_i z^{i-1}+\kappa\sum_{i=0}^{l}a_i z^i=0$$

$$\sum_{i=2}^{l}i(i-1)a_i z^{i-2}-\sum_{i=2}^{l}i(i-1)a_i z^i-\sum_{i=1}^{l}2i a_i z^i+\kappa\sum_{i=0}^{l}a_i z^i=0$$

取z^k的係數為零

$$(k+1)(k+2)a_{k+2}=[k(k-1)-2k-\kappa]a_k$$

$$a_{k+2}=\frac{k(k+1)-\kappa}{(k+1)(k+2)}a_k$$

Recursion Relation

$$a_{k+2} = \frac{k(k+1)-\kappa}{(k+1)(k+2)} a_k$$ Recursion Relation

如果κ不是整數，這個遞迴關係會一直繼續到$k \to \infty$。

而當k很大時， $a_{k+2} = \frac{k(k+1)-\kappa}{(k+1)(k+2)} a_k \to 1 a_k$ 。

$$P(z) = \sum_{i=0}^{\infty} a_i z^i \leftrightarrow \sum_{i=0}^{\infty} z^i = 1 + z + z^2 + z^3 + \cdots = \frac{1}{1-z}$$

兩者的差是有限的。

$\frac{1}{1-z}$在$z = 1$是發散的，因此$P(z) = \sum_{i=0}^{\infty} a_i z^i$ 在$z = 1$也是發散的。

若要$P(z)$在$z = 1$不發散，κ必須是整數，遞迴關係一定要停止於某個m。

當κ是整數，遞迴關係停止於某個$m = l$，$a_{m+2} = 0$。

$$a_{l+2} = \frac{l(l+1)-\kappa}{(l+1)(l+2)} a_l$$

此式的分子必須為零：

$\kappa = l(l+1)$

$$a_{k+2} = \frac{k(k+1)-l(l+1)}{(k+1)(k+2)} a_m$$

→ $a_{l+2} = 0$ l為正整數

$P(z) \equiv P_l(z)$是l次的多項式。

and that $P(z)$ is a *polynomial of order l* in the variable z. We will label the polynomial as $P_l(z)$. These polynomials are known as *Legendre* polynomials. A short list follows:

Legendre Polynomials：

$$P_0(z) = 1$$
$$P_1(z) = z$$
$$P_2(z) = \tfrac{1}{2}(3z^2 - 1)$$
$$P_3(z) = \tfrac{1}{2}(5z^3 - 3z)$$
$$P_4(z) = \tfrac{1}{8}(35z^4 - 30z^2 + 3)$$

$$P_l(z) = \frac{1}{2^l l!}\frac{d^l}{dz^l}(z^2-1)^l$$

若$m \neq 0$：已確認$\kappa = l(l+1)$

$$(1-z^2)\frac{d^2P(z)}{dz^2} - 2z\frac{dP(z)}{dz} - \left(\frac{m^2}{1-z^2} - l(l+1)\right)P(z) = 0$$

注意式中只出現m^2，所以若m為負，結果與正值完全相同。

因為多了$\frac{m^2}{1-z^2}$，此項當$z^2 \to 1$會發散，此式的的解不再是z的有限次多項式。

我們可以取法SHO，解可能是$1-z^2$的函數乘上一個多項式$F(z)$：

要找到這函數，取$z^2 \to 1$，方程式趨近：

$$\frac{d}{dz}\left[(1-z^2)\frac{dP}{dz}\right] \sim -\left(\frac{m^2}{1-z^2}\right)P$$

$$P \to (1-z^2)^{m/2}$$

因此猜想解$P(z)$可能是$(1-z^2)^{m/2}$乘上一個多項式$F(z)$：

$$P(z) = (1-z^2)^{m/2}F(z)$$

代入上式，經過整理，可以得到$F(z)$需要滿足的方程式：

$$(1-z^2)\frac{d^2F}{dz^2} - 2z(m+1)\frac{dF}{dz} - (l-m)(l+m+1)F = 0$$

比較起原式，這樣的選擇使$1/(1-z^2)$項被除掉了，方程式中無發散的項。

解F會是一個有限次多項式。

$$\frac{d^2u}{dy^2} - y^2u + \varepsilon u = 0$$ SHO

此式沒有有限次多項式解。第二項在無限遠處$y \to \infty$會發散。

退而求其次，薛丁格猜想解可能是一個非多項式函數u_0乘上多項式$h(y)$。

他的想法是：非多項式函數$u_0(y)$在無限遠處$y \to \infty$比較重要。

$$\frac{d^2u}{dy^2} - y^2u + \varepsilon u = 0 \quad \xrightarrow{y \to \infty} \quad \frac{d^2u_0}{dy^2} - y^2u_0 = 0$$

解出此方程式就可以得到u_0：

$$u_0(y) = e^{-\frac{y^2}{2}}$$

$$u(y) = e^{-\frac{y^2}{2}} \times h(y)$$

$$\frac{d^2h}{dy^2} - 2y\frac{dh}{dy} + (\varepsilon - 1)h = 0$$

此式真的有多項式解。

這時可以代入有限次多項式，找到Recursion Relation。

$$(1-z^2)\frac{d^2F}{dz^2}-2z(m+1)\frac{dF}{dz}-(l-m)(l+m+1)F=0$$

但有一更快的作法：把上式微分，得到：

$$(1-z^2)\frac{d^2}{dz^2}\frac{dF}{dz}-2z(m+2)\frac{d}{dd}\frac{dF}{dz}-(l-m-1)(l+m+2)\frac{dF}{dz}=0$$

比較兩式，這是一樣的式子當$m\to m+1, F\to\frac{dF}{dZ}$。

所以若F是某一個m的解，$\frac{dF}{dz}$就是$m+1$的解。

因此我們可以推論：$F(z)$就是$P_l(z)$（$m=0$的解）的m次微分。

$$F(z)=\left(\frac{d}{dz}\right)^m P_l(z)$$

綜合兩個公式的結果：

$$P_l^m(z)=(1-z^2)^{m/2}\left(\frac{d}{dz}\right)^m P_l(z)$$

$P_l^m(\theta)$就是標準的Associated Legendre Function。

Table of Spherical Harmonics

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,1} = -\sqrt{\frac{3}{8\pi}} e^{i\varphi} \sin\theta$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$Y_{2,2} = \sqrt{\frac{15}{32\pi}} e^{2i\varphi} \sin^2\theta$$

$$Y_{2,1} = -\sqrt{\frac{15}{8\pi}} e^{i\varphi} \sin\theta\cos\theta$$

$$Y_{2,0} = \sqrt{\frac{5}{16\pi}} (3\cos^2\theta - 1)$$

$$Y_{3,3} = -\sqrt{\frac{35}{64\pi}} e^{3i\varphi} \sin^3\theta$$

$$Y_{3,2} = \sqrt{\frac{105}{64\pi}} e^{2i\varphi} \sin^2\theta\cos\theta$$

$$Y_{3,1} = -\sqrt{\frac{21}{64\pi}} e^{i\varphi} \sin\theta(5\cos^2\theta - 1)$$

$$Y_{3,0} = \sqrt{\frac{7}{16\pi}} (5\cos^3\theta - 3\cos\theta)$$

$$P_l^m(z) = (1-z^2)^{|m|/2}\left(\frac{d}{dz}\right)^{|m|} P_l(z)$$

P_l是l次的多項式，微分次數不能超過l。因此

$|m| \le l$ P_l^m是$l-m$次的多項式

確認$\hat{L}_z$的本徵值滿足$|m| \le l$。

$z = \cos\theta$

$$P_l^m(\theta) = \sin^{|m|}\theta \cdot (\cos\theta\,, l-m\text{次的多項式})$$

$|m| \le l$ 才有解

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

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi}$$

$$Y_{lm}(\theta,\phi) = P_l^m(\theta)\cdot\Phi_m(\phi)$$

捷徑的解法：先寫下Y_{ll}，有最大m值的本徵態$|l, m = m_{\max} = l\rangle$：

$L_+|l, l\rangle = 0$

$L_+ Y_{ll}(\theta, \phi) = 0$

$$L_+ Y_{ll} = \hbar e^{i\phi}\left(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)e^{il\phi}\cdot P_l^l(\theta) = 0$$

$$Y_{lm} = P_l^m(\theta)\frac{1}{\sqrt{2\pi}}e^{im\phi}$$

$$e^{il\phi}\frac{\partial}{\partial\theta}P_l^l(\theta) + i\cot\theta\frac{\partial e^{il\phi}}{\partial\phi}P_l^l(\theta) = 0$$

等同於$\frac{\partial}{\partial\phi}$可以$il$取代。

$$e^{il\phi}\left(\frac{d}{d\theta} - l\cot\theta\right)P_l^l(\theta) = 0$$

$$\frac{dP_l^l}{d\sin\theta} = \frac{l}{\sin\theta}P_l^l$$

可解出：$P_l^l(\theta) = (\sin\theta)^l$

$$Y_{ll}(\theta, \phi) = (\sin\theta)^l\cdot e^{il\phi}$$

這個結果顯示對於軌道角動量，量子數l不能是半整數。

$$Y_{\frac{1}{2}\frac{1}{2}}(\theta, \phi) = \sqrt{\sin\theta}\cdot e^{i\frac{1}{2}\phi}$$

這個函數不合法！ (Gottfried and Yan)

位置變化產生的軌道角動量$L_z = -i\hbar\left(x\frac{\partial}{\partial y} - y\frac{\partial}{\partial x}\right)$, 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$\left[L_x, L_y\right] = i\hbar L_z$，

l就可能是半自然數。那就是電子的自旋。下下一章會討論。

$Y_{ll}(\theta,\phi) = (\sin\theta)^l \cdot e^{il\phi}$ 由此其餘的本徵態可以用Lowering Operato得出：

$$\frac{\partial e^{il\phi}}{\partial\phi} = ile^{il\phi}$$

$$Y_{lm}(\theta,\phi) \propto (L_-)^{l-m} Y_{ll}(\theta,\phi)$$

$$= \left[\hbar e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)\right]^{l-m} e^{il\phi}\cdot(\sin\theta)^l$$

$\frac{\partial}{\partial\phi}$可以$il$取代。

$$= \left[\hbar e^{-i\phi}\left(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\phi}\right)\right]^{l-m-1} \hbar e^{-i\phi}e^{il\phi}\cdot\left(-\frac{\partial}{\partial\theta} - l\cot\theta\right)(\sin\theta)^l$$

$$= \hbar^{l-m}e^{-i(l-m)\phi}e^{il\phi}\left[\left(-\frac{\partial}{\partial\theta} - l\cot\theta\right)\right]^{l-m}(\sin\theta)^l$$

$$= \hbar^{l-m}e^{im\phi}\left[\left(-\frac{\partial}{\partial\theta} - l\cot\theta\right)\right]^{l-m}(\sin\theta)^l \equiv e^{im\phi}P_l^m(\theta)$$

$$\left[\left(-\frac{\partial}{\partial\theta} - l\cot\theta\right)\right]^{l-m}(\sin\theta)^l \equiv P_l^m(\theta)$$

