

CH12 中心势场问题

(对 Shankar 的 CH12 有重新整理, 小节编号和教材中编号不一致)

$$\hat{H} = \frac{\hat{p}_x^2}{2m} + \frac{\hat{p}_y^2}{2m} + \frac{\hat{p}_z^2}{2m} + V(r), \text{ 其中 } r = \sqrt{x^2 + y^2 + z^2}$$

此类 $V(x, y, z) = V(r)$ 的问题统称为中心力场问题或中心势场问题

§ 12.1 三维欧氏空间的旋转矩阵

回忆 homework 2.

$$R_1(\theta) = \begin{pmatrix} 1 & 0 & 0 \\ 0 & \cos\theta & -\sin\theta \\ 0 & \sin\theta & \cos\theta \end{pmatrix}, \quad R_2(\theta) = \begin{pmatrix} \cos\theta & 0 & \sin\theta \\ 0 & 1 & 0 \\ -\sin\theta & 0 & \cos\theta \end{pmatrix}$$

$$R_3(\theta) = \begin{pmatrix} \cos\theta & -\sin\theta & 0 \\ \sin\theta & \cos\theta & 0 \\ 0 & 0 & 1 \end{pmatrix}$$

为三维欧氏空间中绕 x, y, z 轴旋转 θ 角的矩阵

我们进一步定义了“生成元”

$$\Omega_1 = i \left. \frac{dR_1}{d\theta} \right|_{\theta=0} = \begin{pmatrix} 0 & 0 & 0 \\ 0 & 0 & -i \\ 0 & i & 0 \end{pmatrix}$$

$$\Omega_2 = i \left. \frac{dR_2}{d\theta} \right|_{\theta=0} = \begin{pmatrix} 0 & 0 & i \\ 0 & 0 & 0 \\ -i & 0 & 0 \end{pmatrix}$$

$$\Omega_3 = i \left. \frac{dR_3}{d\theta} \right|_{\theta=0} = \begin{pmatrix} 0 & -i & 0 \\ i & 0 & 0 \\ 0 & 0 & 0 \end{pmatrix}$$

其对应关系为 $[\Omega_1, \Omega_2] = i\Omega_3, \quad [\Omega_1, \Omega_3] = -i\Omega_2$

$$[\Omega_2, \Omega_3] = i\Omega_1$$

$$\Rightarrow [\Omega_i, \Omega_j] = i \epsilon_{ijk} \Omega_k \quad (i, j, k = 1, 2, 3)$$

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$$J^2 \equiv J_1^2 + J_2^2 + J_3^2 = 2I$$

并且我们证明了 $R_i(\theta) = e^{i\theta J_i}$ (Ex. 1.47)

对于中心势场问题, 可以利用旋转对称性简化计算

§12.2 Hilbert 空间中的角动量算符.

经典物理中的角动量为矢量: $\vec{L} = \vec{x} \times \vec{p} \Rightarrow L_i = \epsilon_{ijk} x^j p^k$

$$L_1 = \epsilon_{1jk} x^j p^k = x^2 p^3 - x^3 p^2$$

$$L_2 = \epsilon_{2jk} x^j p^k = -x^1 p^3 + x^3 p^1$$

$$L_3 = \epsilon_{3jk} x^j p^k = x^1 p^2 - x^2 p^1$$

也常写为 $L_x = y p_z - z p_y$

$$L_y = z p_x - x p_z$$

$$L_z = x p_y - y p_x$$

升级成算符,

$$\hat{L}_x = \hat{y} \hat{p}_z - \hat{z} \hat{p}_y$$

$$\hat{L}_y = \hat{z} \hat{p}_x - \hat{x} \hat{p}_z$$

$$\hat{L}_z = \hat{x} \hat{p}_y - \hat{y} \hat{p}_x$$

没有算符顺序问题

Ex 12.1 证明 (1) $[\hat{L}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{L}_k$

(2) \hat{L}_i 为厄米算符

证明 (1) 用分量形式

$$[\hat{L}_i, \hat{L}_j] = [\epsilon_{imn} \hat{x}^m \hat{p}^n, \epsilon_{jkl} \hat{x}^k \hat{p}^l]$$

$$= \epsilon_{imn} \epsilon_{jkl} [\hat{x}^m \hat{p}^n, \hat{x}^k \hat{p}^l]$$

$$= \epsilon_{imn} \epsilon_{jkl} \{ \hat{x}^m [\hat{p}^n, \hat{x}^k] \hat{p}^l + \hat{x}^k [\hat{x}^m, \hat{p}^l] \hat{p}^n \}$$

$$= \epsilon_{imn} \epsilon_{kjl} \{ \hat{x}^m (-i\hbar) \delta^{kn} \hat{p}^l + \hat{x}^k i\hbar \delta^{ml} \hat{p}^n \}$$

$$= i\hbar (\epsilon_{imn} \epsilon_{jkl} \delta^{ml}) \hat{x}^k \hat{p}^n - i\hbar (\epsilon_{imn} \epsilon_{kjl} \delta^{kn}) \hat{x}^m \hat{p}^l$$

$$\begin{aligned} \text{利用 } \epsilon_{imn} \epsilon_{jkl} \delta^{ml} &= -\epsilon_{min} \epsilon_{mjk} \\ &= -(\delta_{ij} \delta_{nk} - \delta_{ik} \delta_{jn}) \end{aligned}$$

$$\begin{aligned} \epsilon_{imn} \delta_{jkl} \delta^{kn} &= -\epsilon_{nim} \epsilon_{kjl} \\ &= -(\delta_{ij} \delta_{ml} - \delta_{il} \delta_{mj}) \end{aligned}$$

$$\begin{aligned} [\hat{L}_i, \hat{L}_j] &= (-i\hbar) (\delta_{ij} \delta_{nk} - \delta_{ik} \delta_{jn}) \hat{X}^k \hat{P}^n \\ &\quad + i\hbar (\delta_{ij} \delta_{ml} - \delta_{il} \delta_{mj}) \hat{X}^m \hat{P}^l \\ &= i\hbar \hat{X}^i \hat{P}^j - i\hbar \hat{X}^j \hat{P}^i \\ &= i\hbar (\hat{X}^i \hat{P}^j - \hat{X}^j \hat{P}^i) \end{aligned}$$

$$\begin{aligned} \text{另一方面 } \epsilon_{ijk} \hat{L}_k &= \epsilon_{ijk} \epsilon_{kmn} \hat{X}^m \hat{P}^n \\ &= \epsilon_{kij} \epsilon_{kmn} \hat{X}^m \hat{P}^n \\ &= (\delta_{im} \delta_{jn} - \delta_{in} \delta_{jm}) \hat{X}^m \hat{P}^n \\ &= \hat{X}^i \hat{P}^j - \hat{X}^j \hat{P}^i \end{aligned}$$

$$\Rightarrow [\hat{L}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{L}_k \quad //$$

