第四周高等量子力学作业

隋源 2000011379

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1

由对易关系

$$[\hat{J}_\alpha, \hat{J}_\beta] = i\hbar\varepsilon_{\alpha\beta\gamma}\hat{J}_\gamma$$

可知

$$\begin{aligned}
[\hat{J}^2, \hat{J}_\alpha] &= [\hat{J}_\alpha^2, \hat{J}_\alpha] + [\hat{J}_\beta^2, \hat{J}_\alpha] + [\hat{J}_\gamma^2, \hat{J}_\alpha] \\
&= -i\hbar\varepsilon_{\alpha\beta\gamma}\{\hat{J}_\beta, \hat{J}_\gamma\} - i\hbar\varepsilon_{\alpha\gamma\beta}\{\hat{J}_\gamma, \hat{J}_\beta\} \\
&= 0
\end{aligned}$$

2

旋转算符

$$\mathscr{D}_y(\phi) = \exp(-\frac{i}{\hbar}\hat{J}_y\phi)$$

根据 Baker-Hausdorff 公式

$$e^{-\hat{A}}\hat{B}e^{\hat{A}} = \hat{B} + [\hat{B}, \hat{A}] + \frac{1}{2!}[[\hat{B}, \hat{A}], \hat{A}] + \dots$$

结合对易关系 $[\hat{J}_\alpha, \hat{J}_\beta] = i\hbar\varepsilon_{\alpha\beta\gamma}\hat{J}_\gamma$ 可知

$$\begin{aligned}
\mathscr{D}_y(-\phi)\hat{J}_z\mathscr{D}_y(\phi) &= \hat{J}_z - \phi\hat{J}_x - \frac{1}{2!}\phi^2\hat{J}_z + \frac{1}{3!}\phi^3\hat{J}_x + \dots \\
&= \left(1 - \frac{1}{2!}\phi^2 + \frac{1}{4!}\phi^4 - \dots\right)\hat{J}_z - \left(\phi - \frac{1}{3!}\phi^3 + \frac{1}{5!}\phi^5 - \dots\right)\hat{J}_x \\
&= \hat{J}_z\cos\phi - \hat{J}_x\sin\phi
\end{aligned}$$

故

$$-\mathscr{D}_y(-\pi)\hat{J}_z\mathscr{D}_y(\pi)|j,m\rangle = \hat{J}_z|j,m\rangle = -m\hbar|j,m\rangle$$

等式左乘 $\mathscr{D}_y(\pi)$ 即可得到

$$\hat{J}_z\mathscr{D}_y(\pi)|j,m\rangle = -m\hbar\mathscr{D}_y(\pi)|j,m\rangle$$

即 $\mathscr{D}_y(\pi)|j,m\rangle$ 相当于 $|j,-m\rangle$(正比于一个模为 1 的复数)

3

$\hat{S}_z$ 本征态表象下 $\hat{S}_x$ 和 $\hat{S}_y$ 的矩阵形式为

$$\hat{S}_x = \frac{\hbar}{2}\sigma_x = \frac{\hbar}{2}\begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}, \quad \hat{S}_y = \frac{\hbar}{2}\sigma_y = \frac{\hbar}{2}\begin{pmatrix} 0 & -i \\ i & 0 \end{pmatrix}$$

于是 $\hat{S}_x+$ 和 $\hat{S}_y-$ 的本征态为

$$|\hat{S}_x+\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ 1 \end{pmatrix}, \quad |\hat{S}_y-\rangle = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 \\ -i \end{pmatrix}$$

密度矩阵

$$\begin{aligned}
\rho &= \frac{3}{10}|\hat{S}_x+\rangle\langle\hat{S}_x+| + \frac{7}{10}|\hat{S}_y-\rangle\langle\hat{S}_y-| \\
&= \frac{3}{20}\begin{pmatrix} 1 & 1 \\ 1 & 1 \end{pmatrix} + \frac{7}{20}\begin{pmatrix} 1 & i \\ -i & 1 \end{pmatrix} \\
&= \frac{1}{2}\left(1 + \frac{3}{10}\sigma_x - \frac{7}{10}\sigma_y\right)
\end{aligned}$$