常數由歸一化條件決定。

$$\int \sin\theta\, d\theta d\phi\, |Y_{lm}(\theta,\phi)|^2 = 1$$

$$Y_{lm}(\theta,\phi) = (-1)^m\sqrt{\frac{2l+1}{4\pi}\frac{(l-m)!}{(l+m)!}}\,e^{im\phi}P_l^m(\theta)$$

$$Y_{lm}(\theta,\phi) = Ce^{im\phi}P_l^m(\theta)$$

Table of Spherical Harmonics

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,1} = -\sqrt{\frac{3}{8\pi}}e^{i\varphi}\sin\theta$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}}\cos\theta$$

$$Y_{2,2} = \sqrt{\frac{15}{32\pi}}e^{2i\varphi}\sin^2\theta$$

$$Y_{2,1} = -\sqrt{\frac{15}{8\pi}}e^{i\varphi}\sin\theta\cos\theta$$

$$Y_{2,0} = \sqrt{\frac{5}{16\pi}}(3\cos^2\theta - 1)$$

$$Y_{3,3} = -\sqrt{\frac{35}{64\pi}}e^{3i\varphi}\sin^3\theta$$

$$Y_{3,2} = \sqrt{\frac{105}{64\pi}}e^{2i\varphi}\sin^2\theta\cos\theta$$

$$Y_{3,1} = -\sqrt{\frac{21}{64\pi}}e^{i\varphi}\sin\theta(5\cos^2\theta - 1)$$

$$Y_{3,0} = \sqrt{\frac{7}{16\pi}}(5\cos^3\theta - 3\cos\theta)$$

$$\left[\left(-\frac{\partial}{\partial\theta} - l\cot\theta\right)\right]^{l-m}(\sin\theta)^l \propto P_l^m(\theta)$$

$$P_l^{l-1}(\theta) \sim \left(-\frac{\partial}{\partial\theta} - l\cot\theta\right)(\sin\theta)^l$$

$$= -2l\cos\theta\,(\sin\theta)^{l-1}$$

例如： $P_1^0(\theta) \sim \cos\theta$ $P_1^1(\theta) \sim \sin\theta$

$$P_l^{l-2}(\theta) \sim 2l\left(\frac{\partial}{\partial\theta} + l\cot\theta\right)\cos\theta\,(\sin\theta)^{l-1}$$

$$= 2l(\sin\theta)^l + 4l^2(\cos\theta)^2(\sin\theta)^{l-2}$$

$$\sim[2l + (-2l + 4l^2)(\cos\theta)^2](\sin\theta)^{l-2}$$

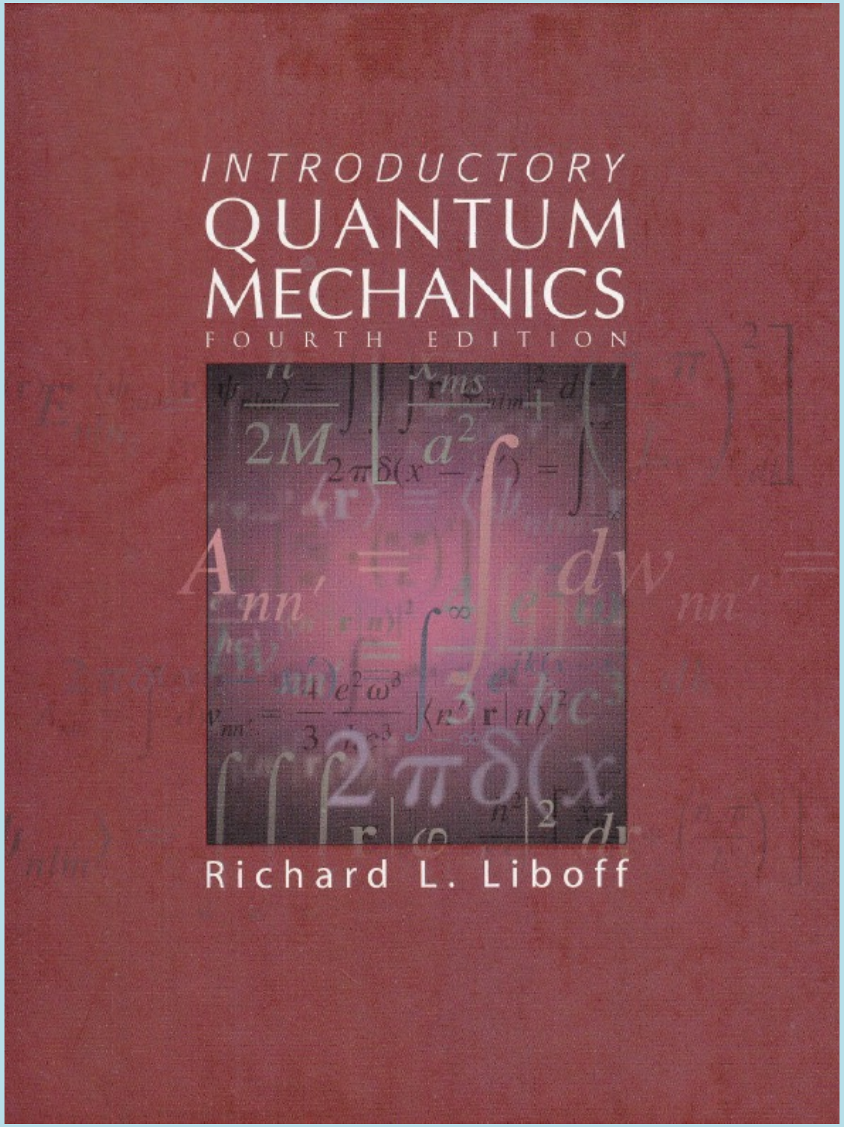
例如： $P_2^0(\theta) \sim [4 + 12(\cos\theta)^2]$

$P_2^1(\theta) \sim \cos\theta\sin\theta$ $P_2^2(\theta) \sim (\sin\theta)^2$

有一個一般的規則：

$$P_l^m(\theta) = \sin^{|m|}\theta \cdot (\cos\theta\,,l - m\text{次的多項式})$$

這些結果將適用於氫原子的定態解。


INTRODUCTORY
QUANTUM
MECHANICS
FOURTH EDITION
Richard L. Liboff

$P_l^m(\theta)$是標準的Associated Legendre Function。

TABLE 9.2 Properties of the Legendre polynomials

Generating formulas

$$(1-2\mu s+s^2)^{-1/2}=\sum_{l=0}^{\infty}P_l(\mu)s^l$$

$$P_l(\mu)=\frac{1}{2^l l!}\left(\frac{d^l}{d\mu^l}\right)(\mu^2-1)^l\begin{cases}-1\le\mu\le 1\\ l=0,1,2,3,\ldots\end{cases}$$

Legendre's Equation

$$(1-\mu^2)\frac{d^2P_l(\mu)}{d\mu^2}-2\mu\frac{dP_l(\mu)}{d\mu}+l(l+1)P_l(\mu)=0$$

Recurrence Relations

$$(l+1)P_{l+1}(\mu)=(2l+1)\mu P_l(\mu)-lP_{l-1}(\mu)$$

$$(1-\mu^2)\frac{d}{d\mu}P_l(\mu)=-l\mu P_l(\mu)+lP_{l-1}(\mu)$$

Normalization and Orthogonality

$$\int_{-1}^{1}P_l(\mu)P_m(\mu)\,d\mu=\frac{2}{2l+1}\qquad(l=m)$$

$$=0\qquad(l\neq m)$$

The First Few Polynomials

$$P_0=1\qquad P_2=\frac{1}{2}(3\mu^2-1)\qquad P_4=\frac{1}{8}(35\mu^4-30\mu^2+3)$$

$$P_1=\mu\qquad P_3=\frac{1}{2}(5\mu^3-3\mu)\qquad P_5=\frac{1}{8}(63\mu^5-70\mu^3+15\mu)$$

Special Values

$$P_l(\mu)=(-1)^lP_l(-\mu),\qquad P_l(1)=1,\qquad P_{2l+1}(0)=0$$

TABLE 9.3 Properties of the associated Legendre functions

Definition

$$P_l^m(\mu) = (-1)^m (1-\mu^2)^{m/2} \frac{d^m}{d\mu^m} P_l(\mu); \qquad P_l^0 = P_l$$

$$P_l^{-m}(\mu) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(\mu); \qquad P_l^{-1} = \frac{1}{2^l l!} \sin^l \theta$$

For these equations, m is taken as ≥ 0. In the formulas below, however, m may be < 0 also; $l = 0, 1, 2, \ldots, |m| \leq l$.

Differential Equation

$$(1-\mu^2)\frac{d^2 P_l^m(\mu)}{d\mu^2} - 2\mu \frac{d P_l^m(\mu)}{d\mu} + \left[l(l+1) - \frac{m^2}{1-\mu^2} \right] P_l^m(\mu) = 0$$

Recurrence Relations

$$(2l+1)\mu P_l^m(\mu) = (l-m+1) P_{l+1}^m(\mu) + (l+m) P_{l-1}^m(\mu)$$

$$(2l+1)(1-\mu^2)^{1/2} P_l^m(\mu) = P_{l-1}^{m+1}(\mu) - P_{l+1}^{m+1}(\mu)$$

$$(1-\mu^2)\frac{d P_l^m(\mu)}{d\mu} = (l+1)\mu P_l^m(\mu) - (l-m+1) P_{l+1}^m(\mu)$$

$$= -l\mu P_l^m(\mu) + (l+m) P_{l-1}^m(\mu)$$

$$(1-\mu^2)^{1/2} P_l^{m+1}(\mu) = (l-m)\mu P_l^m(\mu) - (l+m) P_{l-1}^m(\mu)$$

$$= -(l+m+1) P_l^m(\mu) + (l-m+1) P_{l+1}^m(\mu)$$

Normalization and Orthogonality

$$\int_{-1}^{1} P_l^m(\mu) P_k^m(\mu)\, d\mu = \frac{2}{2l+1} \frac{(l+m)!}{(l-m)!} \qquad (l = k)$$

$$= 0 \qquad (l \neq k)$$

以下稱Polar Plot以r代表方向θ的機率密度$|Y_{lm}|^2 = \left(P_m^l(\theta)\right)^2$，機率密度與$\phi$無關：