- \hat{L}^i ($i=1,2,3$) 的对易关系和 \hat{J}^i ($i=1,2,3$) 相同

Ex 12.2 (1) 求 $\hat{L}^2 = \hat{L}_x^2 + \hat{L}_y^2 + \hat{L}_z^2$

(2) 证明 $[\hat{L}^2, \hat{L}^i] = 0$

- $[\hat{L}^2, \hat{L}^i] = 0$, 这点和 $[\hat{J}^2, \hat{J}^i]$ 也相同

前面证明了 $R_i(\theta) = e^{i\theta \hat{J}_i}$ 为绕 i 轴转 θ 角,

那么 $e^{\frac{i}{\hbar} \theta \hat{L}_i}$ 有什么物理意义

由于 \hat{L}_i 为 $[x, p]$ 量纲, 所以分母有 \hbar

Ex 12.3 在坐标表象下求 $e^{\frac{i}{\hbar}\theta \hat{L}_i} |\psi\rangle$

解. 因为 \hat{L}_i 定义在 3 维空间, 所以其坐标表象为
先考虑 $i=3$

$$\begin{aligned} & \langle x, y, z | e^{\frac{i}{\hbar}\theta \hat{L}_3} |\psi\rangle \\ &= \int dx' dy' dz' \langle x, y, z | e^{\frac{i}{\hbar}\theta \hat{L}_3} |x', y', z'\rangle \underbrace{\langle x', y', z' | \psi\rangle}_{\equiv \psi(x', y', z')} \end{aligned}$$

$$\hat{L}_3 = \hat{X}_1 \hat{P}_2 - \hat{X}_2 \hat{P}_1$$

$$\langle xy z | \hat{L}_3 | x' y' z' \rangle$$

$$= \langle xy z | \hat{X}_1 \hat{P}_2 | x' y' z' \rangle - \langle xy z | \hat{X}_2 \hat{P}_1 | x' y' z' \rangle$$

$$= \langle x | \hat{X}_1 | x' \rangle \langle y | \hat{P}_2 | y' \rangle \langle z | z' \rangle - \langle x | \hat{P}_1 | x' \rangle \langle y | \hat{X}_2 | y' \rangle \langle z | z' \rangle$$

$$= x' \delta(x-x') (-i\hbar) \delta(y-y') \frac{\partial}{\partial y'} \delta(z-z')$$

$$- (-i\hbar) \delta(x-x') \frac{\partial}{\partial x'} y' \delta(y-y') \delta(z-z')$$

$$= \delta(x-x') \delta(y-y') \delta(z-z') (-i\hbar) \left[x' \frac{\partial}{\partial y'} - y' \frac{\partial}{\partial x'} \right] \quad \text{--- (*)}$$

xy 方向转换成极坐标: $\rho' = \sqrt{x'^2 + y'^2}$, $\theta' = \arctan \frac{y'}{x'}$

$$x' = \rho' \cos \theta', \quad y' = \rho' \sin \theta'$$

$$\cdot x' \frac{\partial}{\partial y'} - y' \frac{\partial}{\partial x'} = \rho' \cos \theta' \left[\frac{\partial}{\partial \rho'} \frac{\partial \rho'}{\partial y'} + \frac{\partial}{\partial \theta'} \frac{\partial \theta'}{\partial y'} \right]$$

$$- \rho' \sin \theta' \left[\frac{\partial}{\partial \rho'} \frac{\partial \rho'}{\partial x'} + \frac{\partial}{\partial \theta'} \frac{\partial \theta'}{\partial x'} \right]$$

$$= \rho' \cos \theta' \left[\frac{2y'}{2\sqrt{x'^2 + y'^2}} \frac{\partial}{\partial \rho'} + \frac{1}{1 + \left(\frac{y'}{x'}\right)^2} \frac{\partial}{\partial \theta'} \right]$$

$$- \rho' \sin \theta' \left[\frac{2x'}{2\sqrt{x'^2 + y'^2}} \frac{\partial}{\partial \rho'} + \frac{1}{1 + \left(\frac{y'}{x'}\right)^2} \left(-\frac{y'}{x'^2}\right) \frac{\partial}{\partial \theta'} \right]$$

$$= \rho' \cos \theta' \left[\cancel{\sin \theta'} \frac{\partial}{\partial \rho'} + \frac{1}{\rho'} \cos \theta' \frac{\partial}{\partial \theta'} \right]$$

$$- \rho' \sin \theta' \left[\cancel{\cos \theta'} \frac{\partial}{\partial \rho'} - \frac{1}{\rho'} \sin \theta' \frac{\partial}{\partial \theta'} \right]$$

$$= [(\cos \theta')^2 + (\sin \theta')^2] \frac{\partial}{\partial \theta'} = \frac{\partial}{\partial \theta'}$$

$$\bullet \delta(x-x') \delta(y-y') = ?$$

$$\text{利用 } \int dx' dy' \delta(x-x') \delta(y-y') = 1$$

$$\Rightarrow \int p' dp' d\theta' \delta(x-x') \delta(y-y') = 1$$

$$\Rightarrow \delta(x-x') \delta(y-y') = \frac{1}{p'} \delta(p-p') \delta(\theta-\theta')$$

检查量纲!

所以

$$(*) \Rightarrow \langle xy z | \hat{L}_3 | x' y' z' \rangle = \frac{1}{p'} \delta(p-p') \delta(\theta-\theta') \delta(z-z') (-i\hbar) \frac{\partial}{\partial \theta'},$$

————— (*2)

$$\langle xy z | \hat{L}_3^2 | x' y' z' \rangle = \int dx'' dy'' dz'' \langle xy z | \hat{L}_3 | x'' y'' z'' \rangle$$

$$* \langle x'' y'' z'' | \hat{L}_3 | x' y' z' \rangle$$

$$= \int dx'' dy'' dz'' \frac{1}{p''} \delta(p-p'') \delta(\theta-\theta'') \delta(z-z'') (-i\hbar) \frac{\partial}{\partial \theta''}$$

$$= p'' dp'' d\theta'' \rightarrow * \frac{1}{p'} \delta(p''-p) \delta(\theta''-\theta') \delta(z''-z') (-i\hbar) \frac{\partial}{\partial \theta'},$$

$$= (-i\hbar)^2 \frac{1}{p} \delta(z-z') \delta(p-p') \int d\theta'' \delta(\theta-\theta'') \frac{\partial}{\partial \theta''} \delta(\theta''-\theta') \frac{\partial}{\partial \theta'}$$

