§ 10 Spherical harmonics

1. Solution of Laplace's equation in spherical coordinates. Spherical harmonics are an important class of special functions that are closely related to the classical orthogonal polynomials. They arise, for example, when Laplace's equation is solved in spherical coordinates. Since continuous solutions of Laplace's equation are *harmonic functions*, these solutions are called *spherical harmonics*; the term *spherical functions* is also used.

Let us find the bounded solutions of Laplace's equation $\Delta u = 0$ in spherical coordinates r, θ, ϕ. We have

$$\Delta u = \Delta_r u + \frac{1}{r^2}\Delta_{\theta,\phi} u,$$

where

$$\Delta_r u = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial u}{\partial r}\right),$$

$$\Delta_{\theta,\phi} u = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial u}{\partial\theta}\right) + \frac{1}{\sin^2\theta}\frac{\partial^2 u}{\partial\phi^2}.$$

We look for particular solutions by assuming $u = R(r)Y(\theta,\phi)$. Substituting this into Laplace's equation, we obtain

$$\frac{r^2\Delta_r R(r)}{R(r)} = -\frac{\Delta_{\theta,\phi}Y(\theta,\phi)}{Y(\theta,\phi)}.$$

Since the left-hand side is independent of θ and ϕ, and the right-hand side is independent of r, we have

$$\frac{r^2\Delta_r R}{R} = -\frac{\Delta_{\theta,\phi}Y(\theta,\phi)}{Y(\theta,\phi)} = \mu,$$

where μ is a constant. Hence we have the equations

$$(r^2R')' = \mu R, \tag{1}$$

$$\Delta_{\theta,\phi}Y + \mu Y = 0. \tag{2}$$

We can also solve (2) by separating variables, by putting

$$Y(\theta,\phi) = \Theta(\theta)\Phi(\phi).$$

This yields

$$\frac{\sin\theta \dfrac{d}{d\theta}\left(\sin\theta \dfrac{d\Theta}{d\theta}\right)}{\Theta(\theta)} + \mu \sin^2\theta = -\frac{\Phi''(\phi)}{\Phi(\phi)} = \nu,$$

where ν is a constant. Therefore we obtain the following equations for $\Phi(\phi)$ and $\Theta(\theta)$:

$$\Phi'' + \nu\Phi = 0, \tag{3}$$

$$\sin\theta \frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + (\mu \sin^2\theta - \nu)\Theta = 0. \tag{4}$$

The requirement that $\Phi(\phi)$ is single-valued yields the periodicity $\Phi(\phi+2\pi) = \Phi(\phi)$. Under this condition, (3) can be solved only when $\nu = m^2$ with m an integer. Thus we obtain the linearly independent solutions of (3):

$$\Phi_m(\phi) = C_m e^{im\phi},$$
$$\Phi_{-m}(\phi) = C_{-m} e^{-im\phi}$$

(C_m is a normalizing constant).

The functions $\Phi_m(\phi) = C_m e^{im\phi}$ $(m = 0, \pm 1, \ldots)$ satisfy the orthogonality condition

$$\int_0^{2\pi} \Phi_m^*(\phi)\Phi_{m'}(\phi)d\phi = A_m \delta_{mm'},$$

where

$$A_m = 2\pi|C_m|^2, \quad \delta_{mm'} = \begin{cases} 1, & m' = m, \\ 0, & m' \neq m. \end{cases}$$

It is convenient to take $A_m = 1$, so that $C_m = 1/\sqrt{2\pi}$, i.e.

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{im\phi} \qquad (m = 0, \pm 1, \pm 2, \ldots).$$

Now let us solve equation (4) with $\nu = m^2$. If we put $\cos\theta = x$, equation (4) becomes the generalized equation of hypergeometric type (see §1)

$$\frac{d}{dx}\left[(1-x^2)\frac{d\Theta}{dx}\right] + \left(\mu - \frac{m^2}{1-x^2}\right)\Theta = 0, \tag{5}$$

with $\sigma(x) = 1 - x^2$, $\tilde{\tau}(x) = -2x$, $\tilde{\sigma}(x) = \mu(1-x^2) - m^2$.