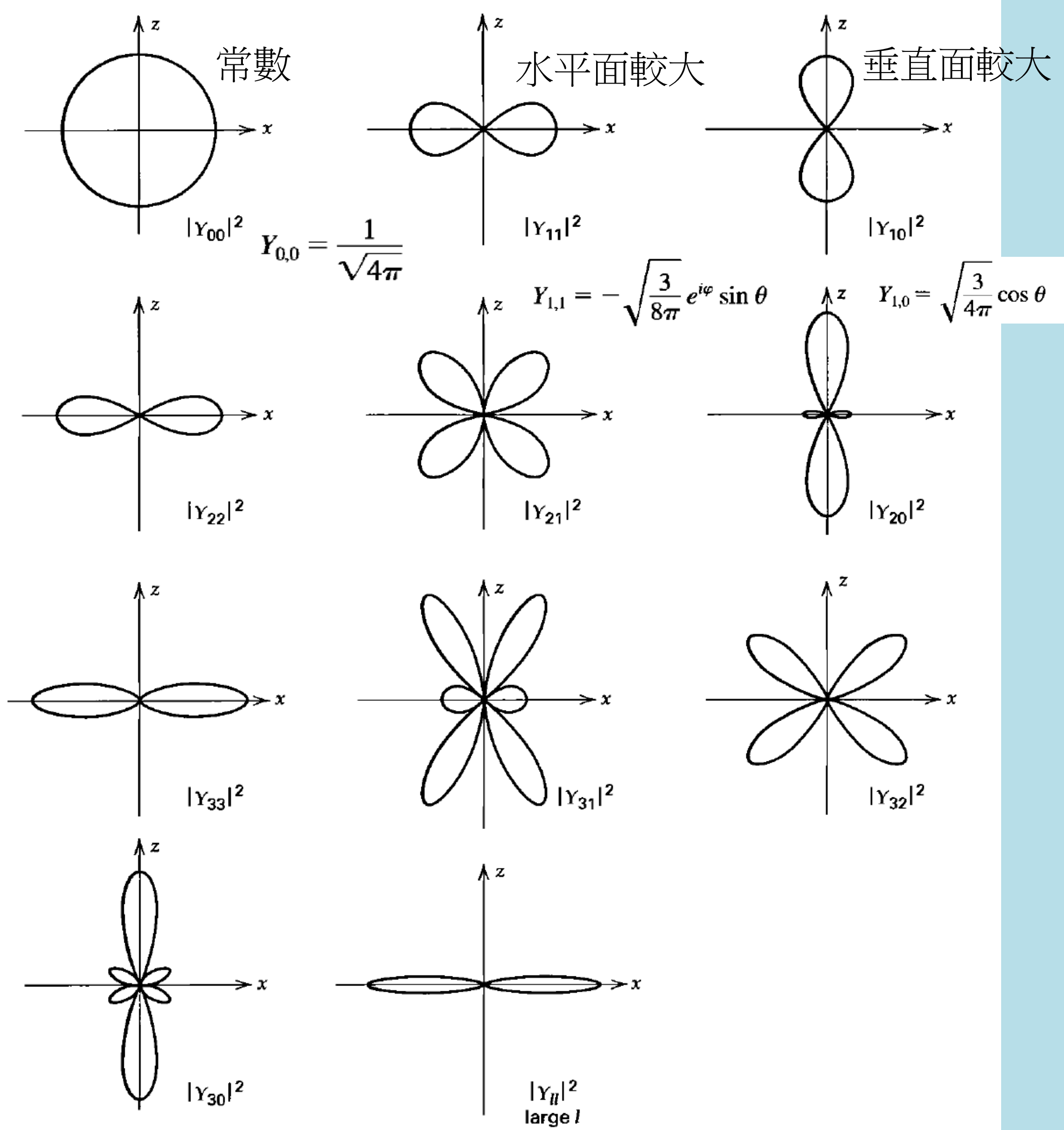


Figure 8-4 Distributions of $|Y_{lm}(\theta, \phi)|^2$. The sketches represent sections of the distributions made in the z-x plane. It should be understood that the three-dimensional distributions are obtained by rotating the figures about the z-axis.

Table of Spherical Harmonics

$$Y_{0,0} = \frac{1}{\sqrt{4\pi}}$$

$$Y_{1,1} = -\sqrt{\frac{3}{8\pi}}\, e^{i\varphi} \sin\theta$$

$$Y_{1,0} = \sqrt{\frac{3}{4\pi}} \cos\theta$$

$$Y_{2,2} = \sqrt{\frac{15}{32\pi}}\, e^{2i\varphi} \sin^2\theta$$

$$Y_{2,1} = -\sqrt{\frac{15}{8\pi}}\, e^{i\varphi} \sin\theta \cos\theta$$

$$Y_{2,0} = \sqrt{\frac{5}{16\pi}}\,(3\cos^2\theta - 1)$$

$$Y_{3,3} = -\sqrt{\frac{35}{64\pi}}\, e^{3i\varphi} \sin^3\theta$$

$$Y_{3,2} = \sqrt{\frac{105}{64\pi}}\, e^{2i\varphi} \sin^2\theta \cos\theta$$

$$Y_{3,1} = -\sqrt{\frac{21}{64\pi}}\, e^{i\varphi} \sin\theta(5\cos^2\theta - 1)$$

$$Y_{3,0} = \sqrt{\frac{7}{16\pi}}\,(5\cos^3\theta - 3\cos\theta)$$

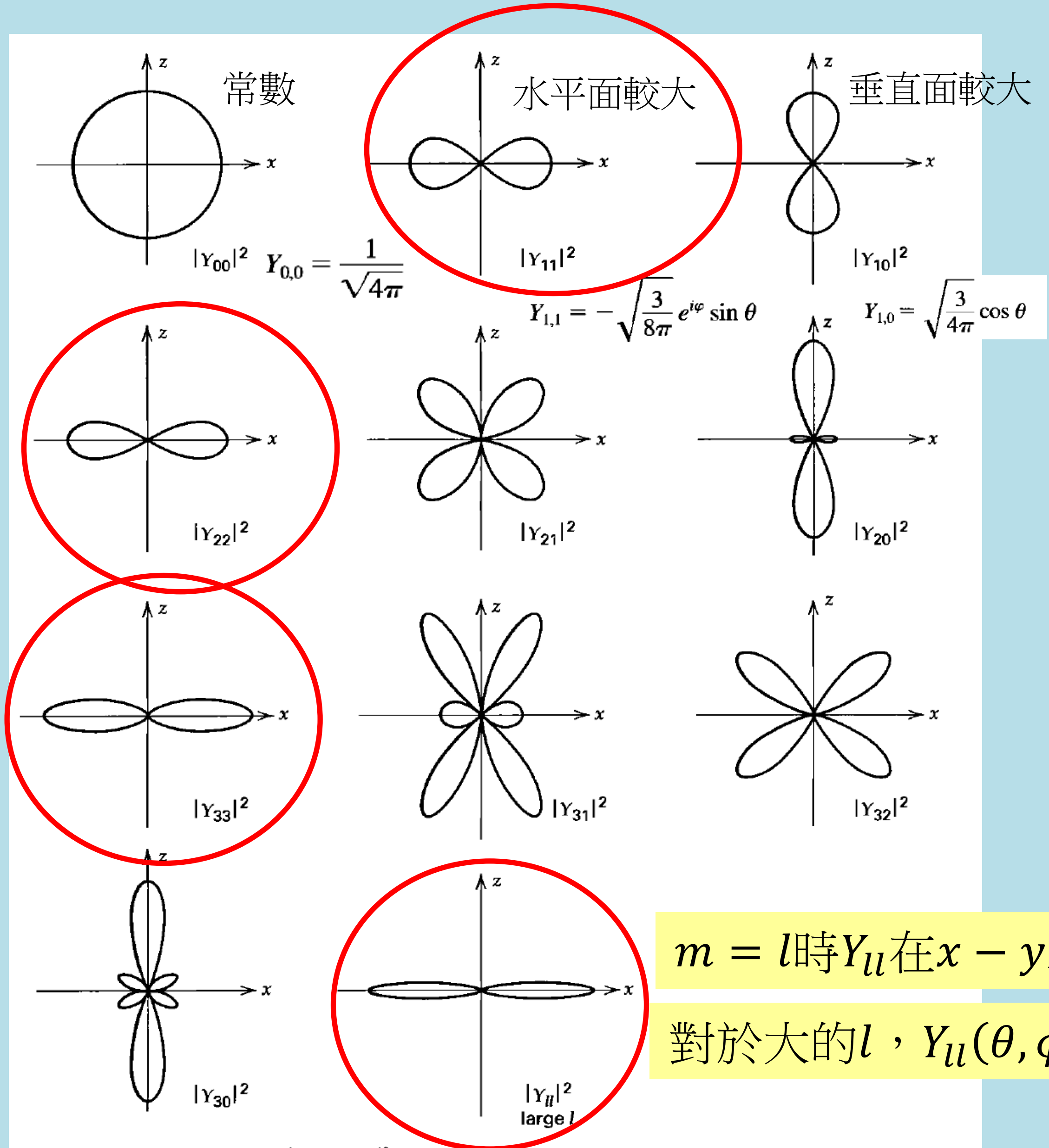
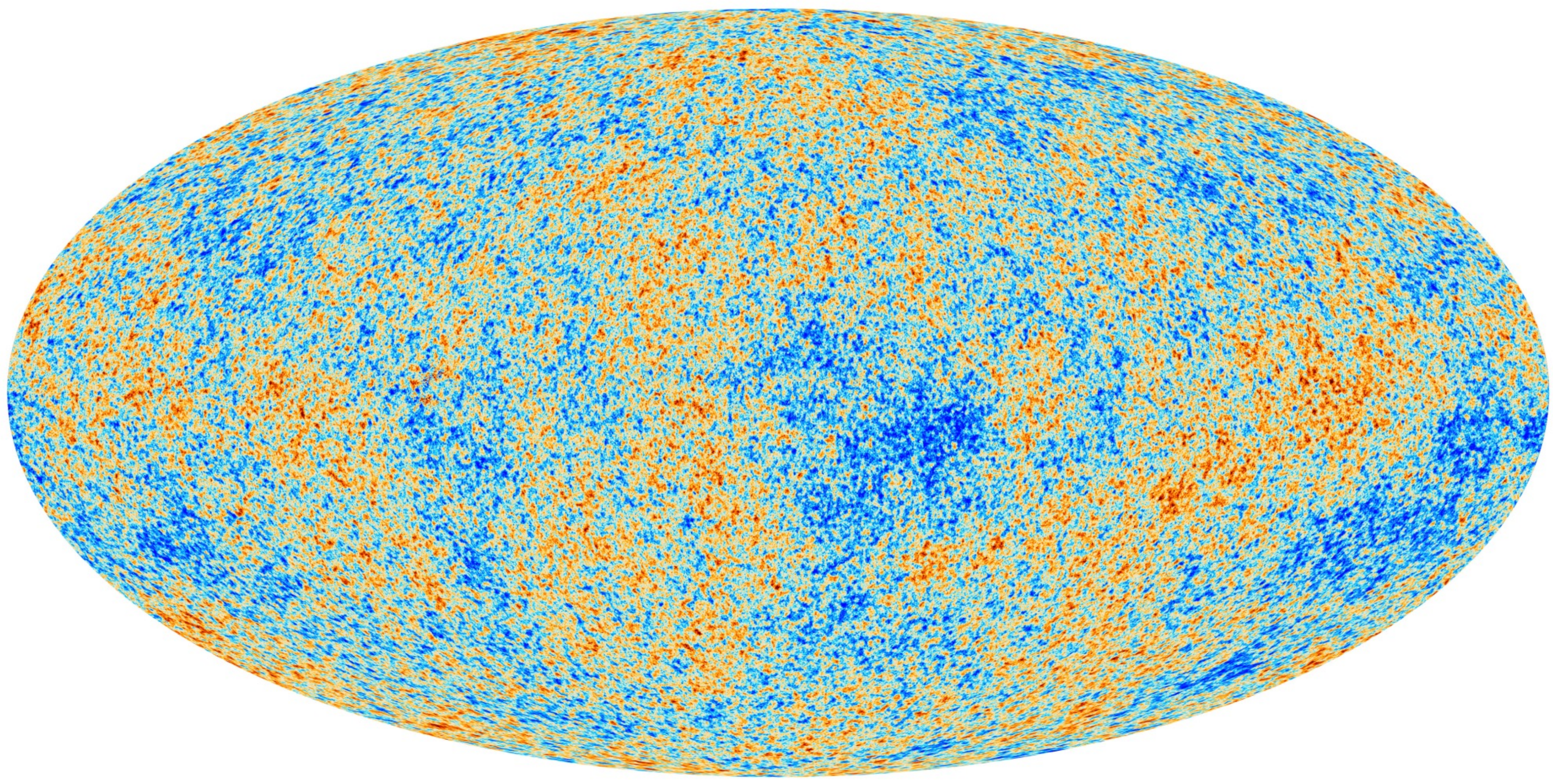


Figure 8-4 Distributions of $|Y_{lm}(\theta, \phi)|^2$. The sketches represent sections of the distributions made in the z-x plane. It should be understood that the three-dimensional distributions are obtained by rotating the figures about the z-axis.