————— (*3)

$$\text{因为 } \int d\theta' \left[\int d\theta'' \delta(\theta-\theta'') \frac{\partial}{\partial \theta''} \delta(\theta''-\theta') \frac{\partial}{\partial \theta'} \right] \psi(\theta')$$

$$= \int d\theta'' \delta(\theta-\theta'') \frac{\partial}{\partial \theta''} \int d\theta' \delta(\theta''-\theta') \frac{\partial}{\partial \theta'} \psi(\theta') = \frac{\partial^2 \psi}{\partial \theta^2}$$

$$\Rightarrow \int d\theta'' \frac{\partial}{\partial \theta''} \delta(\theta''-\theta') \frac{\partial}{\partial \theta'} = \delta(\theta'-\theta'') \frac{\partial^2}{\partial \theta'^2}$$

代入(*)3) 即得

$$\langle x y z | \hat{L}_3^2 | x' y' z' \rangle = \frac{1}{\rho} \delta(z-z') \delta(\rho-\rho') \delta(\theta-\theta') (-i\hbar)^2 \frac{\partial^2}{\partial \theta'^2}$$

用归纳法可证

$$\langle x y z | \hat{L}_3^n | x' y' z' \rangle = \frac{1}{\rho} \delta(z-z') \delta(\rho-\rho') \delta(\theta-\theta') (-i\hbar)^n \frac{\partial^n}{\partial \theta'^n} \quad \text{--- (x4)}$$

所以 $\langle x y z | e^{\frac{i}{\hbar} \varphi \hat{L}_3} | x' y' z' \rangle$

$$= \sum_{n=0}^{+\infty} \frac{1}{n!} \left(\frac{i}{\hbar} \varphi\right)^n \langle x y z | \hat{L}_3^n | x' y' z' \rangle$$

$$= \frac{1}{\rho} \delta(z-z') \delta(\rho-\rho') \delta(\theta-\theta') \sum_{n=0}^{+\infty} \frac{1}{n!} \varphi^n \frac{\partial^n}{\partial \theta'^n}$$

$$\langle x y z | e^{\frac{i}{\hbar} \varphi \hat{L}_3} | \psi \rangle$$

$$= \int dx' dy' dz' \langle x y z | e^{\frac{i}{\hbar} \varphi \hat{L}_3} | x' y' z' \rangle \underbrace{\langle x' y' z' | \psi \rangle}_{\equiv \psi(x', y', z')}$$

$$\equiv \psi(x', y', z')$$

$$= \psi(\rho', \theta', z')$$

$$= \int \rho' d\rho' d\theta' dz' \frac{1}{\rho} \delta(z-z') \delta(\rho-\rho') \delta(\theta-\theta') \sum_{n=0}^{+\infty} \frac{1}{n!} \varphi^n \frac{\partial^n \psi}{\partial \theta'^n}$$

$$= \sum_{n=0}^{+\infty} \frac{1}{n!} \varphi^n \frac{\partial^n \psi}{\partial \theta'^n}$$

$$= \psi(\rho, \theta + \varphi, z)$$

$$\text{令 } |\psi'\rangle = e^{\frac{i}{\hbar} \varphi \hat{L}_3} |\psi\rangle \Rightarrow \psi'(\rho, \theta, z) = \psi(\rho, \theta + \varphi, z) \quad \parallel$$

- $e^{\frac{i}{\hbar} \varphi \hat{L}_3}$ 在坐标空间中将 $\psi(\rho, \theta, z)$ 绕 z 轴旋转 $-\varphi$ 角
同理 $e^{\frac{i}{\hbar} \varphi \hat{L}_1}$ 和 $e^{\frac{i}{\hbar} \varphi \hat{L}_2}$ 为绕 x 轴的 y 轴的相应转动

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- $e^{\frac{i}{\hbar} \phi \hat{L}_i}$ 也有转动的物理含义, 不过是在函数空间中的转动
 \hat{L}_i 即为函数空间中绕 i 轴的无穷小转动

(回忆: 三维欧氏空间中的转动)

- 由 \hat{L}_i 的物理含义, 若 $\hat{H} = \frac{\hat{p}^2}{2m} + V(r)$, 有

$$[\hat{L}_i, \hat{H}] = 0$$

$$\text{和 } [\hat{L}^2, \hat{H}] = [\hat{L}_1^2 + \hat{L}_2^2 + \hat{L}_3^2, \hat{H}] = 0$$

- 一般用 $\hat{H}, \hat{L}^2, \hat{L}_3$ 标记共同的本征态.

Ex 12.4 数学上证明 $[\hat{L}_i, \hat{H}] = 0$

§12.3 \hat{L}^2 和 \hat{L}_z 的共同本征态.

\hat{L}_i 和 \hat{L}_j 虽然具体形式不同, 但都有相同的对易关系, 在这一节中, 我们仅从对易关系出发, 看看能得到关于本征值和本征态的哪些信息.

$$[\hat{L}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{L}_k$$

$$[\hat{L}^2, \hat{L}_i] = 0$$

• 取 \hat{L}^2 和 \hat{L}_3 的共同本征态 $|\alpha, \beta\rangle$, 有

$$\hat{L}^2 |\alpha, \beta\rangle = \alpha |\alpha, \beta\rangle$$

$$\hat{L}_3 |\alpha, \beta\rangle = \beta |\alpha, \beta\rangle$$

$$\text{由于 } [\hat{L}_1, \hat{L}_3] = i\hbar \epsilon_{132} \hat{L}_2 = -i\hbar \hat{L}_2$$

$$[\hat{L}_2, \hat{L}_3] = i\hbar \epsilon_{231} \hat{L}_1 = i\hbar \hat{L}_1$$

所以该本征态不可能是 \hat{L}_1 和 \hat{L}_2 的本征态.

