$(\hat{L}^2,\hat{L}_z)$的共同本征函数组－球谐函数

因$[\hat{L}^2,\hat{L}_z]=0$，它们有共同本征函数组。由对易关系

$$[\hat{L}_z,\hat{L}_x]=i\hbar\hat{L}_y$$

$$[\hat{L}_z,\hat{L}_y]=-i\hbar\hat{L}_x,$$

有

$$[\hat{L}_z,\hat{L}_+]=\hbar\hat{L}_+,$$

$$[\hat{L}_z,\hat{L}_-]=-\hbar\hat{L}_-,$$

其中阶梯算符， $\hat{L}_+=\hat{L}_x+i\hat{L}_y$， $\hat{L}_-=\hat{L}_x-i\hat{L}_y$

A. 本征值

设u_{lm}是它们的共同本征函数，则

$$\hat{L}^2u_{lm}=\eta_l\hbar^2u_{lm}$$

$$\hat{L}_zu_{lm}=m\hbar u_{lm}$$

所以，

$$(\hat{L}^2-\hat{L}_z^2)u_{lm}=(\eta_l-m^2)\hbar^2u_{lm}$$

由于，$\hat{L}^2-\hat{L}_z^2=\hat{L}_x^2+\hat{L}_y^2$，而$\hat{L}_x,\hat{L}_y$是厄密算符，所以，$\hat{L}_x^2,\hat{L}_y^2$的平均值恒为正。因此，

$$\eta_l\geq m^2$$

当l确定，η_l就确定，这时，$|m|\leq\eta_l^{1/2}$，即m有上、下限。由于，

$$\hat{L}_z\hat{L}_--\hat{L}_-\hat{L}_z=-\hbar\hat{L}_-$$

$$\therefore\quad \hat{L}_z\hat{L}_-u_{lm}=\hat{L}_-(\hat{L}_z-\hbar)u_{lm}=(m-1)\hbar\hat{L}_-u_{lm}$$

这表明，如u_{lm}是$\hat{L}^2,\hat{L}_z$的本征态，相应本征值为$\eta_l\hbar^2,m\hbar$，则$\hat{L}_-u_{lm}$也是$\hat{L}^2,\hat{L}_z$的本征态，本征值为$\eta_l\hbar^2,(m-1)\hbar$。所以

$$u_{lm} \quad \hat{L}_- u_{lm} \quad (\hat{L}_-)^2 u_{lm} \quad (\hat{L}_-)^3 u_{lm} \cdots$$

$$m\hbar \quad (m-1)\hbar \quad (m-2)\hbar \quad (m-3)\hbar \cdots$$

称 $\hat{L}_-$ 为降算符（对 $\hat{L}_z$ 而言）。同理

$$\hat{L}_z \hat{L}_+ u_{lm} = \hat{L}_+ (\hat{L}_z + \hbar) u_{lm} = (m+1)\hbar \hat{L}_+ u_{lm}$$

称 $\hat{L}_+$ 为升算符。由于，η_l 固定时，m 有上，下限。若设 m_+ 为上限，m_- 为下限，则

$$\hat{L}_+ u_{lm_+} = 0 \text{，} \qquad \hat{L}_- u_{lm_-} = 0$$

$$\hat{L}_- \hat{L}_+ u_{lm_+} = 0 \text{，} \qquad \hat{L}_+ \hat{L}_- u_{lm_-} = 0$$

$$\Downarrow$$

$$(\hat{L}^2 - \hat{L}_z^2 - \hbar \hat{L}_z) u_{lm_+} = (\eta_l - m_+^2 - m_+)\hbar^2 u_{lm_+} = 0$$

$$(\hat{L}^2 - \hat{L}_z^2 + \hbar \hat{L}_z) u_{lm_-} = (\eta_l - m_-^2 + m_-)\hbar^2 u_{lm_-} = 0$$

$$\Downarrow$$

$$\begin{array}{l} \eta_l = m_+(m_+ + 1) \\ \eta_l = m_-(m_- - 1) \end{array} \Rightarrow \begin{array}{l} m_+ = m_- - 1 \\ m_+ = -m_- \end{array}$$

由于，m_+ 为上限，m_- 为下限，所以，只能取 $m_+ = -m_-$，而

$$\eta_l = m_+(m_+ + 1)\hbar^2$$

若设：$m_+ = l$，则 $\eta_l = l(l+1)\hbar^2$。于是 $m_+ = l$，$m_- = -l$。这表明，l 只能取整数或半整数。但 m 只能取整。于是，$\hat{L}^2$ 的本征值为 $\eta_l = l(l+1)\hbar^2$；$\hat{L}_z$ 本征值可取

$$-l\hbar, \quad (-l+1)\hbar, \quad (-l+2)\hbar, \cdots, \quad 0, \cdots (l-2)\hbar, \quad (l-1)\hbar, \quad l\hbar$$