$m = l$時Y_{ll}在$x - y$水平面最大，而且越來越扁。

對於大的l，$Y_{ll}(\theta, \phi)$，幾乎全部集中在$x - y$平面上



The anisotropies of the Cosmic Microwave Background (CMB) as observed by Planck 2013.

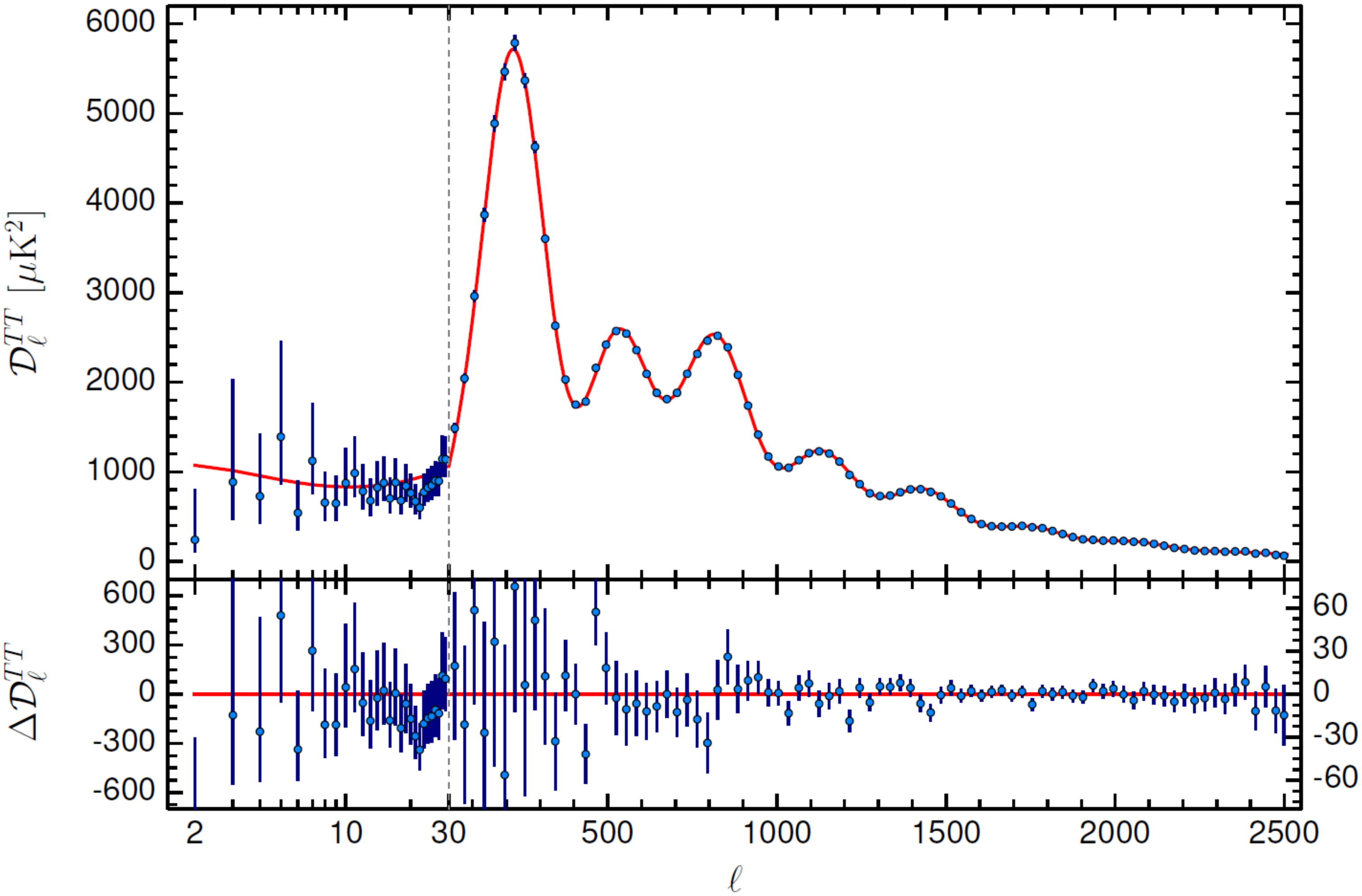
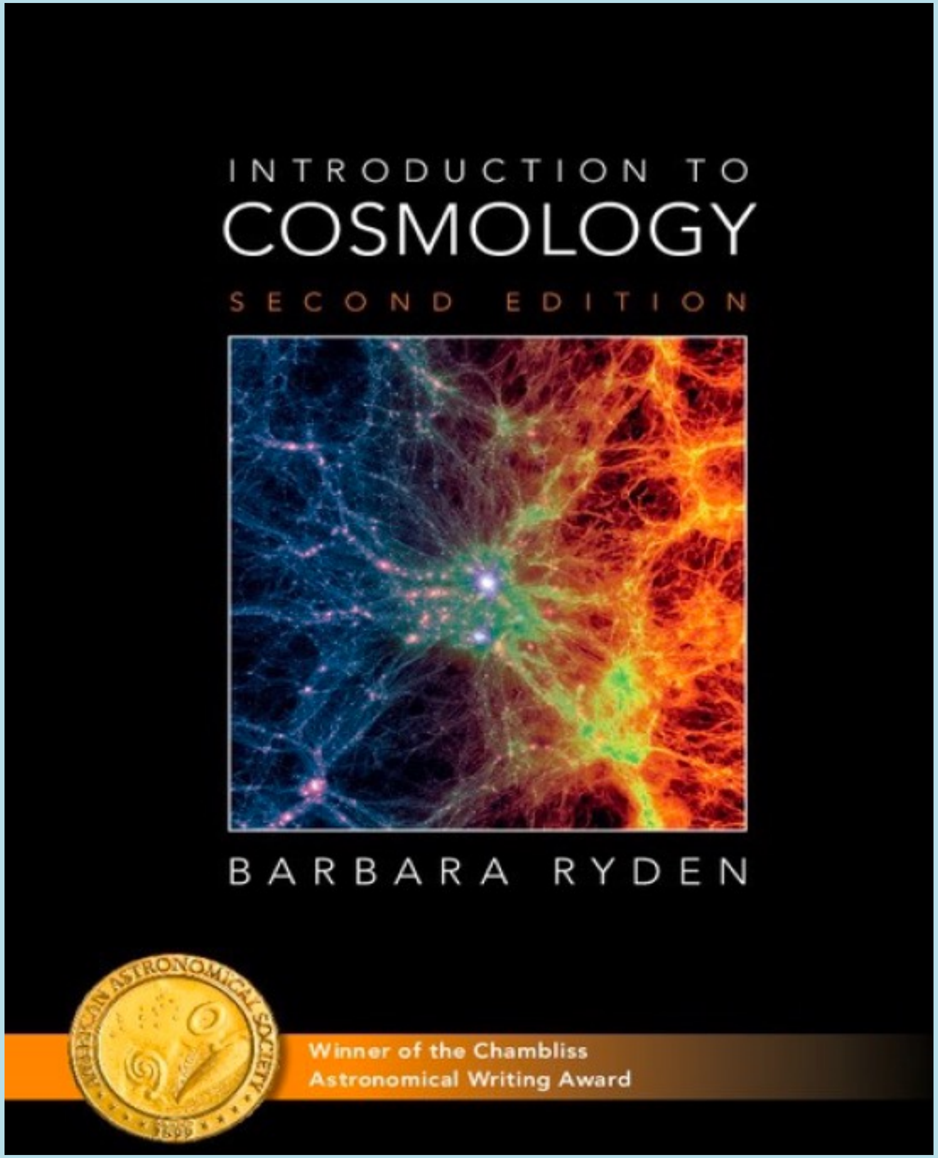


Fig. 1. The *Planck* 2015 temperature power spectrum. At multipoles $\ell \geq 30$ we show the maximum likelihood frequency averaged temperature spectrum computed from the `Plik` cross-half-mission likelihood with foreground and other nuisance parameters determined from the MCMC analysis of the base ΛCDM cosmology. In the multipole range $2 \leq \ell \leq 29$, we plot the power spectrum estimates from the `Commander` component-separation algorithm computed over 94% of the sky. The best-fit base ΛCDM theoretical spectrum fitted to the *Planck* TT+lowP likelihood is plotted in the upper panel. Residuals with respect to this model are shown in the lower panel. The error bars show $\pm 1\,\sigma$ uncertainties.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BARBARA RYDEN
Winner of the Chambliss
Astronomical Writing Award

Consider the density fluctuations $\delta T/T$ of the cosmic microwave background, as shown in Figure 8.3. Since $\delta T/T$ is defined on the surface of a sphere – the celestial sphere in this case – it is useful to expand it in spherical harmonics:

$$\frac{\delta T}{T}(\theta, \phi) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{lm} Y_{lm}(\theta, \phi), \qquad (8.50)$$

where $Y_{lm}(\theta, \phi)$ are the usual spherical harmonic functions. What concerns cosmologists is not the exact pattern of hot spots and cold spots on the sky, but their statistical properties. The most important statistical property of $\delta T/T$ is the correlation function $C(\theta)$. Consider two points on the last scattering surface. Relative to an observer, they are in the directions $\hat{n}$ and $\hat{n}'$, and are separated by an angle θ given by the relation $\cos\theta = \hat{n} \cdot \hat{n}'$. To find the correlation function $C(\theta)$, multiply together the values of $\delta T/T$ at the two points, then average the product over all points separated by the angle θ:

$$C(\theta) = \left\langle \frac{\delta T}{T}(\hat{n}) \frac{\delta T}{T}(\hat{n}') \right\rangle_{\hat{n}\cdot\hat{n}'=\cos\theta}. \qquad (8.51)$$

Using the expansion of $\delta T/T$ in spherical harmonics, the correlation function can be written in the form

$$C(\theta) = \frac{1}{4\pi} \sum_{l=0}^{\infty} (2l+1) C_l P_l(\cos\theta), \qquad (8.52)$$

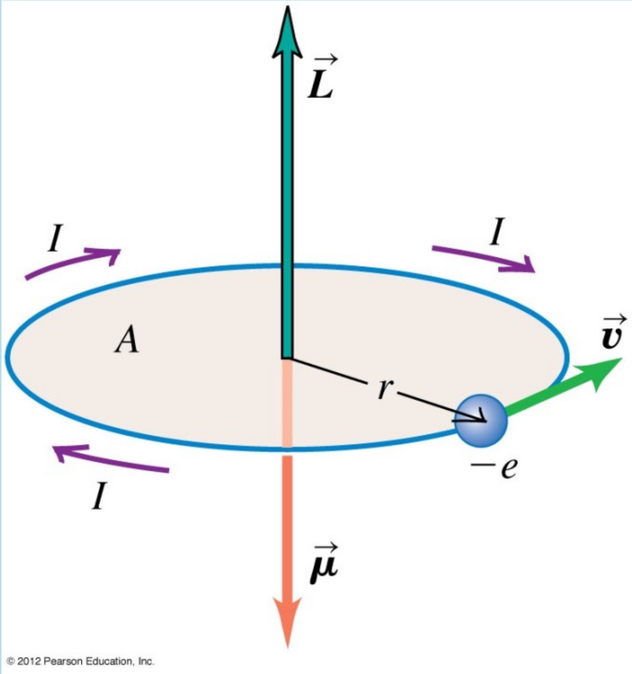
where P_l are the usual Legendre polynomials:

and so forth. In this way, a measured correlation function $C(\theta)$ can be broken down into its multipole moments C_l. The $l = 0$ (monopole) term of the correlation function vanishes if we've defined the mean temperature correctly. The $l = 1$ (dipole) term results primarily from the Doppler shift due to our motion through space. For larger values of l, the termC_l is a measure of temperature fluctuations on an angular scale θ ~ 180°/l. Thus, the multipole l is interchangeable, for all practical purposes, with the angular scale θ. The moments with $l \geq 2$ are of the most interest to astronomers, since they tell us about the fluctuations present at the time of last scattering.