Ex 12.5

$$\text{def } \hat{L}_{\pm} = \hat{L}_1 \pm i\hat{L}_2$$

$$\text{证明 } [\hat{L}_3, \hat{L}_{\pm}] = \pm\hbar \hat{L}_{\pm}$$

$$\text{证明: } [\hat{L}_3, \hat{L}_{\pm}] = [\hat{L}_3, \hat{L}_1] \pm i [\hat{L}_3, \hat{L}_2]$$

$$= i\hbar \hat{L}_2 \pm i (-i)\hbar \hat{L}_1$$

$$= i\hbar \hat{L}_2 \pm \hbar \hat{L}_1 = \pm\hbar (\hat{L}_1 \pm i\hat{L}_2) = \pm\hbar \hat{L}_{\pm} \quad //$$

$$\text{回忆一维谐振子 } [\hat{a}, \frac{\hat{H}}{\hbar\omega}] = \hat{a}, \quad [\hat{a}^{\dagger}, \frac{\hat{H}}{\hbar\omega}] = -\hat{a}^{\dagger}$$

然后我们用梯算符得到了清晰的本征值和本征态结构

Ex 12.6 (1) 计算 $[\hat{L}_+, \hat{L}_-]$
 (2) 计算 $[\hat{L}^2, \hat{L}_\pm]$

解: (1) $[\hat{L}_+, \hat{L}_-] = [\hat{L}_1 + i\hat{L}_2, \hat{L}_1 - i\hat{L}_2]$
 $= -i[\hat{L}_1, \hat{L}_2] + i[\hat{L}_2, \hat{L}_1]$
 $= -i[\hat{L}_1, \hat{L}_2]$
 $= -i \cdot i\hbar \epsilon_{123} \hat{L}_3$
 $= \hbar \hat{L}_3$

(2) $[\hat{L}^2, \hat{L}_\pm] = [\hat{L}_1^2 + \hat{L}_2^2 + \hat{L}_3^2, \hat{L}_\pm]$
 $= [\hat{L}_1^2, \hat{L}_1 \pm i\hat{L}_2] + [\hat{L}_2^2, \hat{L}_1 \pm i\hat{L}_2]$
 $+ [\hat{L}_3^2, \hat{L}_\pm]$
 $= \pm i[\hat{L}_1^2, \hat{L}_2] + [\hat{L}_2^2, \hat{L}_1] + [\hat{L}_3^2, \hat{L}_\pm]$

• $[\hat{L}_1^2, \hat{L}_2] = \hat{L}_1[\hat{L}_1, \hat{L}_2] + [\hat{L}_1, \hat{L}_2]\hat{L}_1$
 $= \hat{L}_1 i\hbar \hat{L}_3 + i\hbar \hat{L}_3 \hat{L}_1$
 $= i\hbar(\hat{L}_1 \hat{L}_3 + \hat{L}_3 \hat{L}_1)$

• $[\hat{L}_2^2, \hat{L}_1] = \hat{L}_2[\hat{L}_2, \hat{L}_1] + [\hat{L}_2, \hat{L}_1]\hat{L}_2$
 $= \hat{L}_2(-i\hbar)\hat{L}_3 + (-i\hbar)\hat{L}_3\hat{L}_2$
 $= -i\hbar(\hat{L}_2 \hat{L}_3 + \hat{L}_3 \hat{L}_2)$

• $[\hat{L}_3^2, \hat{L}_\pm] = \hat{L}_3[\hat{L}_3, \hat{L}_\pm] + [\hat{L}_3, \hat{L}_\pm]\hat{L}_3$
 $= \pm \hbar \hat{L}_3 \hat{L}_\pm \pm \hbar \hat{L}_\pm \hat{L}_3$

$= \mp \hbar(\hat{L}_1 \hat{L}_3 + \hat{L}_3 \hat{L}_1) - i\hbar(\hat{L}_2 \hat{L}_3 + \hat{L}_3 \hat{L}_2)$
 $\pm \hbar \hat{L}_3(\hat{L}_1 \pm i\hat{L}_2) \pm \hbar(\hat{L}_1 \pm i\hat{L}_2)\hat{L}_3$

$= 0$

下面研究 $\hat{L}_{\pm}|\alpha\beta\rangle$ 是否是 \hat{L}^2 和 \hat{L}_3 的本征态。

Ex 12.7 计算 $\hat{L}^2 \hat{L}_{\pm}|\alpha\beta\rangle$ 和 $\hat{L}_3 \hat{L}_{\pm}|\alpha\beta\rangle$

解:
$$\begin{aligned}\hat{L}_3 \hat{L}_{\pm}|\alpha\beta\rangle &= \{[\hat{L}_3, \hat{L}_{\pm}] + \hat{L}_{\pm} \hat{L}_3\} |\alpha\beta\rangle \\ &= \{\pm \hbar \hat{L}_{\pm} + \hat{L}_{\pm} \hat{L}_3\} |\alpha\beta\rangle \\ &= \pm \hbar \hat{L}_{\pm}|\alpha\beta\rangle + \beta \hat{L}_{\pm}|\alpha\beta\rangle \\ &= (\beta \pm \hbar) \hat{L}_{\pm}|\alpha\beta\rangle \quad \text{————— (*)}\end{aligned}$$

$$\begin{aligned}\hat{L}^2 \hat{L}_{\pm}|\alpha\beta\rangle &= \{[\hat{L}^2, \hat{L}_{\pm}] - \hat{L}_{\pm} \hat{L}^2\} |\alpha\beta\rangle \\ &= -\alpha \hat{L}_{\pm}|\alpha, \beta\rangle \quad //\end{aligned}$$

• 可以证明 $|\alpha\beta\rangle$ 没有简并, 所以

$$\hat{L}_{\pm}|\alpha\beta\rangle = C_{\pm}(\alpha, \beta) |\alpha, \beta \pm \hbar\rangle$$

可见 \hat{L}_{\pm} 可以看成升降算符, 将 \hat{L}_3 的本征值改变 \hbar

• 和谐振子类似, 升降不能无休止地进行

$$\forall |\alpha\beta\rangle \quad \langle\alpha\beta| \hat{L}^2 - \hat{L}_3^2 |\alpha\beta\rangle = (\alpha - \beta^2) |\alpha\beta\rangle$$

$$\begin{aligned}\text{另一方面} \quad \langle\alpha\beta| \hat{L}^2 - \hat{L}_3^2 |\alpha\beta\rangle &= \langle\alpha\beta| \hat{L}_x^2 + \hat{L}_y^2 |\alpha\beta\rangle \\ &\geq 0\end{aligned}$$

$$\Rightarrow \alpha > \beta^2$$

\Rightarrow 给定 α , \hat{L}_+ 和 \hat{L}_- 都不能无休止地进行

Ex 12.8 给定 $\alpha > 0$, 有 β_{\max} 和 β_{\min} , 满足

$$\hat{L}_+ |\alpha, \beta_{\max}\rangle = 0$$

$$\hat{L}_- |\alpha, \beta_{\min}\rangle = 0$$

研究 $|\alpha, \beta\rangle$ 的本征值和本征态.