The problem of finding bounded solutions of (5) on $(-1,1)$ leads to the same kind of eigenvalue problem as the one discussed in §9, since in the present case $\sigma(x)|_{x=\pm1} = 0$ and $\tilde{\rho}(x) = 1$. We shall therefore use the method of §9.

We transform (5) to an equation of hypergeometric type by putting $\Theta(x) = \phi(x)y(x)$, where $\phi(x)$ is a solution of $\phi'/\phi = \pi(x)/\sigma(x)$ ($\pi(x)$ is a polynomial of degree at most 1). In the present case

$$\pi(x) = \pm\sqrt{k(1-x^2) + m^2 - \mu(1-x^2)},$$

where k is to be determined by the condition that the expression under the square root sign has a double zero. We obtain the following possibilities for $\pi(x)$:

$$\pi(x) = \begin{cases} \pm m & \text{for } k = \mu, \\ \pm mx & \text{for } k = \mu - m^2. \end{cases}$$

We must choose the form of $\pi(x)$ for which

$$\tau(x) = \tilde{\tau}(x) + 2\pi(x)$$

has a negative derivative and a zero on $(-1,1)$. For $m \geq 0$ these conditions are satisfied by

$$\tau(x) = -2(m+1)x,$$

which corresponds to

$$\begin{aligned} \pi(x) &= -mx, & \phi(x) &= (1-x^2)^{m/2}, \\ \lambda &= \mu - m(m+1), & \rho(x) &= (1-x^2)^m. \end{aligned}$$

The eigenvalues μ are determined by

$$\lambda + n\tau' + \frac{n(n-1)}{2}\sigma'' = 0,$$

which yields $\mu = \mu_n = l(l+1)$, where $l = m+n$ $(n = 0, 1, \ldots)$. The functions $y_n(x)$ have the form

$$y_n(x) = \frac{B_{nm}}{(1-x^2)^m}\frac{d^n}{dx^n}[(1-x^2)^{n+m}]$$

and are, up to constant factors, the Jacobi polynomials $P_n^{(m,m)}(x)$. Since $n = l - m$, where l is an integer such that $l \geq m$, we have, for $m \geq 0$,

$$\Theta(x) \equiv \Theta_{lm}(x) = C_{lm}(1-x^2)^{m/2}P_{l-m}^{(m,m)}(x). \tag{6}$$

Here C_{lm} are normalizing constants. The functions $\Theta_{lm}(x)$ evidently satisfy an orthogonality condition which follows from the orthogonality of the Jacobi polynomials:

$$\int_{-1}^{1} \Theta_{lm}(x)\Theta_{l'm}(x)dx = A_{lm}\delta_{ll'},$$

where

$$A_{lm} = C_{lm}^2 \int_{-1}^{1} \left[P_{l-m}^{(m,m)}(x)\right]^2 (1-x^2)^m dx.$$

It is convenient to take* $A_{lm} = 1$, which yields

$$C_{lm} = \frac{1}{2^m l!}\sqrt{\frac{2l+1}{2}(l-m)!(l+m)!}.$$

A different expression for the functions $\Theta_{lm}(x), m \geq 0$, follows from the properties of the Jacobi polynomials. From the differentiation formula (5.6) for Jacobi polynomials it follows that

$$P_{l-m}^{(m,m)}(x) = \frac{2^m l!}{(l+m)!}\frac{d^m}{dx^m}P_l(x),$$

where $P_l(x) = P_l^{(0,0)}(x)$ are the Legendre polynomials.