In presenting the results of CMB observations, it is customary to plot the function

$$\Delta_T \equiv \left(\frac{l(l+1)}{2\pi} C_l \right)^{1/2} \langle T \rangle \,, \tag{8.54}$$

since this function tells us the contribution per logarithmic interval in l to the total temperature fluctuation δT of the cosmic microwave background. Figure



古典旋轉的帶電粒子就是一個磁偶極$\vec{\mu}$，大小為：

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

方向指向角動量的方向，因此

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

磁偶極矩向量與角動量成正比

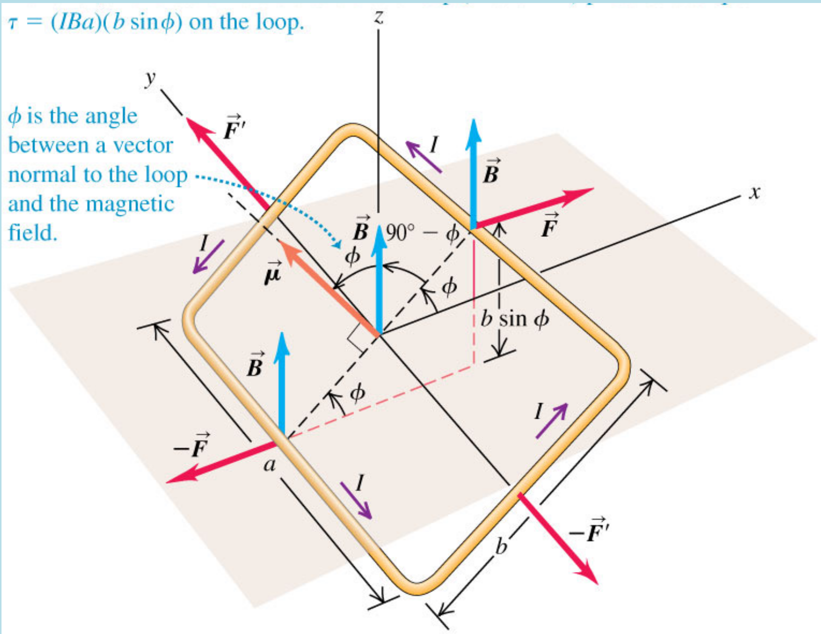
假設此古典的公式對量子力學電子也成立！

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！

如何量磁偶極矩？最容易的就是加一個磁場。

磁偶極在均勻磁場中所受的磁效應：



受力為零，力矩不為零：

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

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

所受力矩只由磁偶極矩向量決定。

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：

$$\Delta U = -W = -\int_{\phi_1}^{\phi_2} (-d\phi)\cdot\tau = -\int_{\phi_1}^{\phi_2} d\phi\cdot\mu B\sin\phi = -\mu B\cos\phi_2 + \mu B\cos\phi_1 = -\Delta\left(\vec{\mu}\cdot\vec{B}\right)$$