即，取 $m\hbar$，$-l \le m \le l$，而 $l = 0, 1, 2, 3, \cdots$。

B．归一化的本征态

设$\mathbf{u_{lm}}$已归一化，而 $\mathbf{u_{lm-1}} \propto \hat{\mathbf{L}}_{-}\mathbf{u_{lm}}$

$$(\hat{L}_{-}u_{lm},\hat{L}_{-}u_{lm}) = (u_{lm},\hat{L}_{+}\hat{L}_{-}u_{lm}) = (l+m)(l-m+1)\hbar^2$$

所以，

$$u_{lm-1} = \frac{\hat{L}_{-}u_{lm}}{\sqrt{(l+m)(l-m+1)}\hbar}$$

$$u_{lm} = \frac{1}{\hbar^{l-m}}\sqrt{\frac{(l+m)!}{(2l)!(l-m)!}}(\hat{L}_{-})^{l-m}u_{ll}$$

$$\hat{L}_{+}u_{ll} = 0$$

这表明，角动量的本征值是量子化的。它与能量量子化不同在于它并不需要粒子是束缚的。自由粒子的角动量是量子化的，这在经典力学看来是非常费解的。这在量子力学看来是非常清楚的，即动量本征态可由角动量的本征态叠加而成。因$[\hat{\mathbf{L}}^2,\frac{\hat{\mathbf{p}}^2}{2\mathbf{m}}]=0$， $[\hat{\mathbf{L}}_z,\frac{\hat{\mathbf{p}}^2}{2\mathbf{m}}]=0$， 所以各个角动量本征态的几率振幅不随时间变，是守恒的。

本征函数

由$\hat{\mathbf{L}}_z\mathbf{u_{lm}} = \mathbf{m}\hbar\mathbf{u_{lm}}$， 即 $-i\frac{\partial}{\partial\varphi}u_{lm} = m\hbar u_{lm}$

有解 $$u_{lm(\theta,\varphi)} = A_{lm}(\theta)e^{im\varphi}$$

而 $$\hat{L}_{+} = \hbar e^{i\varphi}(\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi})$$

$$\hat{L}_{-} = \hbar e^{-i\varphi}(-\frac{\partial}{\partial\theta} + i\cot\theta\frac{\partial}{\partial\varphi})$$

根据 $$\hat{L}_{+}u_{ll} = \hat{L}_{+}A_{ll(\theta)}e^{il\varphi} = 0$$

$$e^{i(l+1)\varphi}(\frac{d}{d\theta}-l\cot\theta)A_{ll}(\theta)=0$$

而 $$(\frac{d}{d\theta}-l\cot\theta)=\sin^l\theta\frac{d}{d\theta}\frac{1}{\sin^l\theta}\text{，}$$

得 $$A_{ll(\theta)}=c\sin^l\theta$$

归一化系数

$$c^2\int_0^\pi\sin^{2l+1}\theta d\theta\int_0^{2\pi}d\varphi=1$$

$$2\pi c^2(-1)^{2l}\frac{2^{2l+1}(l!)^2}{(2l+1)!}=1\text{，}$$

$$c=\frac{(-1)^l}{2^l l!}\sqrt{\frac{(2l+1)!}{4\pi}}$$

所以归一化的 $$A_{ll(\theta)}=(-1)^l\frac{1}{2^l l!}\sqrt{\frac{(2l+1)!}{4\pi}}\sin^l\theta$$

显然， $$u_{lm(\theta,\varphi)}\propto c(\hat{L}_-)^{l-m}\sin^l\theta e^{il\varphi}$$

u_{lm}的归一化问题，以及u_{lm}的具体形式

若u_{lm}是归一化的，由前知有 $$u_{lm-1}=\frac{1}{\sqrt{(l+m)(l-m+1)}\hbar}\hat{L}_-u_{lm}$$

下面给出归一化的波函数

$$\hat{L}_-u_{ll}=c\hat{L}_-\sin^l\theta e^{il\varphi}$$

$$=c\hbar e^{-i\varphi}(-\frac{\partial}{\partial\theta}+i\cot\theta\frac{\partial}{\partial\varphi})\sin^l\theta e^{il\varphi}$$

$$=c\hbar(-\frac{\partial}{\partial\theta}-l\cot\theta)\sin^l\theta e^{i(l-1)\varphi}$$

$$=-c\hbar(\frac{1}{\sin^l\theta}\frac{d}{d\theta}\sin^l\theta)\sin^l\theta e^{i(l-1)\varphi}$$

所以，

$$u_{ll-1}=\frac{c}{\sqrt{2l\cdot 1}}(-1)\frac{1}{\sin^{l}\theta}\frac{d}{d\theta}\sin^{2l}\theta e^{i(l-1)\varphi}$$

$$\hat{L}\_u_{ll-1}=\frac{c\hbar}{\sqrt{2l\cdot 1}}(-1)^{2}e^{-i\varphi}\left(\frac{\partial}{\partial\theta}-ictg\theta\frac{\partial}{\partial\varphi}\right)\frac{1}{\sin^{l}\theta}\frac{d}{d\theta}\sin^{2l}\theta e^{i(l-1)\varphi}$$

$$=\frac{c\hbar}{\sqrt{2l\cdot 1}}(-1)^{2}e^{i(l-2)\varphi}\left(\frac{1}{\sin^{(l-1)}\theta}\frac{d}{d\theta}\sin^{l-1}\right)\frac{1}{\sin^{l}\theta}\frac{d}{d\theta}\sin^{2l}\theta$$

$$u_{ll-2}=\frac{c}{\sqrt{2l\cdot(2l-1)\cdot 1\cdot 2}}(-1)^{2}\frac{1}{\sin^{(l-1)}\theta}\frac{d}{d\theta}\frac{1}{\sin\theta}\frac{d}{d\theta}\sin^{2l}\theta e^{i(l-2)\varphi}$$