4

对自旋 $\frac{1}{2}$ 系统，有

$$\begin{aligned}
\mathscr{D}(\hat{\mathbf{n}}, \theta) &= \exp\left(-\frac{i}{\hbar}\hat{\mathbf{S}}\cdot\hat{\mathbf{n}}\theta\right) \\
&= \exp\left(-\frac{i}{2}\hat{\sigma}\cdot\hat{\mathbf{n}}\theta\right) \\
&= \left[1 - \frac{1}{2!}\left(\frac{\theta}{2}\right)^2 + \frac{1}{4!}\left(\frac{\theta}{2}\right)^4 - \dots\right] \\
&\quad - i(\hat{\sigma}\cdot\hat{\mathbf{n}})\left[\frac{\theta}{2} - \frac{1}{3!}\left(\frac{\theta}{2}\right)^3 + \frac{1}{5!}\left(\frac{\theta}{2}\right)^5 - \dots\right] \\
&= \cos\frac{\theta}{2} - i(\hat{\sigma}\cdot\hat{\mathbf{n}})\sin\frac{\theta}{2} \\
&= \begin{pmatrix} \cos\frac{\theta}{2} - in_z\sin\frac{\theta}{2} & (-in_x - n_y)\sin\frac{\theta}{2} \\ (-in_x + n_y)\sin\frac{\theta}{2} & \cos\frac{\theta}{2} + in_z\sin\frac{\theta}{2} \end{pmatrix}
\end{aligned}$$

为使 $\mathscr{D}(\hat{\mathbf{n}}, \theta) = \mathscr{D}^{(1/2)}(\alpha, \beta, \gamma)$，让两矩阵的迹相等，则

$$2\cos\frac{\theta}{2} = [e^{-i(\alpha+\gamma)/2} + e^{i(\alpha+\gamma)/2}]\cos\frac{\beta}{2}$$

故

$$\theta = 2\arccos\left[\cos\frac{\alpha+\gamma}{2}\cos\frac{\beta}{2}\right]$$

进而可通过 n_x, n_y, n_z 存在解证明二者等价。

第五周高等量子力学作业

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1

$j=1$ 时，J_y 的矩阵元为

$$\langle 1,m'|J_y|1,m\rangle = \frac{\hbar}{2i}\left[\sqrt{(1-m)(2+m)}\delta_{m',m+1} - \sqrt{(1+m)(2-m)}\delta_{m',m-1}\right]$$

写成矩阵形式，容易验证

$$J_y^3 = \hbar^2 J_y$$

因此旋转算符可以展开

$$\begin{aligned}
\exp(-iJ_y\beta/\hbar) &= 1 - i\frac{J_y}{\hbar}\beta - \left(\frac{J_y}{\hbar}\right)^2\frac{\beta^2}{2!} + i\left(\frac{J_y}{\hbar}\right)^3\frac{\beta^3}{3!} + \left(\frac{J_y}{\hbar}\right)^4\frac{\beta^4}{4!} - i\left(\frac{J_y}{\hbar}\right)^5\frac{\beta^5}{5!} \\
&= 1 - i\frac{J_y}{\hbar}\left(\beta - \frac{\beta^3}{3!} + \frac{\beta^5}{5!} - \dots\right) - \left(\frac{J_y}{\hbar}\right)^2\left(\frac{\beta^2}{2!} - \frac{\beta^4}{4!} + \dots\right) \\
&= 1 - i\frac{J_y}{\hbar}\sin\beta - \left(\frac{J_y}{\hbar}\right)^2(1-\cos\beta)
\end{aligned}$$

代入 $d^{(1)}_{m'm}(\beta)\langle 1,m'|\exp(-iJ_y\beta/\hbar)|1,m\rangle$ 和 J_y 的矩阵形式，得到

$$d^{(1)}(\beta) = \begin{pmatrix} \cos^2(\beta/2) & -\frac{1}{\sqrt{2}}\sin\beta & \sin^2(\beta/2) \\ \frac{1}{\sqrt{2}}\sin\beta & \cos\beta & -\frac{1}{\sqrt{2}}\sin\beta \\ \sin^2(\beta/2) & \frac{1}{\sqrt{2}}\sin\beta & \cos^2(\beta/2) \end{pmatrix}$$

这和待证矩阵等价。

2

a. 用球坐标改写波函数

$$\psi(\mathbf{x}) = \sqrt{\frac{8\pi}{3}}\left[\frac{Y_1^{-1}(\theta,\phi) - Y_1^1(\theta,\phi)}{2} - \frac{Y_1^{-1}(\theta,\phi) + Y_1^1(\theta,\phi)}{2i} + \frac{3}{\sqrt{2}}Y_1^0(\theta,\phi)\right] rf(r)$$