Hence for $m \geq 0$

$$\Theta_{lm}(x) = \sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}}P_l^m(x),$$

where

$$P_l^m(x) = (1-x^2)^{m/2}\frac{d^m P_l(x)}{dx^m}$$

are the *associated Legendre functions of the first kind.*

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* This choice of the sign of C_{lm} is not always used. We follow the notation of [B3].

We can obtain explicit expressions for the $\Theta_{lm}(x)$ by using the Rodrigues formulas for $P_l(x)$ and $P_{l-m}^{(m,m)}(x)$:

$$\Theta_{lm}(x) = \frac{(-1)^l}{2^l l!}\sqrt{\frac{2l+1}{2}\frac{(l-m)!}{(l+m)!}}(1-x^2)^{m/2}\frac{d^{l+m}}{dx^{l+m}}(1-x^2)^l, \tag{7}$$

$$\Theta_{lm}(x) = \frac{(-1)^{l-m}}{2^l l!}\sqrt{\frac{2l+1}{2}\frac{(l+m)!}{(l-m)!}}(1-x^2)^{-m/2}\frac{d^{l-m}}{dx^{l-m}}(1-x^2)^l. \tag{8}$$

We define $\Theta_{lm}(x)$ for $m < 0$ by using (7) and (8). This yields

$$\Theta_{l,-m}(x) = (-1)^m \Theta_{lm}(x). \tag{9}$$

It is then clear that, when $m < 0$, $\Theta_{lm}(x)$ is again a solution of (5). Therefore when $\mu = l(l+1)$ equation (2) has the bounded single-valued solutions

$$Y_{lm}(\theta,\phi) = \frac{1}{\sqrt{2\pi}}e^{im\phi}\Theta_{lm}(\cos\theta) \qquad (-l \le m \le l). \tag{10}$$

The functions $Y_{lm}(\theta,\phi)$ are the *spherical harmonics of order l.*

We give the spherical harmonics explicitly for the simplest cases:

$$Y_{l0}(\theta,\phi) = \sqrt{\frac{2l+1}{4\pi}}P_l(\cos\theta), \tag{11}$$

$$\begin{aligned} Y_{10}(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\cos\theta, \\ Y_{1,\pm1}(\theta,\phi) &= \pm\sqrt{\frac{3}{8\pi}}\sin\theta e^{\pm i\phi}. \end{aligned} \tag{12}$$

It is easily verified that the $Y_{lm}(\theta,\phi)$ satisfy the *orthogonality condition*

$$\int_\Omega Y_{lm}(\theta,\phi)Y^*_{l'm'}(\theta,\phi)d\Omega = \delta_{ll'}\delta_{mm'}. \tag{13}$$

The integration in (13) is with respect to solid angle,

$$d\Omega = \sin\theta\, d\theta d\phi \qquad (0 \le \theta \le \pi, 0 \le \phi \le 2\pi).$$

It is clear from (9) and (10) that

$$Y^*_{lm}(\theta,\phi) = \Theta_{lm}(\cos\theta)\Phi_{-m}(\phi) = (-1)^m Y_{l,-m}(\theta,\phi). \tag{14}$$

Hence we have explicitly obtained the functions $Y(\theta,\phi)$ that give the angle dependence of the bounded solutions $u = R(r)Y(\theta,\phi)$ of Laplace's equation.

To determine the functions $R(r)$ we reduce (1) to the Euler equation

$$r^2R'' + 2rR' - l(l+1)R = 0,$$

whose general solution is

$$R(r) = C_1 r^l + C_2 r^{-l-1}$$

(C_1 and C_2 are constants). Hence the functions $r^l Y_{lm}(\theta,\phi)$ and $r^{-l-1}Y_{lm}(\theta,\phi)$ are particular solutions of Laplace's equation; the former are used in solving interior boundary value problems for spherical regions, and the latter, for exterior problems. They are known as *solid spherical harmonics.*

Remark. A different approach to spherical harmonics, based on the representations of the rotation group, is discussed, for example, in [G2]. This approach is useful in the general theory of angular momentum in quantum mechanics.