以此类推

$$u_{lm}=\frac{c}{\sqrt{2l\cdot(2l-1)\cdots(l+m+1)\cdot 1\cdot 2\cdots(l-m)}}(-1)^{l-m}\frac{1}{\sin^{m+1}\theta}\cdot$$

$$\cdot\overbrace{\frac{d}{d\theta}\frac{1}{\sin\theta}\frac{d}{d\theta}\cdots\frac{1}{\sin\theta}\frac{d}{d\theta}}^{l-m}\sin^{2l}\theta e^{im\varphi}$$

$$=\frac{(-1)^{l}}{2^{l}l!}\sqrt{\frac{(2l+1)!}{4\pi}}\sqrt{\frac{(l+m)!}{(2l)!(l-m)!}}(-1)^{l-m}(-1)^{l-m}\frac{1}{\sin^{m}\theta}\left(\frac{d}{d\cos\theta}\right)^{l-m}\sin^{2l}\theta e^{im\varphi}$$

$$=\frac{(-1)^{l}}{2^{l}l!}\sqrt{\frac{(2l+1)}{4\pi}}\sqrt{\frac{(l+m)!}{(l-m)!}}\frac{1}{\sin^{m}\theta}\left(\frac{d}{d\cos\theta}\right)^{l-m}\sin^{2l}\theta e^{im\varphi}$$

于是得（$\hat{L}^{2},L_{z}$）的共同本征函数组−球谐函数

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

而

$$P_{l}^{m}(\cos\theta)=(-1)^{l+m}\frac{1}{2^{l}l!}\sqrt{\frac{(2l+1)}{4\pi}}\frac{(l+m)!}{(l-m)!}\frac{1}{\sin^{m}\theta}\left(\frac{d}{d\cos\theta}\right)^{l-m}\sin^{2l}\theta,$$

称为缔合勒让德函数（***Associated Legendre function***）。

当 l，m 给定，也就是$\hat{L}^{2},L_{z}$的本征值给定，那就唯一地确定了本征函数$Y_{lm}(\theta,\varphi)$。

性质：

1. 正交归一 $\int Y^*_{lm}(\theta,\varphi)Y_{l'm'}(\theta,\varphi)d\Omega = \delta_{ll'}\delta mm'$

2. 封闭性

$$\sum_{l=0}^{\infty}\sum_{m=-l}^{m=l} Y_{lm}(\theta,\varphi)Y^*_{lm}(\theta',\varphi') = \frac{1}{\sin\theta}\delta(\theta-\theta')\delta(\varphi-\varphi')$$

3. $P_l^{-m}(\cos\theta) = (-1)^m \frac{(l-m)!}{(l+m)!} P_l^m(\cos\theta) \qquad m \ge 0$

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

$$= \sqrt{\frac{(2l+1)}{4\pi}}\sqrt{\frac{(l-m)!}{(l+m)!}}P_l^{m}(\cos\theta)e^{-im\varphi}$$

$$\Rightarrow \quad Y_{l-m} = (-1)^m Y^*_{lm}$$

4. 宇称 $r \to -r, \quad \to \quad \theta \to \pi-\theta, \ \varphi \to \varphi+\pi$

$$P_l^m(\cos\theta) \xrightarrow{\text{贡献}} (-1)^{l-m}, e^{im\varphi} \xrightarrow{\text{贡献}} (-1)^m ,$$

$\Rightarrow \quad Y_{lm}(\theta,\varphi)$ 的宇称为 $(-1)^l$

5. 递推关系

$$\cos\theta Y_{lm} = a_{lm}Y_{l+1m} + a_{l-1m}Y_{l-1m}$$

$$\frac{d}{d\theta}Y_{lm} = -a_{lm}Y_{l+1m} + a_{l-1m}(l+1)Y_{l-1m}$$

$$\sin\theta e^{i\varphi}Y_{lm} = b_{l-1(-m-1)}Y_{l-1m+1} - b_{lm}Y_{l+1m+1}$$

$$\sin\theta e^{-i\varphi}Y_{lm} = b_{l-1m-1}Y_{l-1m-1} - b_{l-m}Y_{l+1m-1}$$

$$a_{lm} = \sqrt{\frac{(l+m+1)(l-m+1)}{(2l+1)(2l+3)}},$$

$$b_{lm} = \sqrt{\frac{(l+m+1)(l+m+2)}{(2l+1)(2l+3)}}$$