因此 $\psi(x)$ 是 $\mathbf{L}^2$ 的本征函数，且为 $l=1$ 态。

b. 分别乘复共轭可以得到每个态的相对系数

$$|c_{\pm 1}|^2 = \frac{(1+i)(1-i)}{4} = \frac{1}{2}, \quad |c_0|^2 = \frac{9}{2}$$

故 $m=\pm 1$ 态的概率都是 $(1/2)/(1+9/2) = 1/11$, $m=0$ 态的概率是 $(9/2)/(1+9/2) = 9/11$。

c. 定态薛定谔方程

$$\left(\frac{\mathbf{P}^2}{2m} + V(r)\right)\psi(\mathbf{x}) = E\psi(\mathbf{x})$$

将动能项分解为径向和角向，后者可直接由角动量算符表示。由于 $l=1$，径向方程可化简为

$$\left[-\frac{\hbar^2}{2mr^2}\frac{\mathrm{d}}{\mathrm{d}r}\left(r^2\frac{\mathrm{d}}{\mathrm{d}r}\right) + \frac{\hbar^2}{mr^2} + V(r)\right] rf(r) = Erf(r)$$

由此可求出 $V(r)$。

3

角动量叠加

$$J^2 = J_1^2 + J_2^2 + 2J_1 \cdot J_2$$

其中 $2J_1 \cdot J_2 = 2J_{1z}J_{2z} + J_{1+}J_{2-} + J_{1-}J_{2+}$。对于九个态，思路是通过计算 $(2J_1 \cdot J_2)_{ij}$ 的值，写出其矩阵形式，并通过矩阵对角化求出本征态（可通过写出态转换进行简化），其中用到

$$J_z = m\hbar, \qquad J_\pm = \hbar\sqrt{(J \mp m)(J \pm m + 1)}\delta_{m,m\pm 1}$$

对角化后初步得到如下本征态

$$|+0\rangle \pm |0+\rangle, \quad |-0\rangle \pm |0-\rangle, \quad |++\rangle, \quad |--\rangle, \quad |+-\rangle + |-+\rangle \pm |00\rangle$$

其中 $+,-,0$ 分别对应 $m = 1, -1, 0$。接下来分别通过 J^2 和 $J_z = J_{1z} + J_{2z}$ 计算系统的 j, m，将最后结果归类，$l=2$ 的五个本征态为

$$\begin{aligned}
|2,2\rangle &= |++\rangle \\
|2,1\rangle &= \frac{1}{\sqrt{2}}(|0+\rangle + |+0\rangle) \\
|2,0\rangle &= \frac{1}{\sqrt{6}}(|+-\rangle + |-+\rangle + 2|00\rangle) \\
|2,-1\rangle &= \frac{1}{\sqrt{2}}(|0-\rangle + |-0\rangle) \\
|2,2\rangle &= |--\rangle
\end{aligned}$$

$l=1$ 的三个本征态为

$$|1,1\rangle = \frac{1}{\sqrt{2}}(|+0\rangle + |0+\rangle)$$
$$|1,0\rangle = \frac{1}{\sqrt{2}}(|+-\rangle - |-+\rangle)$$
$$|1,-1\rangle = \frac{1}{\sqrt{2}}(|-0\rangle + |0-\rangle)$$

$l=0$ 仅有一个本征态

$$|0,0\rangle = \frac{1}{\sqrt{3}}(|+-\rangle + |-+\rangle - |00\rangle)$$

以上的所有系数都由正交归一给出。

4

a.

$$\begin{aligned}\sum_{m=-j}^{j} |d^{(j)}_{mm'}(\beta)|^2 m &= \sum_{m=-j}^{j} \langle j,m'|e^{iJ_y\beta/\hbar}|j,m\rangle m \langle j,m|e^{-iJ_y\beta/\hbar}|j,m'\rangle \\ &= \frac{1}{\hbar}\langle j,m'|e^{iJ_y\beta/\hbar}J_z e^{-iJ_y\beta/\hbar}|j,m'\rangle \\ &= \frac{1}{\hbar}\langle j,m'|J_z\cos\beta + J_x\sin\beta|j,m'\rangle \\ &= m'\cos\beta\end{aligned}$$

利用

$$d^{(\frac{1}{2})}(\beta) = \begin{pmatrix}\cos(\beta/2) & -\sin(\beta/2) \\ \sin(\beta/2) & \cos(\beta/2)\end{pmatrix}$$