解: 利用 $\hat{L}_- \hat{L}_+ = (\hat{L}_1 - i\hat{L}_2)(\hat{L}_1 + i\hat{L}_2) = \hat{L}_1^2 + \hat{L}_2^2 + i[\hat{L}_1, \hat{L}_2]$

$$= \hat{L}^2 - \hat{L}_3^2 + i\hbar\hat{L}_3$$

$$= \hat{L}^2 - \hat{L}_3^2 - \hbar\hat{L}_3$$

可得 $0 = \hat{L}_- \hat{L}_+ |\alpha, \beta_{\max}\rangle$

$$= (\hat{L}^2 - \hat{L}_3^2 - \hbar\hat{L}_3) |\alpha, \beta_{\max}\rangle$$

$$= (\alpha - \beta_{\max}^2 - \hbar\beta_{\max}) |\alpha, \beta_{\max}\rangle$$

$$\Rightarrow \alpha = \beta_{\max}(\beta_{\max} + \hbar) \quad \text{—————} \quad (*1)$$

利用 $\hat{L}_+ \hat{L}_- = (\hat{L}_1 + i\hat{L}_2)(\hat{L}_1 - i\hat{L}_2) = \hat{L}_1^2 + \hat{L}_2^2 + i[\hat{L}_2, \hat{L}_1]$

$$= \hat{L}^2 - \hat{L}_3^2 + i(-i\hbar)\hat{L}_3$$

$$= \hat{L}^2 - \hat{L}_3^2 + \hbar\hat{L}_3$$

可得 $0 = \hat{L}_+ \hat{L}_- |\alpha, \beta_{\min}\rangle = (\hat{L}^2 - \hat{L}_3^2 + \hbar\hat{L}_3) |\alpha, \beta_{\min}\rangle$

$$= (\alpha - \beta_{\min}^2 + \hbar\beta_{\min}) |\alpha, \beta_{\min}\rangle$$

$$\Rightarrow \alpha = \beta_{\min}(\beta_{\min} - \hbar) \quad \text{—————} \quad (*2)$$

比较 (*1) (*2), 可得

$$\beta_{\max}^2 + \hbar\beta_{\max} = \beta_{\min}^2 - \hbar\beta_{\min}$$

$$\Rightarrow (\beta_{\max} - \beta_{\min})(\beta_{\max} + \beta_{\min}) + \hbar(\beta_{\max} + \beta_{\min}) = 0$$

$$\Rightarrow (\beta_{\max} - \beta_{\min} + \hbar)(\beta_{\max} + \beta_{\min}) = 0$$

$$\Rightarrow \beta_{\max} = -\beta_{\min} \quad \text{—————} \quad (*3)$$

若从 $|\alpha\beta_{\min}\rangle$ 经过 k 次 \hat{L}_+ 升到 $|\alpha\beta_{\max}\rangle$
可知 $\beta_{\max} = \beta_{\min} + k\hbar \quad (k=0, 1, 2, \dots)$

$$\text{结合} (*3) \Rightarrow \beta_{\max} = \frac{k\hbar}{2} \quad \text{—————} \quad (*4)$$

$$\Rightarrow \alpha = \beta_{\max}(\beta_{\max} + \hbar) = \frac{k\hbar}{2} \left(\frac{k\hbar}{2} + \hbar \right) = \hbar^2 \frac{k}{2} \left(\frac{k}{2} + 1 \right) \quad \text{—————} \quad (*5) //$$

总结, \hat{L}^2 和 \hat{L}_3 的共同本征态 $|\alpha\beta\rangle$:

$$\hat{L}^2 |\alpha\beta\rangle = \alpha |\alpha\beta\rangle$$

$$\hat{L}_3 |\alpha\beta\rangle = \beta |\alpha\beta\rangle$$

其中 α 只能取 $\hbar^2 \frac{k}{2} \left(\frac{k}{2} + 1 \right) \quad (k=0, 1, 2, \dots)$

给定 α 后, β 只能取 $-\frac{k\hbar}{2}, (-\frac{k}{2} + 1)\hbar, \dots, \frac{k\hbar}{2}$

共 $(k+1)$ 个

习惯上用 $l = \frac{k}{2}, m = \frac{\beta}{\hbar}$ 取代 $|\alpha\beta\rangle$

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

$$\hat{L}_3 |l, m\rangle = m\hbar |l, m\rangle$$

$l = \frac{k}{2}$ 为整数或半整数, $m = -\frac{k}{2}, -\frac{k}{2} + 1, \dots, \frac{k}{2}$

即为 $m = -l, -l+1, \dots, l-1, l$, 共 $2l+1$ 个

由 $\hat{L}_{\pm} |\alpha\beta\rangle = C_{\pm}(\alpha, \beta) |\alpha, \beta \pm \hbar\rangle$ 可得

$$\hat{L}_{\pm} |l, m\rangle = C_{\pm}(l, m) |l, m \pm 1\rangle$$

所以 \hat{L}_{\pm} 只能联系相同 l , 但不同 m 的态.

Ex 12.9 计算归一化因子 $C_{\pm}(l, m)$

解: 假设 $|l, m\rangle$ 为归一化态矢: $\langle l', m' | l, m\rangle = \delta_{ll'} \delta_{mm'}$

因为 $\hat{L}_{\pm} = \hat{L}_x \pm i\hat{L}_y$ 互为厄米共轭算符

$$\begin{aligned} \langle l, m | \hat{L}_+ \hat{L}_- |l, m\rangle &= |C_-(l, m)|^2 \langle l, m-1 | l, m-1\rangle \\ &= |C_-(l, m)|^2 \end{aligned}$$

又因为 $\hat{L}_+ \hat{L}_- = \hat{L}^2 - \hat{L}_3^2 + \hbar \hat{L}_3$ 见 Ex 12.8

$$\begin{aligned} \Rightarrow \langle l, m | \hat{L}_+ \hat{L}_- |l, m\rangle &= \langle l, m | (\hat{L}^2 - \hat{L}_3^2 + \hbar \hat{L}_3) |l, m\rangle \\ &= l(l+1)\hbar^2 - m^2\hbar^2 + m\hbar^2 \\ &= [l(l+1) - m(m-1)]\hbar^2 \end{aligned}$$

$$\Rightarrow C_-(l, m) = \sqrt{l(l+1) - m(m-1)} \hbar$$

自洽性检查

$$\hat{L}_- |l, -l\rangle \propto \sqrt{l(l+1) - (-l)(-l-1)} \hbar = 0$$

所以 $|l, -l\rangle$ 是“最低”的本征态.