2. Properties of spherical harmonics. We now obtain the basic properties of the spherical harmonics $Y_{lm}(\theta,\phi)$.

1) From the recursion relation for the Jacobi polynomials and the connection of $\Theta_{lm}(x)$ with $P_{l-m}^{(m,m)}(x)$, it is easy to derive the recursion relation (on l) for $Y_{lm}(\theta,\phi)$:

$$\cos\theta\cdot Y_{lm} = \left(\frac{(l+1)^2-m^2}{4(l+1)^2-1}\right)^{1/2} Y_{l+1,m} + \left(\frac{l^2-m^2}{4l^2-1}\right)^{1/2} Y_{l-1,m}.$$

This formula remains valid for $m < 0$, as is easily seen by using (14).

2) Differentiating (7), we obtain the differentiation formula

$$\frac{d\Theta_{lm}}{dx} = -\frac{mx}{1-x^2}\Theta_{lm} + \left(\frac{l(l+1)-m(m+1)}{1-x^2}\right)^{1/2}\Theta_{l,m+1}.$$

Replacing m by $-m$ and using (9), we can obtain another differentiation formula

$$\frac{d\Theta_{lm}}{dx} = -\frac{mx}{1-x^2}\Theta_{lm} - \left(\frac{l(l+1)-m(m-1)}{1-x^2}\right)^{1/2}\Theta_{l,m-1}.$$

In these formulas we take $\Theta_{lm}(x) = 0$ for $m = \pm(l+1)$.

By eliminating $d\Theta_{lm}/dx$ from the differentiation formulas, we obtain a recursion on m for $\Theta_{lm}(x)$:

$$\frac{2mx}{\sqrt{1-x^2}}\Theta_{lm} = \left[\sqrt{l(l+1)-m(m+1)}\Theta_{l,m+1} \right.$$
$$\left. +\sqrt{l(l+1)-m(m-1)}\Theta_{l,m-1}\right].$$

By using (10), we can obtain a *differentiation formula for spherical harmonics*. Since

$$\frac{\partial Y_{lm}(\theta,\phi)}{\partial\theta} = -\sin\theta\frac{e^{im\phi}}{\sqrt{2\pi}}\left.\frac{d\Theta_{lm}(x)}{dx}\right|_{x=\cos\theta},$$

the differentiation formulas for $\Theta_{lm}(x)$ can be written in the form

$$e^{\pm i\phi}\left(\pm\frac{\partial Y_{lm}}{\partial\theta} + m\cot\theta\cdot Y_{lm}\right) = \sqrt{l(l+1)-m(m\pm 1)}Y_{l,m\pm 1}. \tag{15}$$

Here we are to put $Y_{lm}(\theta,\phi) = 0$ if $m = \pm(l+1)$.

The following *differentiation formula* can be derived from the explicit form of the spherical harmonics:

$$\frac{\partial Y_{lm}(\theta,\phi)}{\partial\phi} = imY_{lm}(\theta,\phi). \tag{16}$$

3. Integral representation. Let us obtain an *integral representation* for the $Y_{lm}(\theta,\phi)$. Starting from the expression (7) for $\Theta_{lm}(x)$, let us represent $(d^{l+m}/dx^{l+m})\,(1-x^2)^l$ by Cauchy's integral formula:

$$\frac{d^{l+m}}{dx^{l+m}}(1-x^2)^l = \frac{(l+m)!}{2\pi i}\int\limits_C \frac{(1-s^2)^l}{(s-x)^{l+m+1}}ds$$

(C is a contour surrounding the point $s = x$). Let us take C to be a circumference with center at $s = x$ and radius $\sqrt{1-x^2}$. Then, putting $s = x + \sqrt{1-x^2}e^{i\alpha}$, we obtain

$$\frac{d^{l+m}}{dx^{l+m}}(1-x^2)^l$$
$$= \frac{(-2)^l(l+m)!}{2\pi}(1-x^2)^{-m/2}\int\limits_0^{2\pi} e^{-im\alpha}(x+i\sqrt{1-x^2}\sin\alpha)^l d\alpha.$$