可以验证 $m=\pm\frac{1}{2}$ 时符合。

b. 和 a 同理，有

$$\sum_{m=-j}^{j} |d^{(j)}_{mm'}(\beta)|^2 m^2 = \frac{1}{\hbar^2}\langle j,m'|e^{iJ_y\beta/\hbar}J_z^2 e^{-iJ_y\beta/\hbar}|j,m'\rangle$$

为了计算，引入球矢量语言，改写为

$$J_z^2 = \frac{1}{3}\mathbf{J}^2 + \left(J_z^2 - \frac{1}{3}\mathbf{J}^2\right)$$

根据张量积，括号内的张量算符为 $T_0^{(2)}$，前者是 $T_0^{(0)}$。于是

$$\begin{aligned}\sum_{m=-j}^{j} |d^{(j)}_{mm'}(\beta)|^2 m^2 &= \frac{1}{3}j(j+1) + \frac{1}{\hbar^2}\mathcal{D}^{(2)}_{00}(\beta)\langle j,m'|J_z^2 - \mathbf{J}^2/3|j,m'\rangle \\ &= \frac{1}{3}j(j+1) + P_2(\cos\beta)\left(m'^2 - \frac{1}{3}j(j+1)\right) \\ &= \frac{1}{2}j(j+1)\sin^2\beta + \frac{1}{2}m'^2(3\cos^2\beta - 1)\end{aligned}$$

第六周高等量子力学作业

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1

矢量构造的秩为 1 的球张量

$$U_{+1} = -(U_x + iU_y)/\sqrt{2}, \quad U-1 = (U_x - iU_y)/\sqrt{2}, \quad U_0 = U_z$$

a. 用矢量 U, V 构造秩为 1 球张量的表达式

$$T_q^{(1)} = \sum_{q_1}\sum_{q_2}\langle 11; q_1 q_2 | 11; 1q\rangle U_{q_1} V_{q_2}$$

通过计算 CG 系数直接得到

$$\begin{aligned}
T_{+1}^{(1)} &= \frac{1}{\sqrt{2}}(-U_0V_{+1} + U_{+1}V_0) = \frac{1}{2}(U_zV_x - U_xV_z) + \frac{i}{2}(U_zV_y - U_yV_z) \\
T_0^{(1)} &= \frac{1}{\sqrt{2}}(-U_{-1}V_{+1} + U_{+1}V_{-1}) = \frac{i}{2}(U_xV_y - U_yV_x) \\
T_{-1}^{(1)} &= \frac{1}{\sqrt{2}}(-U_{-1}V_0 + U_0V_{-1}) = \frac{1}{2}(U_zV_x - U_xV_z) + \frac{i}{2}(U_yV_z - U_zV_y)
\end{aligned}$$

b. 用矢量 U, V 构造秩为 2 球张量的表达式

$$T_q^{(2)} = \sum_{q_1}\sum_{q_2}\langle 11; q_1 q_2 | 11; 2q\rangle U_{q_1} V_{q_2}$$

通过计算 CG 系数直接得到

$$\begin{aligned}
T_{+2}^{(2)} &= U_{+1}V_{+1} = \frac{1}{2}(U_xV_x - U_yV_y) + \frac{i}{2}(U_yV_x - U_xV_y) \\
T_{+1}^{(2)} &= \frac{1}{\sqrt{2}}(U_0V_{+1} + U_{+1}V_0) = -\frac{1}{2}(U_zV_x + U_xV_z) - \frac{i}{2}(U_zV_y + U_yV_z) \\
T_0^{(2)} &= \frac{1}{\sqrt{6}}(U_{-1}V_{+1} + U_{+1}V_{-1} + 2U_0V_0) = -\frac{1}{\sqrt{6}}(U_xV_x + U_yV_y + 2U_zV_z) \\
T_{-1}^{(2)} &= \frac{1}{\sqrt{2}}(U_{-1}V_0 + U_0V_{-1}) = \frac{1}{2}(U_zV_x + U_xV_z) - \frac{i}{2}(U_yV_z + U_zV_y) \\
T_{-2}^{(2)} &= U_{-1}V_{-1} = \frac{1}{2}(U_xV_x - U_yV_y) - \frac{i}{2}(U_yV_x + U_xV_y)
\end{aligned}$$