同样地 $\langle l, m | \hat{L}_- \hat{L}_+ |l, m\rangle = |C_+(l, m)|^2$

$$\begin{aligned} \text{且有 } \langle l, m | \hat{L}_- \hat{L}_+ |l, m\rangle &= \langle l, m | \hat{L}^2 - \hat{L}_3^2 - \hbar \hat{L}_3 |l, m\rangle \\ &= l(l+1)\hbar^2 - m^2\hbar^2 - m\hbar^2 \\ &= [l(l+1) - m(m+1)]\hbar^2 \end{aligned}$$

$$\Rightarrow C_+(l, m) = \sqrt{l(l+1) - m(m+1)} \hbar$$

自洽性检查 $\hat{L}_+ |l, l\rangle \propto \sqrt{l(l+1) - l(l+1)} = 0$

所以 $|l, l\rangle$ 是“最高”的本征态 //

总结: 在这一节, 我们仅利用 $[\hat{L}_i, \hat{L}_j] = i\hbar \epsilon_{ijk} \hat{L}_k$, 即得到了关于本征值和本征态大量的信息

\hat{L}_2, \hat{L}_3 的共同本征态可写成 $|l, m\rangle$ 的形式

$$\hat{L}_2^2 |l, m\rangle = l(l+1)\hbar^2 |l, m\rangle$$

$$\hat{L}_3 |l, m\rangle = m\hbar |l, m\rangle$$

其中 $l \geq 0$ 可取整数或半整数.

$m = -l, -l+1, \dots, l-1, l$ 共 $2l+1$ 个取值

$\hat{L}_\pm = \hat{L}_x \pm i\hat{L}_y$ 可作为升降算符连接相同 l 但不同 m 的态

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

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

$$\hat{L}_+ |l, l\rangle = 0$$

$$\hat{L}_- |l, -l\rangle = 0$$

Ex 12.10 三维欧氏空间中的转动矩阵的“生成元” J_i 也满足

$$[J_i, J_j] = i \epsilon_{ijk} J_k$$

所以 $J^2 = J_1^2 + J_2^2 + J_3^2$ 和 J_3 的本征向量也可写成 $|l, m\rangle$ 的形式

(1) 求 l 的取值.

(2) 求 $|l, -l\rangle \dots |l, l\rangle$ 的列向量形式

(3) 定义 $J_{\pm} = J_1 \pm iJ_2$, 写出 J_{\pm} 的矩阵表示, 并用矩阵计算表明

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

$$J_- |l, -l\rangle = 0$$

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

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

§12.4 角动量算符本征态波函数

在本节中, 我们进一步利用角动量算符 \hat{L}_i 的具体形式,

$$\hat{L}_i = \epsilon_{ijk} \hat{x}_j \hat{p}_k$$

计算 $|l, m\rangle$ 在坐标空间中的波函数.

思路: 给定 l , 先求 $|l, l\rangle$ 在坐标表象下的波函数, 再用 L_- 求其他的 $|l, m\rangle$

Ex 12.11 求 $\hat{L}_3, \hat{L}_1, \hat{L}_2, \hat{L}^2, \hat{L}_\pm$ 在坐标表象下的表示 (用球坐标)

解: (1) $\langle x, y, z | \hat{L}_3 | x', y', z' \rangle$ 在 §12.2 节算过柱坐标下的表象, 现在我们改成球坐标

$$\begin{aligned} \langle x, y, z | \hat{L}_3 | x', y', z' \rangle &= \langle x, y, z | \hat{x}_1 \hat{p}_2 - \hat{x}_2 \hat{p}_1 | x', y', z' \rangle \\ &= \langle x | \hat{x}_1 | x' \rangle \langle y | \hat{p}_2 | y' \rangle \langle z | z' \rangle \\ &\quad - \langle x | \hat{p}_1 | x' \rangle \langle y | \hat{x}_2 | y' \rangle \langle z | z' \rangle \\ &= \delta(x-x') \delta(y-y') \delta(z-z') \left[x' (-i\hbar) \frac{\partial}{\partial y'} - y' (-i\hbar) \frac{\partial}{\partial x'} \right] \\ &= \delta(x-x') \delta(y-y') \delta(z-z') (-i\hbar) \left[x' \frac{\partial}{\partial y'} - y' \frac{\partial}{\partial x'} \right] \end{aligned}$$

球坐标下

$$\begin{cases} x = r \sin \theta \cos \varphi \\ y = r \sin \theta \sin \varphi \\ z = r \cos \theta \end{cases} \quad \begin{cases} r = \sqrt{x^2 + y^2 + z^2} \\ \theta = \arctan \frac{\sqrt{x^2 + y^2}}{z} \\ \varphi = \arctan \frac{y}{x} \end{cases}$$

$$\begin{aligned} \bullet \quad x' \frac{\partial}{\partial y'} - y' \frac{\partial}{\partial x'} &= r' \sin \theta' \cos \varphi' \left[\frac{\partial r'}{\partial y'} \frac{\partial}{\partial r'} + \frac{\partial \theta'}{\partial y'} \frac{\partial}{\partial \theta'} + \frac{\partial \varphi'}{\partial y'} \frac{\partial}{\partial \varphi'} \right] \\ &\quad - r' \sin \theta' \sin \varphi' \left[\frac{\partial r'}{\partial x'} \frac{\partial}{\partial r'} + \frac{\partial \theta'}{\partial x'} \frac{\partial}{\partial \theta'} + \frac{\partial \varphi'}{\partial x'} \frac{\partial}{\partial \varphi'} \right] \end{aligned}$$

$$\begin{aligned}
&= x' \left\{ \frac{y'}{r'} \frac{\partial}{\partial r'} + \frac{\frac{1}{z'} \sqrt{x'^2 + y'^2}}{1 + \frac{x'^2 + y'^2}{z'^2}} \frac{\partial}{\partial \theta'} + \frac{\frac{1}{x'}}{1 + \frac{y'^2}{x'^2}} \frac{\partial}{\partial \varphi'} \right\} \\
&\quad - y' \left\{ \frac{x'}{r'} \frac{\partial}{\partial r'} + \frac{\frac{1}{z'} \sqrt{x'^2 + y'^2}}{1 + \frac{x'^2 + y'^2}{z'^2}} \frac{\partial}{\partial \theta'} + \frac{\frac{(-y')}{x'^2}}{1 + \frac{y'^2}{x'^2}} \frac{\partial}{\partial \varphi'} \right\} \\
&= \frac{x'^2}{x'^2 + y'^2} \frac{\partial}{\partial \varphi'} + \frac{y'^2}{x'^2 + y'^2} \frac{\partial}{\partial \varphi'} \\
&= \frac{\partial}{\partial \varphi'}
\end{aligned}$$

$$\begin{aligned}
&\bullet \int dx' dy' dz' \delta(x-x') \delta(y-y') \delta(z-z') \\
&= \int r'^2 \sin \theta' dr' d\theta' d\varphi' \delta(r-r') \delta(\theta-\theta') \delta(\varphi-\varphi') \\
&\Rightarrow \delta(x-x') \delta(y-y') \delta(z-z') = \frac{1}{r'^2 \sin \theta'} \delta(r-r') \delta(\theta-\theta') \delta(\varphi-\varphi')
\end{aligned}$$