Substituting this into (7) and using (10), we obtain the integral representation for $Y_{lm}(\theta,\phi)$:

$$
\begin{aligned}
Y_{lm}(\theta,\phi) &= B_{lm}\int_0^{2\pi} e^{-im(\alpha-\phi)}(\cos\theta + i\sin\theta\sin\alpha)^l d\alpha \\
&= B_{lm}\int_{-\phi}^{2\pi-\phi} e^{-im\alpha}[\cos\theta + i\sin\theta\sin(\alpha+\phi)]^l d\alpha.
\end{aligned}
$$

where

$$B_{lm} = \frac{1}{4\pi l!}\left(\frac{2l+1}{\pi}(l-m)!(l+m)!\right)^{1/2}.$$

Since the integral of a periodic function is the same over any interval whose length is a period, we have

$$Y_{lm}(\theta,\phi) = B_{lm}\int_0^{2\pi} e^{-im\alpha}[\cos\theta + i\sin\theta\sin(\alpha+\phi)]^l d\alpha. \tag{17}$$

4. Connection between homogeneous harmonic polynomials and spherical harmonics. When we solved Laplace's equation $\Delta u = 0$ in spherical coordinates, we found the solutions that are bounded as $r \to 0$:

$$u_{lm}(r,\theta,\phi) = r^l Y_{lm}(\theta,\phi).$$

We can write the integral representation (17) for $u_{lm}(r,\theta,\phi)$ in Cartesian coordinates $x = r\sin\theta\cos\phi$, $y = r\sin\theta\sin\phi$, $z = r\cos\theta$:

$$
\begin{aligned}
u_{lm}(r,\theta,\phi) &= B_{lm}\int_0^{2\pi} e^{-im\alpha}[r\cos\theta + ir\sin\theta\sin(\alpha+\phi)]^l d\alpha \\
&= B_{lm}\int_0^{2\pi} e^{-im\alpha}(z + ix\sin\alpha + iy\cos\alpha)^l d\alpha.
\end{aligned}
$$

It is then clear that the functions $u_{lm}(r,\theta,\phi)$ are the homogeneous polynomials of degree l in x, y, z.

Recall that a homogeneous polynomial of degree l has the form

$$u_l(x,y,z) = \sum_{l_1,l_2,l_3} C_{l_1 l_2 l_3} x^{l_1} y^{l_2} z^{l_3},$$

where the summation is over all nonnegative indices $l_1 \geq 0, l_2 \geq 0, l_3 \geq 0$ whose sum is l. For example, $r^2 = x^2 + y^2 + z^2$ is a homogeneous polynomial.

Let us find the number of linearly independent homogeneous polynomials of degree l. It is enough to find all combinations of l_1 and l_2, since for a given l the value of l_3 is then determined: $l_3 = l - l_1 - l_2$. For a given l_1 the value of l_2 varies from $l_2 = 0$ to $l_2 = l - l_1$, i.e. it takes $l - l_1 + 1$ values. Hence the number of linearly independent homogeneous polynomials of degree l is

$$N_1 = \sum_{l_1=0}^{l} (l - l_1 + 1) = \frac{(l+1)(l+2)}{2}.$$

A homogeneous polynomial that satisfies Laplace's equation is a *homogeneous harmonic polynomial.* The function $r^l Y_{lm}(\theta,\phi)$ is an example.