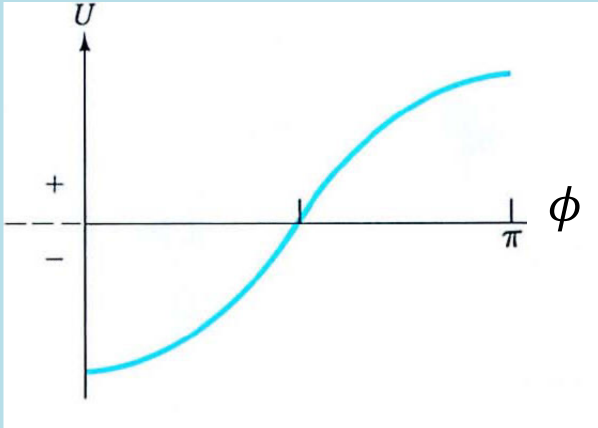


圖 23.28
電偶極的位能為其方向角度的函數

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

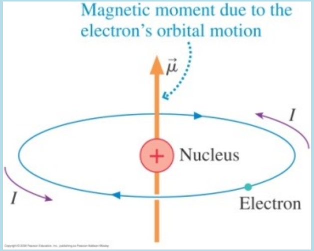
量測磁偶極在磁場中能量，就是量磁偶極矩。

量測磁偶極在磁場中能量，就是量磁偶極矩。

原子能階的能量與角動量無關，完全由主量子數n決定。

但若加一 z方向磁場B，原子能量會被磁偶極修正，就與z方向角動量L_z有關。

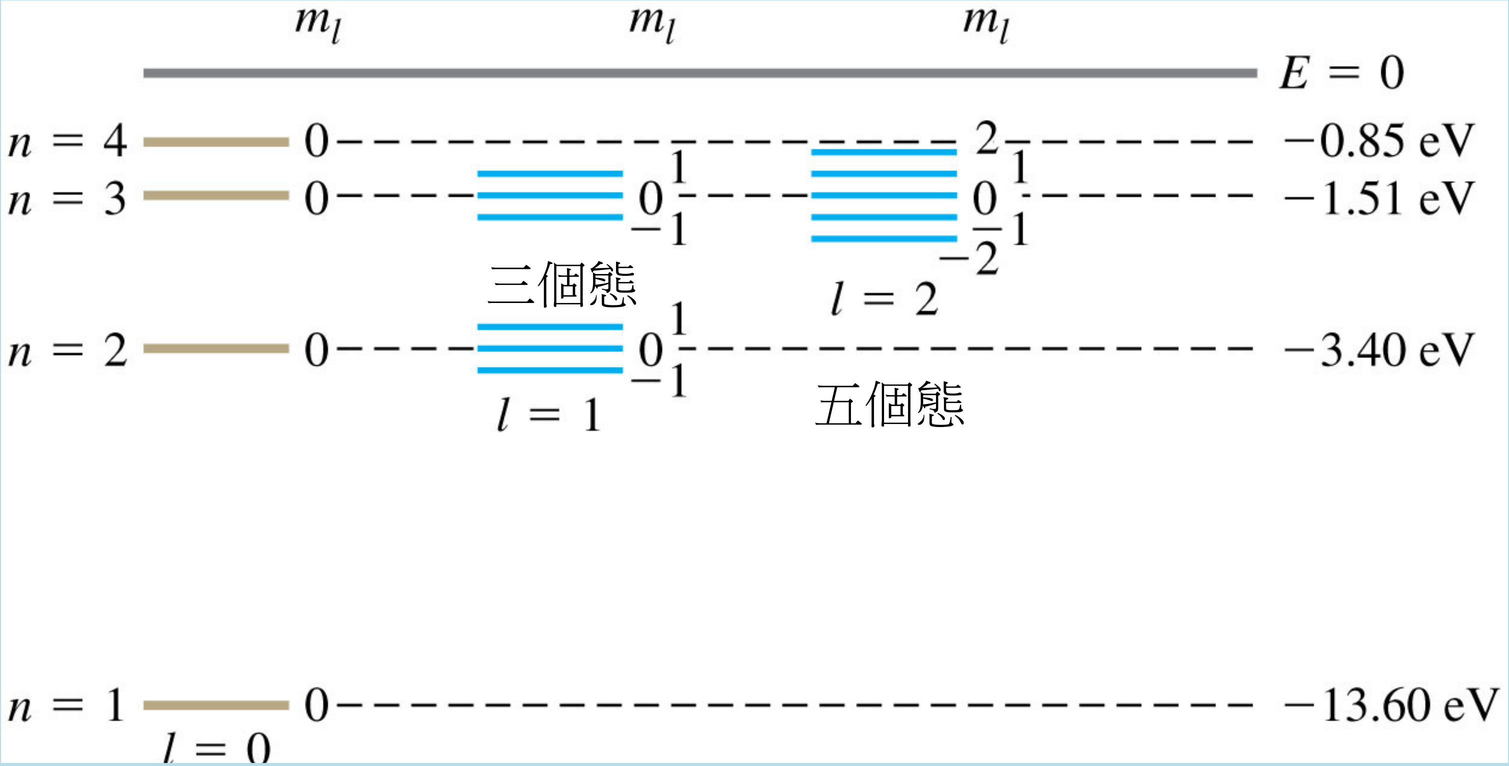
因此加磁場再觀察原子光譜，即可以測角動量L_z 。



$$H \supset -\vec{\mu}\cdot\vec{B} = \mu_z B$$

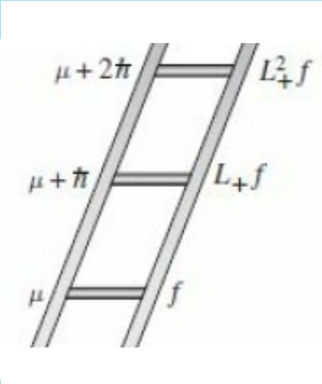
$$\mu_z = -\frac{e}{2m} m_z \hbar$$

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

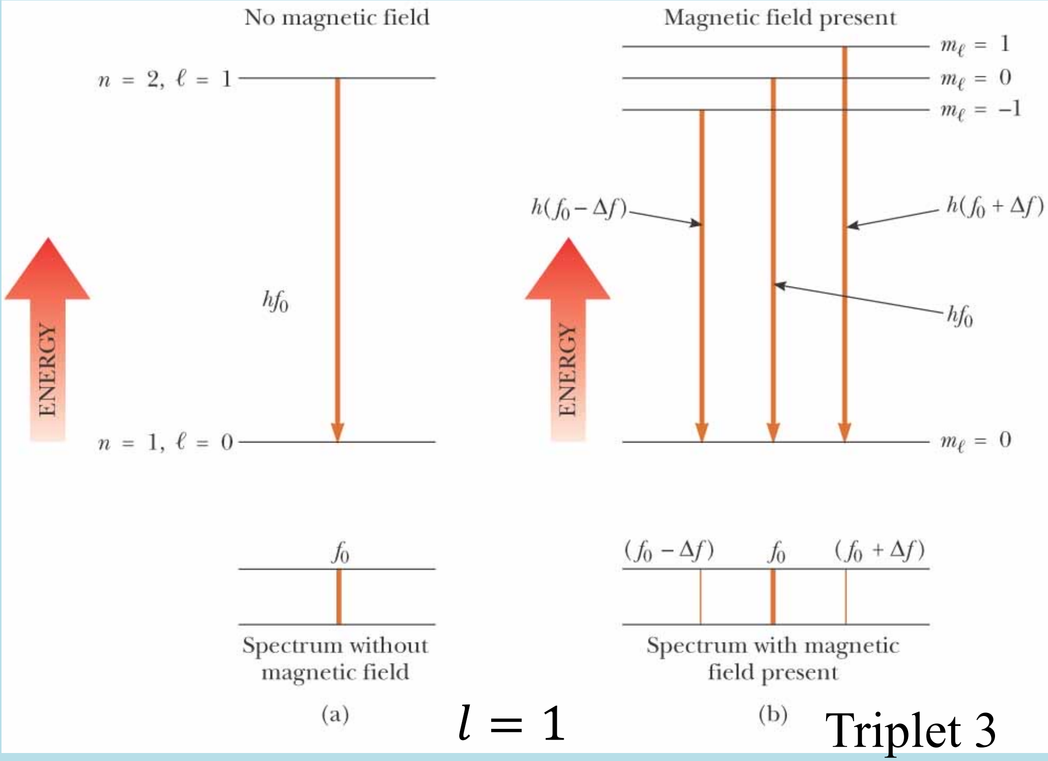


角動量量子化，因此磁偶極矩也是量子化！

Zeeman Effect：外加磁場後原子光譜的分裂

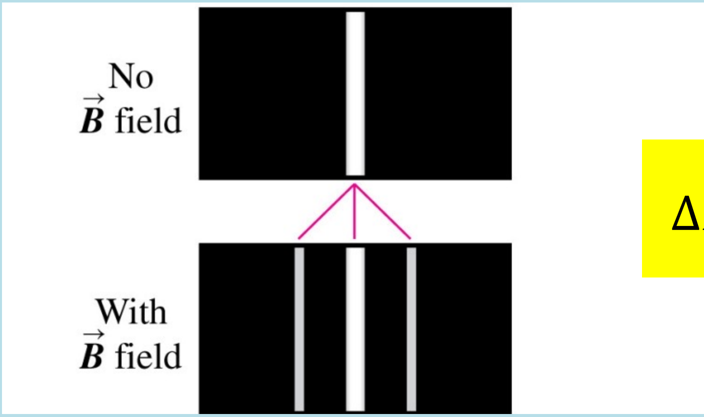


$$\begin{pmatrix} |1,1\rangle \\ |1,0\rangle \\ |1,-1\rangle \end{pmatrix}$$



$l = 1$

Triplet 3



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

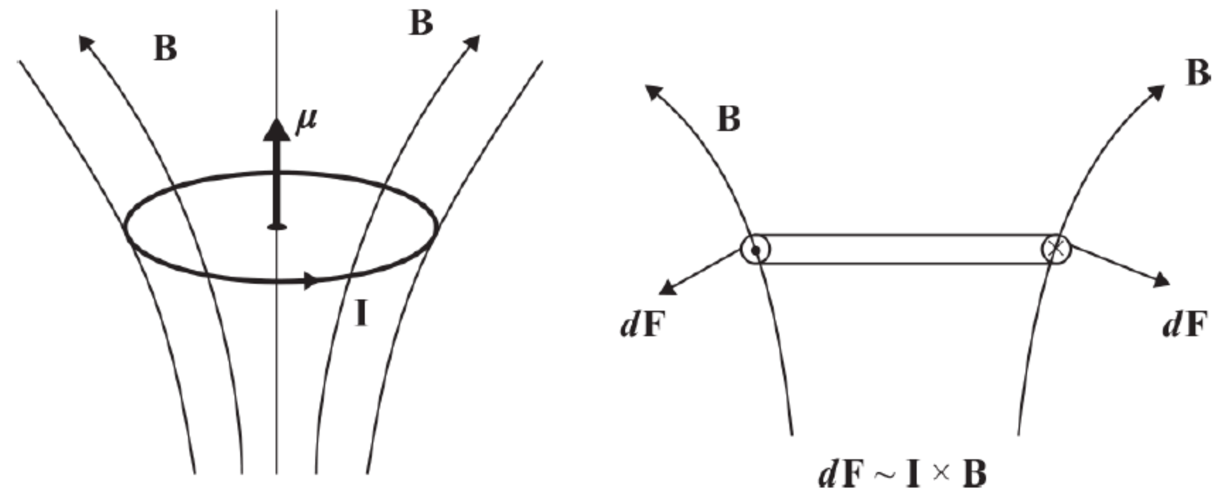


Figure 12.2
A magnetic dipole in a nonuniform magnetic field will experience a force. The force points in the direction for which $\mu \cdot \mathbf{B}$ grows the fastest. In this case the force is downward.

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

此式在不均勻磁場中也成立。此時磁偶極會受一個力。

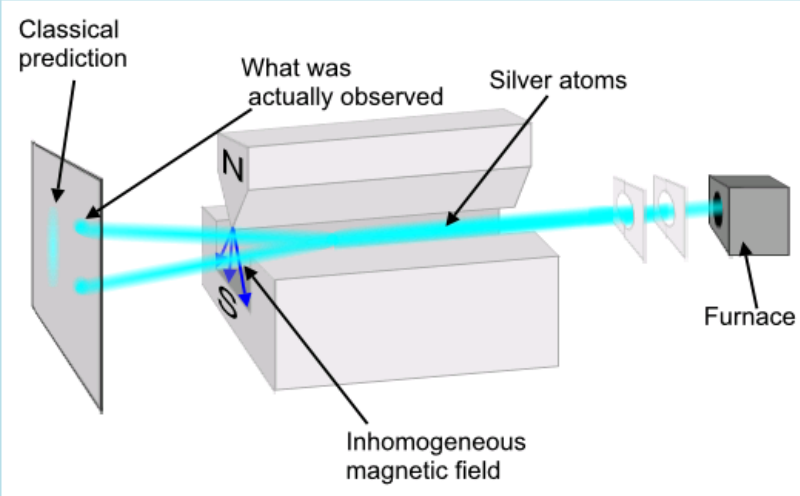
$$F = -\nabla U = \nabla(\vec{\mu} \cdot \vec{B})$$

量測磁偶極在不均勻磁場中的軌跡，就是量磁偶極矩。

Stern-Gerlach Experiment 1922

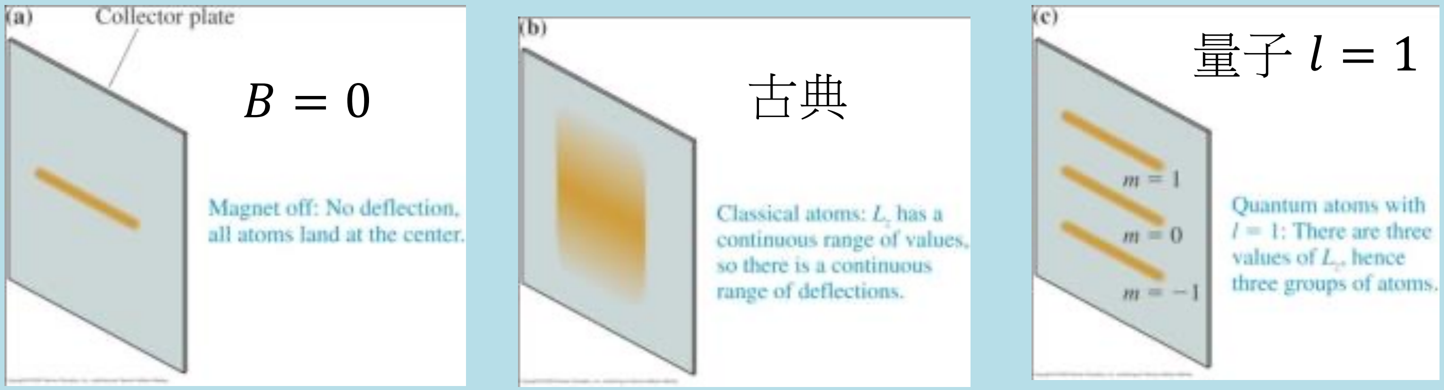
使氣態銀原子通過一不均勻的z方向磁場B，它會受z方向的力。

$$F = -\nabla U = \nabla(\vec{\mu}\cdot\vec{B}) = \mu_z \nabla B \qquad F_z = \mu_z \frac{dB}{dz} \propto L_z$$



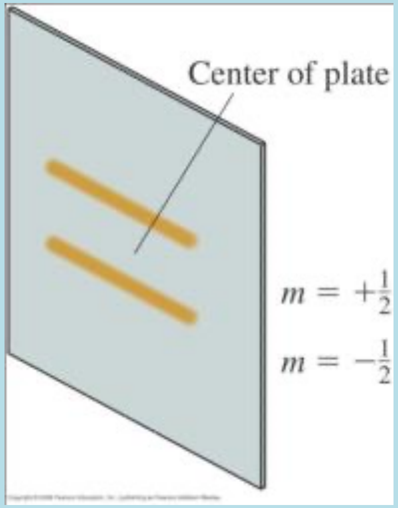
這個實驗等於是對z方向角動量L_z的測量。

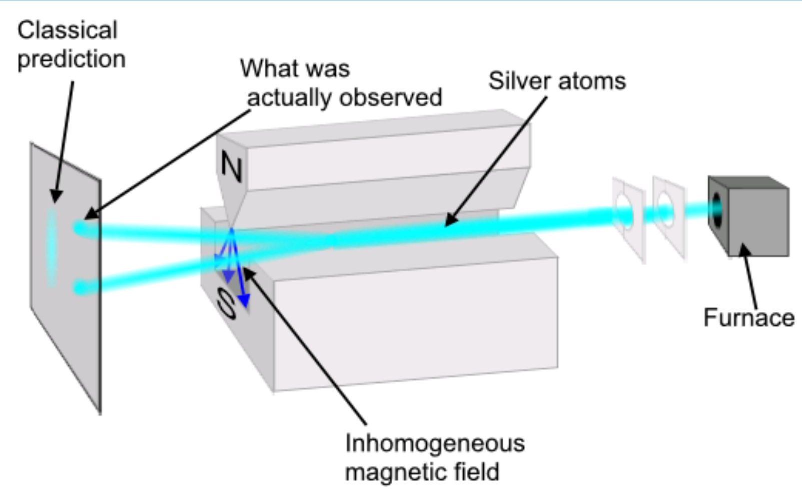
例如若是$l = 1$，會有三條分離軌跡。

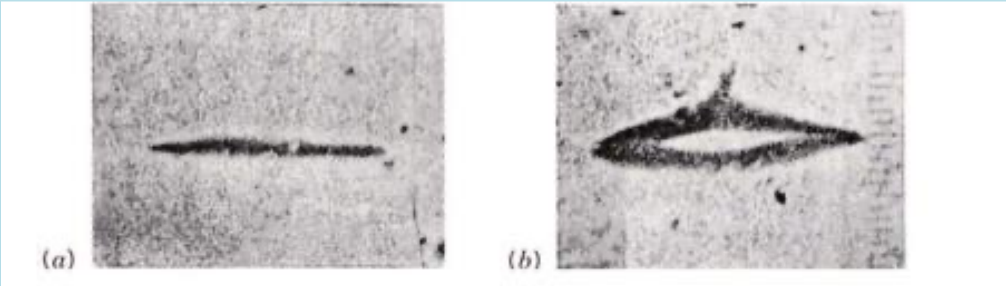


銀原子內電子的軌道角動量為零，

沒有軌道角動量！照理應該沒有偏折。







但的確量到氫原子有磁偶極矩，因此有角動量。

而且此角動量非常異乎尋常，只有兩種可能的狀態！ $2l+1=2, l=\dfrac{1}{2}$

已知軌道角動量的量子數l不能是半整數。所以這不是軌道角動量。

In 1922, at the University of Frankfurt in Germany, Otto Stern and Walther Gerlach conducted fundamental experiments to measure the deflection of beams of silver atoms as they were sent through nonhomogeneous magnetic fields. As we will explain below, the silver atom has a magnetic dipole moment, and magnetic dipoles get deflected when exposed to spatially varying magnetic fields. Rather than finding the expected continuous range of deflections, however, the incoming beam was split into two beams, as deduced from the two separate spots on the target screen. These experiments demonstrated that these silver atoms have quantized magnetic moments that can have one of two values.