所以

$$\langle x y z | \hat{L}_3 | x' y' z' \rangle = \frac{1}{r'^2 \sin \theta'} \delta(r-r') \delta(\theta-\theta') \delta(\varphi-\varphi') (-i\hbar) \frac{\partial}{\partial \varphi'}$$

Ex 12.12 利用 Ex 12.11 的结果, 计算 $\langle xy z | \hat{L}_z | \ell \ell \rangle$

解: $\langle xy z | \hat{L}_z | \ell \ell \rangle = \langle \hat{L}_z \langle xy z | \ell \ell \rangle = \psi_{\ell \ell}(r, \theta, \varphi)$

另一方面

$$\begin{aligned} \langle xy z | \hat{L}_z | \ell \ell \rangle &= \int dx' dy' dz' \langle xy z | \hat{L}_z | x' y' z' \rangle \langle x' y' z' | \ell \ell \rangle \\ &= \int r'^2 \sin \theta' dr' d\theta' d\varphi' \frac{1}{r'^2 \sin \theta'} \delta(r-r') \delta(\theta-\theta') \delta(\varphi-\varphi') \\ &\quad * (-i\hbar) \frac{\partial}{\partial \varphi'} \psi_{\ell \ell}(r', \theta', \varphi') \\ &= (-i\hbar) \frac{\partial}{\partial \varphi} \psi_{\ell \ell}(r, \theta, \varphi) \end{aligned}$$

$$\Rightarrow (-i\hbar) \frac{\partial}{\partial \varphi} \psi_{\ell \ell}(r, \theta, \varphi) = \langle \hat{L}_z \psi_{\ell \ell}(r, \theta, \varphi) \rangle$$

$$\Rightarrow \psi_{\ell \ell}(r, \theta, \varphi) \propto e^{i\ell\varphi}$$

令 $\psi_{\ell \ell}(r, \theta, \varphi) = f_{\ell \ell}(r, \theta) e^{i\ell\varphi}$, 下面求 $f_{\ell \ell}(r, \theta)$

$$\langle xy z | \hat{L}_+ | \ell \ell \rangle = 0$$

$$\Rightarrow \int r'^2 \sin \theta' dr' d\theta' d\varphi' \langle xy z | \hat{L}_+ | x' y' z' \rangle \langle x' y' z' | \ell \ell \rangle$$

$$= \int r'^2 \sin \theta' dr' d\theta' d\varphi' \frac{1}{r'^2 \sin \theta'} \delta(r-r') \delta(\theta-\theta') \delta(\varphi-\varphi')$$

$$* \hbar e^{i\varphi'} \left[\frac{\partial}{\partial \theta'} + i \cot \theta' \frac{\partial}{\partial \varphi'} \right] f_{\ell \ell}(r', \theta') e^{i\ell\varphi'}$$

$$= \hbar e^{i\varphi} \left[\frac{\partial f_{\ell \ell}}{\partial \theta} e^{i\ell\varphi} + i \cot \theta f_{\ell \ell}(r, \theta) (i\ell) e^{i\ell\varphi} \right]$$

$$= \hbar e^{i\varphi} e^{i\ell\varphi} \left[\frac{\partial f_{\ell \ell}}{\partial \theta} - \ell \cot \theta f_{\ell \ell}(r, \theta) \right] = 0$$

$$\Rightarrow \frac{\partial f_{\ell \ell}}{\partial \theta} - \ell \cot \theta f_{\ell \ell}(r, \theta) = 0$$

只与 θ 有关, 令 $f_{\ell \ell}(r, \theta) = R_{\ell \ell}(r) g_{\ell \ell}(\theta) \Rightarrow \frac{dg_{\ell \ell}}{g_{\ell \ell}} = \frac{\ell \cos \theta}{\sin \theta} d\theta$

$$\Rightarrow d \log g_{ll} = l d \log \sin \theta \Rightarrow g_{ll} = C_{ll} (\sin \theta)^l$$

$$\Rightarrow \psi_{ll}(r, \theta, \varphi) = C_{ll} R_{ll}(r) (\sin \theta)^l e^{i l \varphi}$$

接下来求归一化常数 C_{ll}

$$\int r^2 \sin \theta dr d\theta d\varphi |\psi_{ll}(r, \theta, \varphi)|^2$$

$$= \int r^2 |R_{ll}(r)|^2 dr * |C_{ll}|^2 \int \sin \theta d\theta d\varphi (\sin \theta)^{2l}$$

若要求径向波函数 $R_{ll}(r)$ 满足 $\int_0^{+\infty} r^2 |R_{ll}(r)|^2 dr = 1$

$$\text{则有 } |C_{ll}|^2 \int \sin \theta d\theta d\varphi (\sin \theta)^{2l} = 1$$

$$\int_0^{2\pi} \int_0^{\pi} \sin \theta d\theta d\varphi (\sin \theta)^{2l} = (2\pi) \int_{-1}^1 d(\cos \theta) (1 - \cos^2 \theta)^l$$

$$= 4\pi \int_0^1 (1 - \cos^2 \theta)^l d(\cos \theta)$$

$$\stackrel{x = \cos \theta}{=} 4\pi \int_0^1 (1-x)^l \frac{dx}{2\sqrt{x}}$$

$$= 2\pi \int_0^1 (1-x)^l x^{-\frac{1}{2}} dx$$

$$\downarrow \text{ recall } B(p, q) = \int_0^1 x^{p-1} (1-x)^{q-1} dx$$

$$\stackrel{\downarrow}{=} 2\pi B\left(\frac{1}{2}, l+1\right)$$

$$= 2\pi \frac{\Gamma(\frac{1}{2})\Gamma(l+1)}{\Gamma(l+\frac{3}{2})} = 2\pi \frac{l!}{(l+\frac{1}{2})(l-\frac{1}{2})\dots\frac{1}{2}}$$

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

$$\Rightarrow C_{ll} = \sqrt{\frac{4\pi}{(2l+1)!}} 2^l l!$$

所以归一化波函数为

$$\psi_{ll}(r, \theta, \varphi) = R_{ll}(r) \sqrt{\frac{4\pi}{(2l+1)!}} 2^l l! (\sin \theta)^l e^{i l \varphi}$$