From the homogeneous polynomials r^2 and $r^{l-2n} Y_{l-2n,m}(\theta,\phi)$ we can construct homogeneous polynomials of degree l,

$$u_{lmn}(x,y,z) = (r^2)^n r^{l-2n} Y_{l-2n,m}(\theta,\phi) = r^l Y_{l-2n,m}(\theta,\phi).$$

Here the indices m and n can take integral values satisfying

$$0 \leq 2n \leq l, -(l-2n) \leq m \leq l - 2n.$$

Since the spherical harmonics $Y_{l-2n,m}(\theta,\phi)$ are linearly independent (as follows from their orthogonality), the homogeneous polynomials $u_{lmn}(x,y,z)$ are linearly independent. For a given $l - 2n$ there are $2(l-2n)+1$ possible values of m. Hence the total number of these homogeneous polynomials is

$$\sum_n [2(l-2n)+1] = \frac{(l+1)(l+2)}{2}.$$

Since we have constructed as many homogeneous polynomials as the total number of linearly independent homogeneous polynomials of degree l, every homogeneous polynomial of degree l can be represented as a linear combination of $r^l Y_{l-2n,m}(\theta,\phi)$, i.e.

$$u_l(x,y,z) = r^l \sum_{m,n} C_{mn} Y_{l-2n,m}(\theta,\phi). \tag{18}$$

We have thus obtained an expansion of an arbitrary homogeneous polynomial in terms of spherical harmonics. It is easy to show by using (18) that *every homogeneous harmonic polynomial of degree l is a linear combination of the homogeneous harmonic polynomials $r^l Y_{lm}(\theta, \phi)$.*

In fact, let $u_l(x, y, z)$ be a homogeneous harmonic polynomial, $\Delta u_l = 0$. If we apply the Laplacian $\Delta_r + (1/r^2)\Delta_{\theta,\phi}$ to (18), we obtain

$$\begin{aligned}\Delta u_l &= r^{l-2} \sum_{m,n} [l(l+1) - (l-2n)(l-2n+1)] C_{mn} Y_{l-2n,m}(\theta, \phi) \\ &= r^{l-2} \sum_{m,n} 2n(2l - 2n + 1) C_{mn} Y_{l-2n,m}(\theta, \phi) = 0.\end{aligned}$$

Since the spherical harmonics $Y_{l-2n,m}(\theta, \phi)$ are linearly independent, we obtain

$$2n(2l - 2n + 1)C_{mn} = 0,$$

that is, $C_{mn} = 0$ for $n > 0$, as required.

5. Generalized spherical harmonics. Under rotations of the coordinate system, a homogeneous polynomial becomes a homogeneous polynomial of the same degree. On the other hand, the Laplacian is invariant under rotations, $\Delta_{xyz} = \Delta_{x'y'z'}$. Therefore every homogeneous harmonic polynomial becomes a homogeneous harmonic polynomial of the same degree under a rotation. Hence

$$u_{lm}(x, y, z) = \sum_{m'} D^l_{mm'} u_{lm'}(x', y', z'),$$

where

$$u_{lm}(x, y, z) = r^l Y_{lm}(\theta, \phi).$$

Consequently

$$Y_{lm}(\theta, \phi) = \sum_{m'} D^l_{mm'} Y_{lm'}(\theta', \phi'). \tag{19}$$

Thus the linear combinations of the $Y_{lm}(\theta, \phi)$ with a given l form a $(2l+1)$-dimensional space that is invariant under rotation.

The coefficients $D^l_{mm'}$ evidently depend on the parameters that determine the rotation. Every rotation of the coordinate system about the origin is completely determined by three real parameters. In fact, every rotation can be described by giving the direction of the rotation axis (two parameters) and the angle of rotation (one parameter). A more commonly used set of parameters that determine the rotation are the *Euler angles* α, β, γ. Every rotation can be realized by three successive rotations about the coordinate axes:

a) a rotation about the z axis through the angle α;

b) a rotation about the new y axis through the angle β;

c) a rotation about the new z axis through the angle* γ.

