Chapter 17
Spherical Harmonics

17.1 Angular Momentum in Quantum Mechanics

The angular momentum operator $\hat{\boldsymbol{J}}$ is defined [18] in such a way that $\hat{U} = \exp\left(-\mathrm{i}\hat{\boldsymbol{J}} \cdot \delta\boldsymbol{\varphi}\right)$ is the operator of an infinitesimal rotation with the angle $\delta\boldsymbol{\varphi}$: if $|\psi>$ is a state, then $\hat{U}\,|\psi>$ is the same state rotated by $\delta\boldsymbol{\varphi}$. Therefore, the average value $\boldsymbol{V}'$ of a vector operator $\hat{\boldsymbol{V}}$ over $\hat{U}\,|\psi>$ is related to its average value $\boldsymbol{V}$ over $|\psi>$ by the formula $\boldsymbol{V}' = \boldsymbol{V} + \delta\boldsymbol{\varphi} \times \boldsymbol{V}$ and hence $\hat{U}^{+}\hat{\boldsymbol{V}}\hat{U} = \hat{\boldsymbol{V}} + \mathrm{i}\left[\hat{\boldsymbol{J}} \cdot \delta\boldsymbol{\varphi}, \hat{\boldsymbol{V}}\right] = \hat{\boldsymbol{V}} + \delta\boldsymbol{\varphi} \times \hat{\boldsymbol{V}}$. Therefore, for any vector operator $\hat{\boldsymbol{V}}$ the commutation relation $\left[\hat{V}_i, \hat{J}_j\right] = \mathrm{i}\varepsilon_{ijk}\hat{V}_k$ holds. The average value of a scalar operator $\hat{S}$ does not change at rotations; hence $\left[\hat{S}, \hat{J}_i\right] = 0$. In particular, the angular momentum $\hat{\boldsymbol{J}}$ is a vector operator, and its square $\hat{\boldsymbol{J}}^2 = \hat{J}_x^2 + \hat{J}_y^2 + \hat{J}_z^2$ is a scalar one:

$$\left[\hat{J}_i, \hat{J}_j\right] = \mathrm{i}\varepsilon_{ijk}\hat{J}_k\,, \qquad \left[\hat{\boldsymbol{J}}^2, \hat{J}_i\right] = 0\,.$$

Therefore, a system of common eigenstates of $\hat{\boldsymbol{J}}^2$ and $\hat{J}_z$ exists. Let's introduce the operators $\hat{J}_\pm = \hat{J}_x \pm \mathrm{i}\hat{J}_y$, $\hat{J}_\pm^+ = \hat{J}_\mp$; we have $\left[\hat{J}_z, \hat{J}_\pm\right] = \pm\hat{J}_\pm$. This means that if $|\psi>$ is an eigenstate of $\hat{J}_z$ ($\hat{J}_z\,|\psi> = m\,|\psi>$), then $\hat{J}_\pm\,|\psi>$ are also eigenstates of $\hat{J}_z$: $\hat{J}_z\hat{J}_\pm\,|\psi> = (m \pm 1)\hat{J}_\pm\,|\psi>$ (if they don't vanish). Therefore, eigenvalues m of $\hat{J}_z$ form a progression with unit step, and the ladder operators $\hat{J}_\pm$ increase and decrease m.

Let's consider states with a given eigenvalue of $\hat{\boldsymbol{J}}^2$. For these states, eigenvalues of $\hat{J}_z$ are bounded from above and from below because the operator $\hat{\boldsymbol{J}}^2 - \hat{J}_z^2 = \hat{J}_x^2 + \hat{J}_y^2$ is positive definite. Let $|m_\pm>$ be the eigenstates with the maximum and the minimum eigenvalues of $\hat{J}_z$ equal to $m_\pm$. Then these eigenvalues cannot be further increased and decreased by the operators $\hat{J}_\pm$ correspondingly: $\hat{J}_\pm\,|m_\pm> = 0$. We have

$$\hat{J}_\pm\hat{J}_\mp = \hat{\boldsymbol{J}}^2 - \hat{J}_z^2 \pm \hat{J}_z\,.$$

A. Grozin, *Introduction to Mathematica® for Physicists*, Graduate Texts in Physics,
DOI 10.1007/978-3-319-00894-3_17,

Therefore, $\hat{J}_\mp \hat{J}_\pm |m_\pm\rangle = 0 = \left[\hat{\boldsymbol{J}}^2 - m_\pm(m_\pm \pm 1)\right] |m_\pm\rangle$, i.e., the eigenvalue of the operator $\hat{\boldsymbol{J}}^2$ for these states (as well as for all the other states being considered) is $m_+(m_+ + 1) = m_-(m_- - 1)$. Hence $(m_+ + m_-)(m_+ - m_- + 1) = 0$; taking into account $m_+ \geqslant m_-$ we obtain $m_- = -m_+$ or $m_\pm = \pm j$. The number j must be integer or half-integer because m_+ and m_- differ by an integer.