A little knowledge of chemistry shows that a silver atom in the Stern-Gerlach experiment acts like a heavy electron. The silver atom has forty-seven electrons; twenty-eight of them completely fill the $n = 1$, 2, and 3 shells, and eighteen more fill the *s*, *p*, and *d* orbitals of the $n = 4$ shell. Finally, there is just one electron with $n = 5$ and $\ell = 0$: the zero angular momentum 5*s* state. Since this is the only unpaired electron, the magnetic dipole moment of the silver atom is to a good approximation just the magnetic dipole moment of the 5*s* electron; the nucleus has a much smaller dipole moment and can be ignored. For a charged particle like the electron, a magnetic moment arises because the particle has spin.

Although the quantized magnetic moments found by Stern and Gerlach were consistent with the idea that the electron had spin, this suggestion took some time to develop. Pauli introduced a “two-valued” degree of freedom for electrons, without suggesting a physical interpretation. Ralph Kronig suggested in 1925 that this degree of freedom originated from the self-rotation of the electron. This idea was severely criticized by Pauli, and Kronig did not publish it. George Uhlenbeck and Samuel Goudsmit had a similar idea, and Paul Ehrenfest encouraged them to publish it. They did so in 1925 and are now credited with discovering that the electron has an intrinsic spin with value “one-half.” Much of the mathematics of spin one-half was developed by Pauli himself in 1927 and goes along the lines we followed in the previous section. In fact, it took until 1927 for anyone to realize that the Stern-Gerlach experiment measured the magnetic moment of the electron.

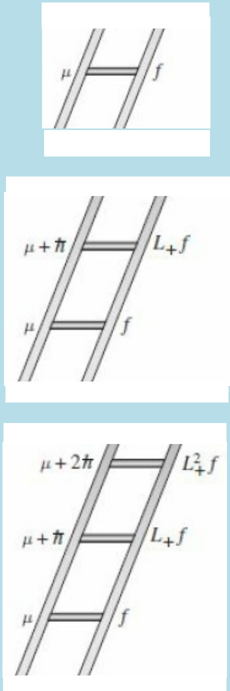
The postcard sent by Stern to Bohr showing the results of the Stern–Gerlach experiment. The left image shows the rectangular beam in the absence of the magnetic field gradient; the right-hand image shows the splitting of the beam into two components. The greatest field gradient occurs in the centre of the beam.

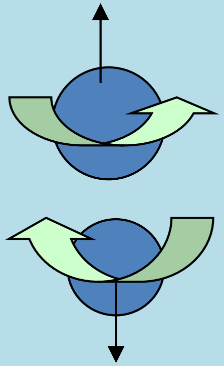
A plaque at the Frankfurt institute commemorating the experiment 1922

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

$|0,0\rangle$

$l = 0$





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

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

$l = \frac{1}{2}$

二維

$|1,1\rangle$

$|1,0\rangle$

$|1,-1\rangle$

$l = 1$

三維

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

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

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

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

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

整數l的本徵態有奇數個。 半整數l的本徵態有偶數個。

所以此實驗結果顯示：即使靜止時，電子也有角動量，稱為自旋 Spin。

電子自旋只有兩個態，因此猜測：$l \equiv s = \frac{1}{2}$

測量偏轉的程度，可以確認z方向角動量：$= m_s \hbar = \pm \frac{1}{2} \hbar$

這個內在的角動量是粒子位置不變時還擁有的角動量，

因此自旋角動量就不再能寫成位置微分：$S_z \neq x p_y - y p_x$

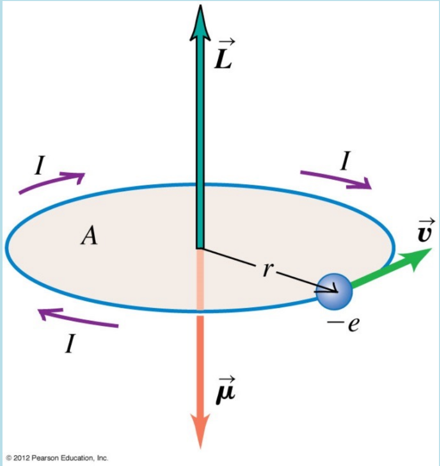
這樣的角動量就稱為自旋角動量，以新的符號S, S_i來區別。

科學家猜想，後來實驗也證實：軌道角動量的對易關係對自旋還是對的：

$[S_y, S_z] = i\hbar S_x$ $[S_z, S_x] = i\hbar S_y$ $[S_x, S_y] = i\hbar S_z$

如此，之前推導的本徵值依舊正確！

$$S = \sqrt{s(s+1)}\hbar = \frac{\sqrt{3}}{2}\hbar$$



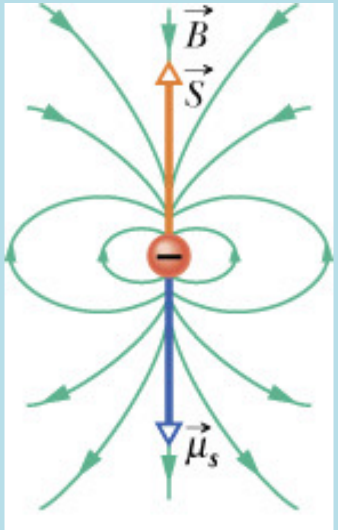
確定了電子自旋的大小為$s = 1/2$，

Stern-Gerlach實驗直接測量的是磁偶極矩，有一驚人結果：

帶電粒子磁偶極矩向量與軌道角動量成正比。

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

$$\mu_B = \frac{e\hbar}{2m}$$



自旋也產生磁偶極矩，也與自旋角動量成正比。

但磁偶極矩與角動量的比例是軌道角動量的兩倍！

$$\vec{\mu} = -\frac{e}{m}\vec{S} \equiv g\mu_B \frac{\vec{S}}{\hbar}$$

$$g = 2$$

Called gyromagnetic ratio or g-factor.

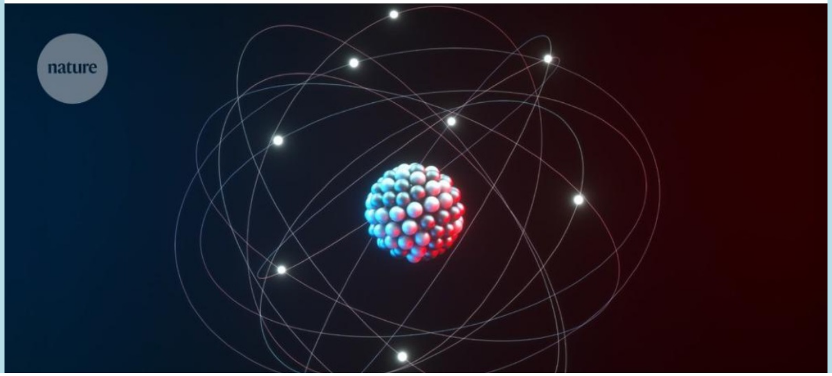
可見自旋角動量不同於軌道角動量。

電子在磁場中，能量將多一個項：

$$H \supset -\vec{\mu}\cdot\vec{B} = \frac{e}{2m}\vec{L}\cdot\vec{B} + \frac{e}{m}\vec{S}\cdot\vec{B}$$

Nature
16小時 ·

Physicists nail down the most precise value yet of the electron magnetic moment, surpassing a value measured 14 years ago.



Measurement of the Electron Magnetic Moment

X. Fan,[1,2,*] T. G. Myers,[2] B. A. D. Sukra,[2] and G. Gabrielse[2,†]
[1]*Department of Physics, Harvard University, Cambridge, Massachusetts 02138, USA*
[2]*Center for Fundamental Physics, Department of Physics and Astronomy, Northwestern University, Evanston, Illinois 60208, USA*

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The electron magnetic moment, $-\mu/\mu_B = g/2 = 1.001\,159\,652\,180\,59\,(13)$ [0.13 ppt], is determined 2.2 times more accurately than the value that stood for fourteen years. The most precisely determined property of an elementary particle tests the most precise prediction of the standard model (SM) to 1 part in 10^{12}. The test would improve an order of magnitude if the uncertainty from discrepant measurements of the fine structure constant α is eliminated since the SM prediction is a function of α. The new measurement and SM theory together predict $\alpha^{-1} = 137.035\,999\,166\,(15)$ [0.11 ppb] with an uncertainty 10 times smaller than the current disagreement between measured α values.

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The quest to find physics beyond the standard model of particle physics (BSM) is well motivated because the SM is incomplete. No known *CP* violation mechanism [1] is large enough to keep the matter and antimatter produced in the big bang [2] from annihilating as the universe cooled, dark matter [3,4] has not been identified, and neither dark energy [5,6] nor inflation [7–10] has a SM explanation. The most precise SM prediction is the electron magnetic moment in Bohr magnetons, $-\mu/\mu_B = g/2$, with $\mu_B = e\hbar/(2m)$ for electron charge $-e$ and mass m, and the reduced Planck constant $\hbar$. It

$$\boldsymbol{\mu} = -\frac{g}{2}\mu_B \frac{\mathbf{S}}{\hbar/2}, \qquad (1)$$

is proportional to its spin $\mathbf{S}$, normalized to its spin eigenvalue $\hbar/2$. The energy levels are

$$E = h\nu_s m_s + h\nu_c\left(n + \frac{1}{2}\right), \qquad (2)$$

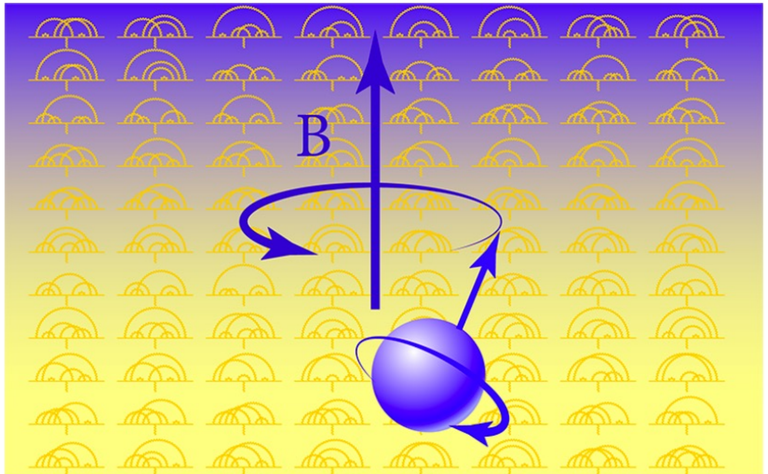
where $h = 2\pi\hbar$. The cyclotron frequency is $\nu_c = eB/(2\pi m)$

Searching for New Physics with the Electron's Magnetic Moment

Measurements of the magnetic moment of the electron have achieved unprecedented accuracy, showing great potential for the search for physics beyond the standard model.