所以我们得到所有归一化波函数

$$\langle xyz | l m \rangle = R_{ll}(r) Y_{lm}(\theta, \varphi)$$

其中 $R_{ll}(r)$ 满足 $\int_0^{\infty} r^2 |R_{ll}(r)|^2 dr = 1$

Ex 12.14 考虑 $l=2$ 的态, 从 $Y_{22}(\theta, \varphi)$ 开始, 用 \hat{L}^- 得到所有 $|2, m\rangle$ 在坐标表象下的波函数, 验证得到的结果即为球谐函数

讨论:

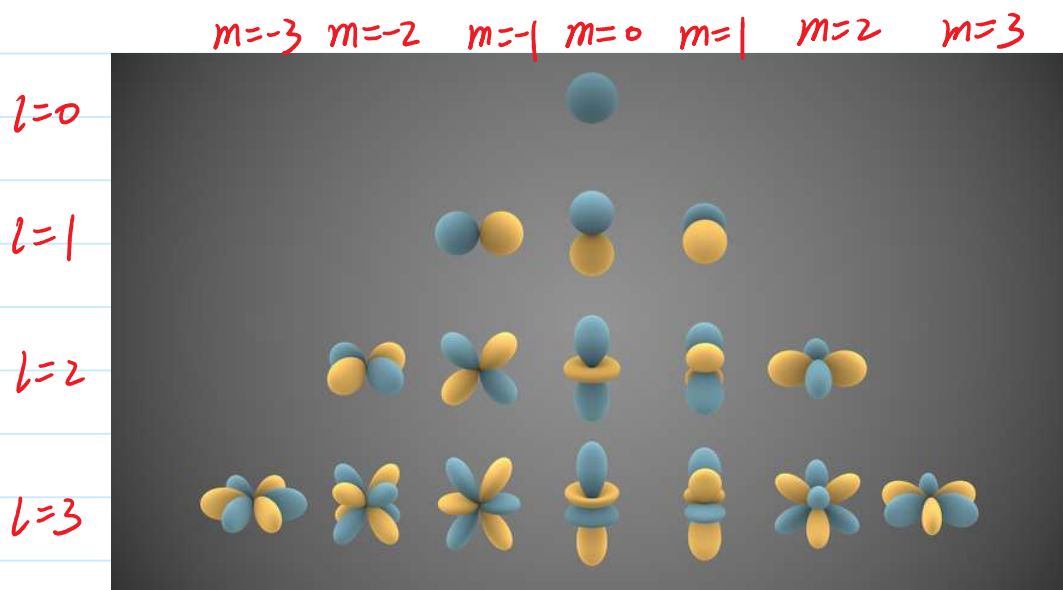
(1) 在上一节是, 我们推导出 $|l, m\rangle$ 中的 l 可以取 $\frac{k}{2}$ ($k=0, 1, 2, \dots$) 而 m 可以取 $-l, -l+1, \dots, l-1, l$

在本节推导中, 我们得到 $\psi_{ll}(r, \theta, \varphi) \propto e^{im\varphi}$. 从物理图像上考虑, 必须有 $\psi_{ll}(r, \theta, \varphi + 2\pi) = \psi_{ll}(r, \theta, \varphi)$, 由此可得 l 必为整数, $m = -l \dots l$ 也必为整数.

(2) 在 Ex. 12.12 和 Ex 12.13 的推导中, 可知 $\psi_{lm}(r, \theta, \varphi)$ 可写成分离变量的形式 $R_{ll}(r) g_{lm}(\theta) e^{im\varphi}$ 的形式, 每个函数均为一维, 因为一维问题没有简并, 所以 $|l, m\rangle$ 没有简并

(3) 由 Ex 12.13 的推导, 可知径向波函数 $R(r)$ 不依赖于 m 的取值, 所以可记 $R_{ll}(r) = R_l(r)$

(4) 球谐函数的几何图像



球谐函数

$$\begin{aligned}
 m \geq 0 \quad Y_l^m(\theta, \phi) &= (-1)^l \left[\frac{(2l+1)!}{4\pi} \right]^{1/2} \frac{1}{2^l l!} \left[\frac{(l+m)!}{(2l)!(l-m)!} \right]^{1/2} e^{im\phi} (\sin \theta)^{-m} \\
 &\quad \times \frac{d^{l-m}}{d(\cos \theta)^{l-m}} (\sin \theta)^{2l} \quad (12.5.35)
 \end{aligned}$$

对于 $m < 0$, 有 $Y_{lm}(\theta, \phi) = (-1)^m (Y_{l, -m}(\theta, \phi))^*$

正交关系为

$$\begin{aligned}
 &\int d\Omega Y_{lm}(\theta, \phi) Y_{l'm'}^*(\theta, \phi) \\
 &= \int_0^\pi d\theta \int_0^{2\pi} d\phi \sin \theta Y_{lm}(\theta, \phi) Y_{l'm'}^*(\theta, \phi) \\
 &= 1
 \end{aligned}$$

由 $\psi_{lm}(r, \theta, \phi) = R_l(r) Y_{lm}(\theta, \phi)$, 可得

$$R_l(r) = \int d\Omega \psi_{lm}(r, \theta, \phi) Y_{lm}^*(\theta, \phi)$$

(5) $|l, m\rangle$ 在坐标表示下的波函数也可直接用

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

$$\text{和 } \hat{L}_z |l, m\rangle = m\hbar |l, m\rangle$$

以及 Ex 12.11 的结论得到, 见如下练习

Ex 12.15 (1) 用 $\hat{L}_z |l, m\rangle = m\hbar |l, m\rangle$ 证明

$$\langle x, y, z | l, m \rangle \propto e^{im\varphi}$$

(2) 设 $\langle x, y, z | l, m \rangle = f_{lm}(r, \theta) e^{im\varphi}$, 代入

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

求关于 $f_{lm}(r, \theta)$ 的微分方程.

(3) 该微分方程与 r 无关, 所以可以令 $f_{lm}(r, \theta) = R_{lm}(r) P_{lm}(\theta)$

求关于 $P_{lm}(\theta)$ 的微分方程

设 $u = \cos\theta$, 将 $P_{lm}(\theta)$ 的微分方程中的 θ 换成 u

$$(4) \text{ 令 } P_{lm}(u) = \sum_{n=0}^{+\infty} C_n^{lm} u^n$$

代入 (3) 中得到的微分方程, 求 C_n^{lm} 的递推关系

(5) 证明 $\lim_{n \rightarrow \infty} \frac{C_{n+2}^{lm}}{C_n^{lm}} = 1$, 所以为了让 $P_{lm}(u)$ 有限,

$$P_{lm}(u) = \sum_{n=0}^{+\infty} C_n^{lm} u^n \text{ 必须在某个 } n \text{ 处截断.}$$

求出最前面几项的表达式, 验证其是否为连带勒让德函数.