2

a. 利用球谐函数构造

$$Y_2^{\pm 2} = \sqrt{\frac{15}{32\pi}} \frac{x^2 - y^2 \pm 2ixy}{r^2}$$
$$Y_2^{\pm 1} = \mp\sqrt{\frac{15}{8\pi}} \frac{(x \pm iy)z}{r^2}$$
$$Y_2^0 = \sqrt{\frac{15}{16\pi}} \frac{3z^2 - r^2}{r^2}$$

得到

$$xy = i\sqrt{\frac{2\pi}{15}}(Y_2^{-2} - Y_2^2)r^2$$
$$xz = \sqrt{\frac{2\pi}{15}}(Y_2^{-1} - Y_2^1)r^2$$
$$x^2 - y^2 = \sqrt{\frac{8\pi}{15}}(Y_2^{-2} + Y_2^2)r^2$$

b. 将四极距和待求值分别用 CG 系数表示

$$Q = e\sqrt{\frac{16\pi}{5}}\langle \alpha, j, j|Y_2^0 r^2|\alpha, j, j\rangle = e\sqrt{\frac{16\pi}{5}} \frac{\langle \alpha, j||Y^{(2)}||\alpha, j\rangle}{\sqrt{2j+1}} \langle j2; j0|j2; jj\rangle$$

$$\begin{aligned} e\langle \alpha, j, m'|x^2 - y^2|\alpha, j, j\rangle &= e\sqrt{\frac{8\pi}{5}}\langle \alpha, j, m'|(Y_2^{-2} + Y_2 2)r^2|\alpha, j, j\rangle \\ &= e\sqrt{\frac{8\pi}{5}} \frac{\langle \alpha, j||Y^{(2)}||\alpha, j\rangle}{\sqrt{2j+1}} [\langle j2; j-2|j2; jm'\rangle + \langle j2; j2|j2; jm'\rangle] \end{aligned}$$

因为 $m = j, j-1, j-2, \ldots$ 所以 $\langle j2; j2|j2; jm'\rangle = 0$，故

$$e\langle \alpha, j, m'|x^2 - y^2|\alpha, j, j\rangle = \frac{Q}{\sqrt{2}} \frac{\langle j2; j-2|j2; jm'\rangle}{\langle j2; j0|j2; jj\rangle}$$

3

a.

$$\mathscr{T}_{\boldsymbol{d}}\mathscr{T}_{\boldsymbol{d}'} = \exp(i\boldsymbol{p}\cdot\boldsymbol{d})\exp(i\boldsymbol{p}\cdot\boldsymbol{d}') = \exp(i\boldsymbol{p}\cdot\boldsymbol{d}')\exp(i\boldsymbol{p}\cdot\boldsymbol{d}) = \mathscr{T}_{\boldsymbol{d}'}\mathscr{T}_{\boldsymbol{d}}$$

故 $\mathscr{T}_{\boldsymbol{d}}$ 和 $\mathscr{T}_{\boldsymbol{d}'}$ 对易。

b. 不同轴的有限角度转动是不对易的，因此 $\mathscr{D}(\hat{\boldsymbol{n}}, \phi)$ 与 $\mathscr{D}(\hat{\boldsymbol{n}}', \phi')$ 不对易。

c.

$$\mathscr{T}_{\boldsymbol{d}}\boldsymbol{\pi}|\boldsymbol{x}\rangle = |-\boldsymbol{x}+\boldsymbol{d}\rangle, \quad \boldsymbol{\pi}\mathscr{T}_{\boldsymbol{d}}|\boldsymbol{x}\rangle = |-(\boldsymbol{x}+\boldsymbol{d})\rangle$$

故 $\mathscr{T}_{\boldsymbol{d}}$ 和 $\boldsymbol{\pi}$ 不对易。

d. 由于旋转操作和坐标宇称之间互不影响，因此 $\mathscr{D}(\hat{\boldsymbol{n}}, \phi)$ 和 $\boldsymbol{\pi}$ 对易。

4

设

$$A|\psi\rangle = a|\psi\rangle, \quad B|\psi\rangle = b|\psi\rangle$$

由于

$$(AB+BA)|\psi\rangle = (ab+ba)|\psi\rangle = 0$$

故 a 和 b 中至少一个为 0。举例：$\boldsymbol{\pi}$ 和 $\boldsymbol{p}$ 反对易，显然要使二者有共同本征态只能让 $\boldsymbol{p}=0$ 即本征值等于 0。