Finally, we have a system of common eigenstates $|j,m\rangle$ of the operators $\hat{\boldsymbol{J}}^2$ and $\hat{J}_z$:

$$\hat{\boldsymbol{J}}^2 |j,m\rangle = j(j+1)|j,m\rangle, \qquad \hat{J}_z|j,m\rangle = m|j,m\rangle,$$

where j is integer or half-integer, and m varies from $-j$ to j by 1. The operators $\hat{J}_\pm$ increase and decrease m correspondingly: $\hat{J}_\pm|j,m\rangle = a_\pm(j,m)|j,m\pm 1\rangle$. Tuning the phases of $|j,m\rangle$ we can make $a_\pm(j,m)$ real and positive. They can be found from the normalization: $|a_\pm(j,m)|^2 = \langle j,m|\hat{J}_\mp \hat{J}_\pm|j,m\rangle = j(j+1) - m(m\pm 1)$. Finally we arrive at

$$\hat{J}_\pm|j,m\rangle = \sqrt{j(j+1) - m(m\pm 1)}\,|j,m\pm 1\rangle = \sqrt{(j\pm m+1)(j\mp m)}\,|j,m\pm 1\rangle.$$

The orbital angular momentum of a particle $\hat{\boldsymbol{l}} = \boldsymbol{r} \times \hat{\boldsymbol{p}}$ (where $\hat{\boldsymbol{p}} = -\mathrm{i}\boldsymbol{\nabla}$ in the coordinate representation) is an example of angular momentum. In spherical coordinates

$$\hat{l}_z = -\mathrm{i}\frac{\partial}{\partial\varphi}, \qquad \hat{l}_\pm = \mathrm{e}^{\pm\mathrm{i}\varphi}\left(\pm\frac{\partial}{\partial\theta} + \mathrm{i}\cot\theta\frac{\partial}{\partial\varphi}\right).$$

The eigenfunctions of $\hat{l}_z$ are $\mathrm{e}^{\mathrm{i}m\varphi}$; they must not change at $\varphi \to \varphi + 2\pi$; hence m must be integer. The common eigenfunctions of $\hat{\boldsymbol{l}}^2$ and $\hat{l}_z$ are called spherical harmonics:

$$\hat{\boldsymbol{l}}^2 Y_{lm}(\theta,\varphi) = l(l+1)Y_{lm}(\theta,\varphi), \qquad \hat{l}_z Y_{lm}(\theta,\varphi) = mY_{lm}(\theta,\varphi),$$

where l is integer, and m varies from $-l$ to l by 1; $Y_{lm}(\theta,\varphi) = P_{lm}(\theta)\mathrm{e}^{\mathrm{i}m\varphi}$. They are orthonormalized:

$$\int Y^*_{l'm'}(\theta,\varphi)Y_{lm}(\theta,\varphi)\mathrm{d}\Omega = \delta_{l'l}\delta_{m'm}.$$

Here are the operators $\hat{l}_\pm$ in *Mathematica*:

In[1] := lp[f_] := Together[Exp[I ∗ φ] ∗ (D[f, θ] + I ∗ Cot[θ] ∗ D[f, φ])]
In[2] := lm[f_] := Together[Exp[−I ∗ φ] ∗ (−D[f, θ] + I ∗ Cot[θ] ∗ D[f, φ])]

17.2 $Y_{ll}(\theta,\varphi)$

The angular momentum projection of this state cannot be raised by $\hat{l}_+$.

In[3] := Eq = lp[Exp[I ∗ l ∗ φ] ∗ P[θ]] == 0
Out[3] = $-\mathrm{e}^{\mathrm{i}\varphi+\mathrm{i}l\varphi}\left(l\,\mathrm{Cot}[\theta]P[\theta] - P'[\theta]\right) == 0$

In[4] := s = DSolve[Eq, P[θ], θ]

$$\text{Out[4]} = \left\{\left\{P[\theta] \to C[1]\text{Sin}[\theta]^l\right\}\right\}$$

In[5] := P = P[θ]/.s[[1]]

$$\text{Out[5]} = C[1]\text{Sin}[\theta]^l$$

The normalization integral.