By **Saïda Guellati-Khelifa**

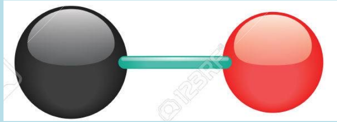
Despite its remarkable successes, the standard model of particle physics clearly isn't complete—dark matter, dark energy, and the matter–antimatter asymmetry of the Universe are some of its most flagrant deficiencies. Experimenters thus eagerly search for anomalies that could provide hints on a theory that could complete or replace the standard model. The electron is a key player in this quest: its magnetic moment is both the most precisely measured elementary-particle property and the most accurately verified standard model prediction to date. New measurements by Gerald Gabrielse's group at Northwestern University in Illinois [1] have determined the value of the electron's magnetic



$$\vec{\mu} = -\frac{e}{m}\vec{S} \equiv g\mu_B\frac{\vec{S}}{\hbar}$$

$$\frac{g}{2} = 1.001\,159\,652\,180\,59(13)$$

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：

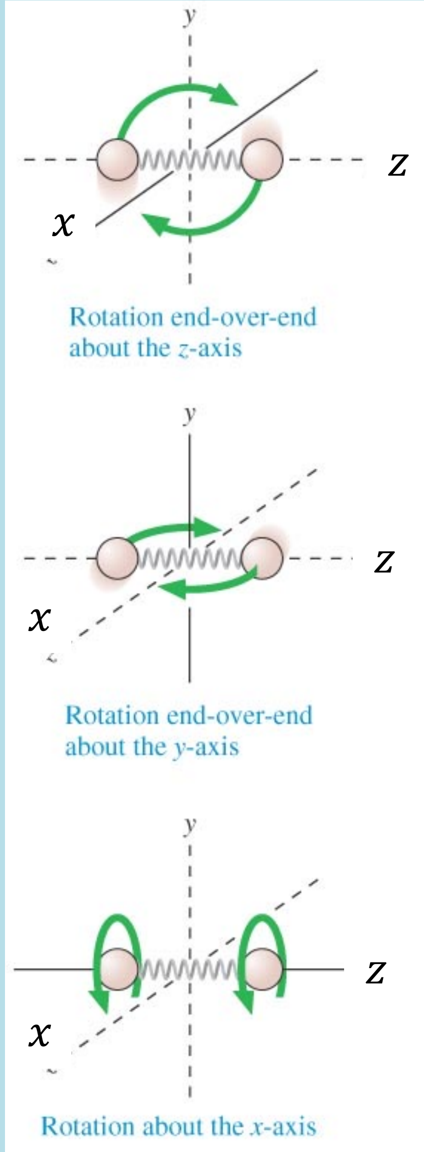
$$L_x^2 + L_y^2 = L^2 - L_z^2$$

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

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：

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



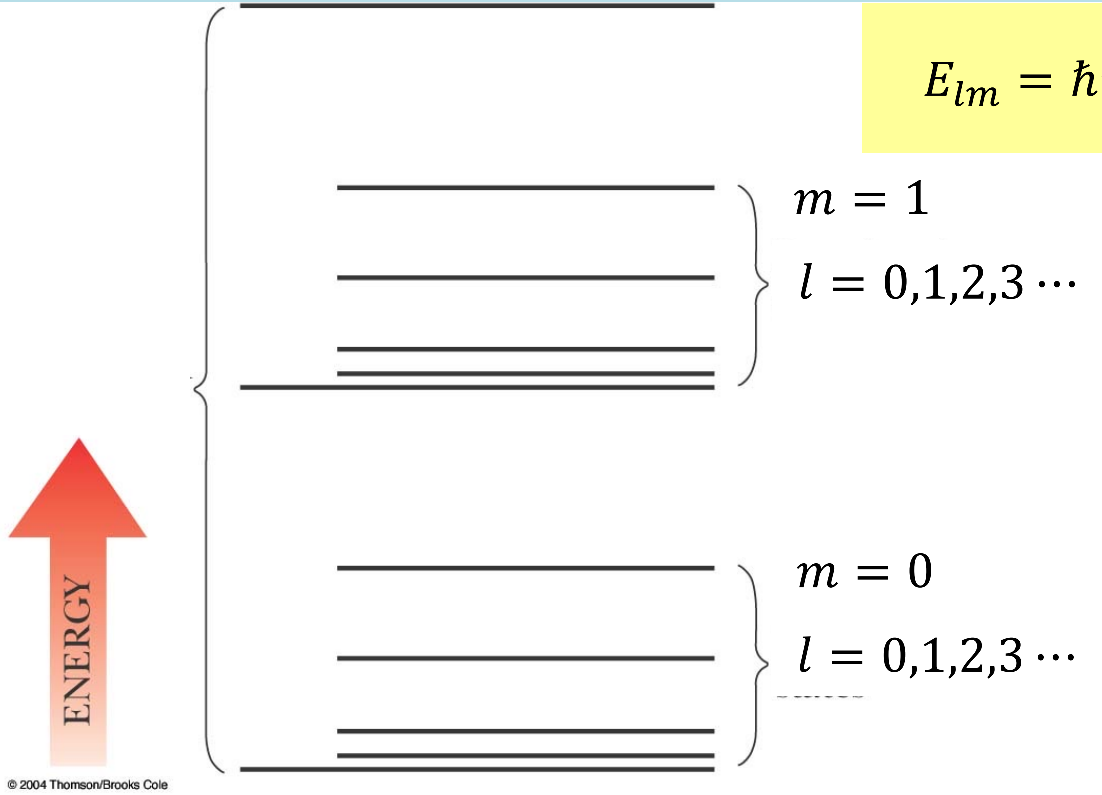
5. The Hamiltonian for an axially symmetric rotator is

$$H = \frac{L_x^2 + L_y^2}{2I_1} + \frac{L_z^2}{2I_3}$$

(a) What are the eigenvalues of H?

(b) Sketch the spectrum, assuming that $I_1 > I_3$. For b) try $l = 0,1,2$.

(c) What is the spectrum in the limit that I_1 is much larger than I_3?



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

$I > I_z$，第二項$\frac{\hbar^2 m^2}{2I_z}$較大

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:

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

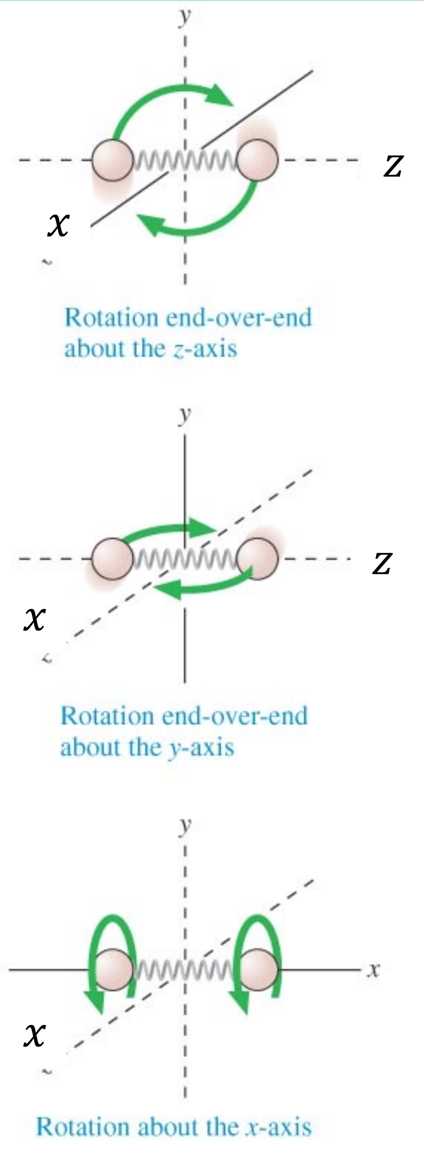
The best justification for adopting this formula is that it leads us to results that are confirmed by experiments.

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！

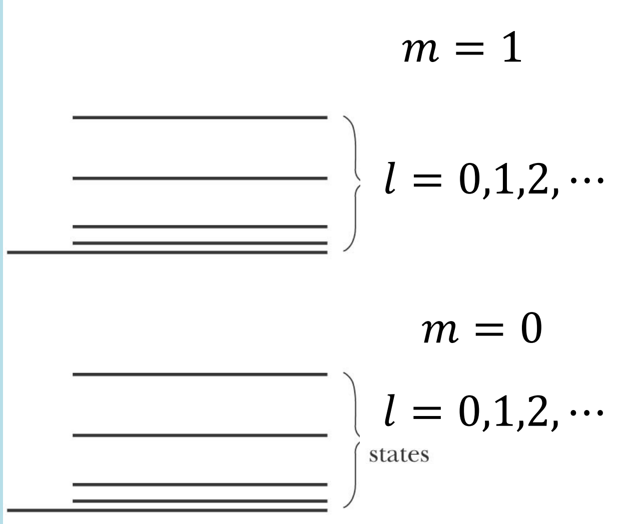
只有$m^2 = 0$的能階留下！能量由l決定：

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

因角動量受恆，發射光子的前後態$\Delta l = \pm 1$

光譜線對應$l+1 \to l$的躍遷，能差為：

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



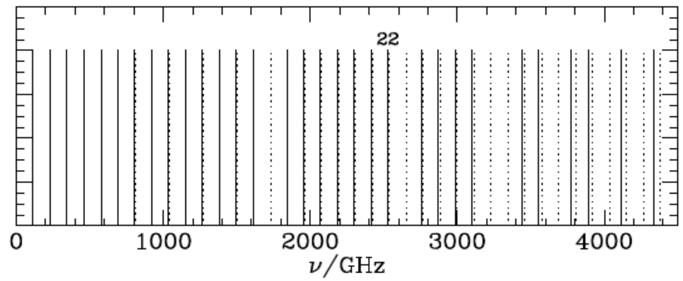
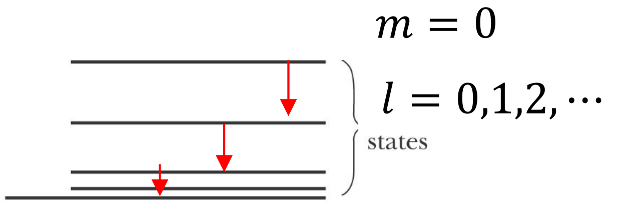


Figure 7.2 The rotation spectrum of CO. The full lines show the measured frequencies for transitions up to $j = 38 \to 37$, while the dotted lines show integer multiples of the lowest measured frequency. Up to the line for $j = 22 \to 21$ the dotted lines are obscured by the full lines except at one 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.

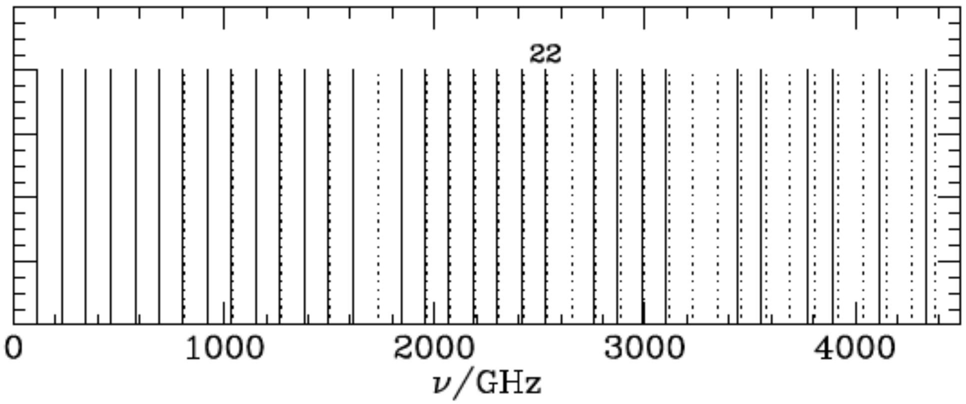


Figure 7.2 The rotation spectrum of CO. The full lines show the measured frequencies for transitions up to $j = 38 \to 37$, while the dotted lines show integer multiples of the lowest measured frequency. Up to the line for $j = 22 \to 21$ the dotted lines are obscured by the full lines except at one 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.