**In[6] := NI = 2 * Pi * Integrate[P^2 * Sin[θ], {θ, 0, Pi}, Assumptions−>{l ≥ 0}]/.
Gamma[−l]−> − Pi/(Sin[Pi * l] * Gamma[l + 1])**

$$\text{Out[6]} = \frac{2\pi^{3/2}C[1]^2\text{Gamma}[1+l]}{\text{Gamma}\left[\frac{3}{2}+l\right]}$$

In[7] := s = Solve[NI == 1, C[1]]

$$\text{Out[7]} = \left\{\left\{C[1] \to -\frac{\sqrt{\text{Gamma}\left[\frac{3}{2}+l\right]}}{\sqrt{2}\pi^{3/4}\sqrt{\text{Gamma}[1+l]}}\right\}, \left\{C[1] \to \frac{\sqrt{\text{Gamma}\left[\frac{3}{2}+l\right]}}{\sqrt{2}\pi^{3/4}\sqrt{\text{Gamma}[1+l]}}\right\}\right\}$$

In[8] := P = P/.s[[2]]

$$\text{Out[8]} = \frac{\sqrt{\text{Gamma}\left[\frac{3}{2}+l\right]}\text{Sin}[\theta]^l}{\sqrt{2}\pi^{3/4}\sqrt{\text{Gamma}[1+l]}}$$

The phase can be chosen arbitrarily. According to Landau–Lifshitz [18]:

In[9] := Y[l_, l_] = (−I)^l * P * Exp[I * l * φ]

$$\text{Out[9]} = \frac{(-\mathrm{i})^l e^{\mathrm{i}l\varphi}\sqrt{\text{Gamma}\left[\frac{3}{2}+l\right]}\text{Sin}[\theta]^l}{\sqrt{2}\pi^{3/4}\sqrt{\text{Gamma}[1+l]}}$$

In[10] := Clear[Eq, s, P]

17.3 $Y_{lm}(\theta,\varphi)$

These states can be obtained from $Y_{ll}(\theta,\varphi)$ by the lowering operator $\hat{l}_-$.

In[11] := S = Cos[x_]^n_−>(1 − Sin[x]^2)^Quotient[n, 2] * Cos[x]^Mod[n, 2];

**In[12] := Y[l_, m_]/; m < l := Y[l, m] =
Factor[Expand[lm[Y[l, m + 1]]/Sqrt[(l − m) * (l + m + 1)]/.S]]**

In[13] := Table[Table[Y[l, m], {m, l, −l, −1}], {l, 0, 4}]

$$\text{Out[13]} = \left\{\left\{\frac{1}{2\sqrt{\pi}}\right\}, \left\{-\frac{1}{2}\mathrm{i}e^{\mathrm{i}\varphi}\sqrt{\frac{3}{2\pi}}\text{Sin}[\theta], \frac{1}{2}\mathrm{i}\sqrt{\frac{3}{\pi}}\text{Cos}[\theta], \frac{1}{2}\mathrm{i}e^{-\mathrm{i}\varphi}\sqrt{\frac{3}{2\pi}}\text{Sin}[\theta]\right\},\right.$$

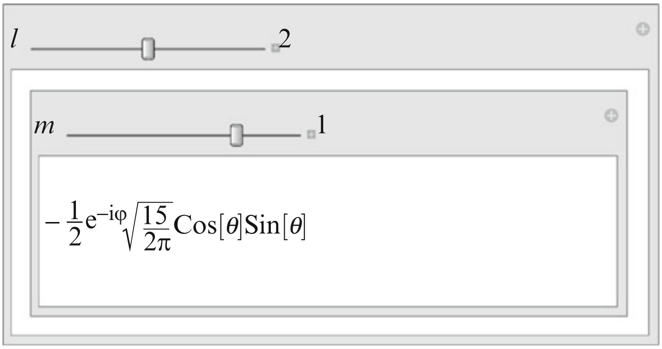
$$\left\{-\frac{1}{4}e^{2\mathrm{i}\varphi}\sqrt{\frac{15}{2\pi}}\text{Sin}[\theta]^2, \frac{1}{2}e^{\mathrm{i}\varphi}\sqrt{\frac{15}{2\pi}}\text{Cos}[\theta]\text{Sin}[\theta], \frac{1}{4}\sqrt{\frac{5}{\pi}}\left(-2+3\text{Sin}[\theta]^2\right),\right.$$

$$\left.-\frac{1}{2}e^{-\mathrm{i}\varphi}\sqrt{\frac{15}{2\pi}}\text{Cos}[\theta]\text{Sin}[\theta], -\frac{1}{4}e^{-2\mathrm{i}\varphi}\sqrt{\frac{15}{2\pi}}\text{Sin}[\theta]^2\right\},$$

$$\left\{\frac{1}{8}\mathrm{i}e^{3\mathrm{i}\varphi}\sqrt{\frac{35}{\pi}}\mathrm{Sin}[\theta]^3, -\frac{1}{4}\mathrm{i}e^{2\mathrm{i}\varphi}\sqrt{\frac{105}{2\pi}}\mathrm{Cos}[\theta]\mathrm{Sin}[\theta]^2,\right.$$
$$-\frac{1}{8}\mathrm{i}e^{\mathrm{i}\varphi}\sqrt{\frac{21}{\pi}}\mathrm{Sin}[\theta]\left(-4+5\mathrm{Sin}[\theta]^2\right), \frac{1}{4}\mathrm{i}\sqrt{\frac{7}{\pi}}\mathrm{Cos}[\theta]\left(-2+5\mathrm{Sin}[\theta]^2\right),$$
$$\frac{1}{8}\mathrm{i}e^{-\mathrm{i}\varphi}\sqrt{\frac{21}{\pi}}\mathrm{Sin}[\theta]\left(-4+5\mathrm{Sin}[\theta]^2\right), -\frac{1}{4}\mathrm{i}e^{-2\mathrm{i}\varphi}\sqrt{\frac{105}{2\pi}}\mathrm{Cos}[\theta]\mathrm{Sin}[\theta]^2,$$
$$\left.-\frac{1}{8}\mathrm{i}e^{-3\mathrm{i}\varphi}\sqrt{\frac{35}{\pi}}\mathrm{Sin}[\theta]^3\right\},$$
$$\left\{\frac{3}{16}e^{4\mathrm{i}\varphi}\sqrt{\frac{35}{2\pi}}\mathrm{Sin}[\theta]^4, -\frac{3}{8}e^{3\mathrm{i}\varphi}\sqrt{\frac{35}{\pi}}\mathrm{Cos}[\theta]\mathrm{Sin}[\theta]^3,\right.$$
$$-\frac{3}{8}e^{2\mathrm{i}\varphi}\sqrt{\frac{5}{2\pi}}\mathrm{Sin}[\theta]^2\left(-6+7\mathrm{Sin}[\theta]^2\right),$$
$$\frac{3}{8}e^{\mathrm{i}\varphi}\sqrt{\frac{5}{\pi}}\mathrm{Cos}[\theta]\mathrm{Sin}[\theta]\left(-4+7\mathrm{Sin}[\theta]^2\right), \frac{3\left(8-40\mathrm{Sin}[\theta]^2+35\mathrm{Sin}[\theta]^4\right)}{16\sqrt{\pi}},$$
$$-\frac{3}{8}e^{-\mathrm{i}\varphi}\sqrt{\frac{5}{\pi}}\mathrm{Cos}[\theta]\mathrm{Sin}[\theta]\left(-4+7\mathrm{Sin}[\theta]^2\right),$$
$$-\frac{3}{8}e^{-2\mathrm{i}\varphi}\sqrt{\frac{5}{2\pi}}\mathrm{Sin}[\theta]^2\left(-6+7\mathrm{Sin}[\theta]^2\right), \frac{3}{8}e^{-3\mathrm{i}\varphi}\sqrt{\frac{35}{\pi}}\mathrm{Cos}[\theta]\mathrm{Sin}[\theta]^3,$$
$$\left.\left.\frac{3}{16}e^{-4\mathrm{i}\varphi}\sqrt{\frac{35}{2\pi}}\mathrm{Sin}[\theta]^4\right\}\right\}$$

In[14] := Manipulate[Manipulate[*Y*[*l*,*m*],
{*m*,−*l*,*l*,1,Appearance−>"Labeled"}],{*l*,0,4,1,Appearance−>"Labeled"}]

Out[14] =



Orthogonality of $Y_{l_1m_1}$ and $Y_{l_2m_2}$ with $m_1 \neq m_2$ is evident; let's check all the rest.

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In[15] := Table[Table[Table[
    Integrate[Y[l1,m] * Conjugate[Y[l2,m]] * Sin[θ], {φ,0,2*Pi}, {θ,0,Pi}],
    {m,l2,-l2,-1}], {l2,0,l1}], {l1,0,4}]
Out[15] = {{{1}}, {{0}, {1,1,1}}, {{0}, {0,0,0}, {1,1,1,1,1}},
    {{0}, {0,0,0}, {0,0,0,0,0}, {1,1,1,1,1,1,1}},
    {{0}, {0,0,0}, {0,0,0,0,0}, {0,0,0,0,0,0,0}, {1,1,1,1,1,1,1,1,1}}}
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