Consequently

$$D^l_{mm'} = D^l_{mm'}(\alpha, \beta, \gamma).$$

We shall denote the matrix with elements $D^l_{mm'}(\alpha, \beta, \gamma)$ by $D(\alpha, \beta, \gamma)$ and call it a *finite rotation matrix.*

Every rotation is uniquely specified by the Euler angles if they are taken so that $0 \leq \alpha < 2\pi, 0 \leq \beta \leq \pi, 0 \leq \gamma < 2\pi$. If the Euler angles are not in these intervals, one must keep in mind that a rotation with angles $(\alpha+2\pi n_1, \beta+2\pi n_2, \gamma+2\pi n_3)$ coincides with the rotation (α, β, γ) if n_1, n_2, n_3 are integers. Therefore

$$D(\alpha + 2\pi n_1, \beta + 2\pi n_2, \gamma + 2\pi n_3) = D(\alpha, \beta, \gamma).$$

Moreover, we observe that the rotation (α, β, γ) is equivalent to the rotation $(\pi + \alpha, -\beta, \pi + \gamma)$.

The inverse rotation is described by the angles

$$\alpha_1 = -\gamma, \quad \beta_1 = -\beta, \quad \gamma_1 = -\alpha,$$

and is equivalent to the rotation

$$(\pi + \alpha_1, -\beta_1, \pi + \gamma_1) = (\pi - \gamma,\ \beta,\ \pi - \alpha).$$

Consequently the matrix of the inverse rotation is the matrix of the rotation $(\pi - \gamma, \beta, \pi - \alpha)$, i.e.

$$D^{-1}(\alpha, \beta, \gamma) = D(\pi - \gamma, \beta, \pi - \alpha).$$

The functions $D^l_{mm'}(\alpha, \beta, \gamma)$ are known as *generalized spherical harmonics*, since in many special cases they coincide with ordinary spherical harmonics. They are also known as *Wigner's D-functions.* They are extensively used in quantum mechanics. (See, for example, [B2], [D1], [E1], [F1], [R2], [V1]. Note that in [B2] the functions $D^l_{mm'}(\alpha, \beta, \gamma)$ are denoted by $D^l_{m',m}(\alpha, \beta, \gamma)$.)

* Sometimes the rotation through the angle β is taken about the new x axis instead of about the new y axis. The Euler angles α', β', γ' defined in this way are connected with α, β, γ by $\alpha'=\alpha+\pi/2$, $\beta'=\beta$, $\gamma'=\gamma-\pi/2$.

We shall present a number of basic properties of generalized spherical harmonics. Since the element of solid angle is invariant under a rotation of coordinates, i.e. $d\Omega = d\Omega'$, the orthogonality conditions

$$\int Y_{lm}(\theta,\phi)Y^*_{lm_1}(\theta,\phi)d\Omega = \delta_{mm_1},$$
$$\int Y_{lm'}(\theta',\phi')Y^*_{lm'_1}(\theta',\phi')d\Omega' = \delta_{m'm'_1}$$

(the superscript * means "complex conjugate") imply the formula

$$\sum_{m'} D^l_{mm'}(\alpha,\beta,\gamma)[D^l_{m_1m'}(\alpha,\beta,\gamma)]^* = \delta_{mm_1},$$

i.e. the matrix $D^\dagger(\alpha,\beta,\gamma)$, the transpose conjugate of $D(\alpha,\beta,\gamma)$, is equal to $D^{-1}(\alpha,\beta,\gamma)$. This means that $D(\alpha,\beta,\gamma)$ is a unitary matrix (see [G1] or [S6]). From (19) we obtain

$$Y_{lm'}(\theta',\phi') = \sum_m [D^l_{mm'}(\alpha,\beta,\gamma)]^* Y_{lm}(\theta,\phi). \tag{20}$$

If we use the equations $D^{-1}(\alpha,\beta,\gamma) = D(\pi-\gamma,\beta,\pi-\alpha)$ and $D^{-1}(\alpha,\beta,\gamma) = D^\dagger(\alpha,\beta,\gamma)$ we obtain the following formula:

$$D^l_{mm'}(\pi-\gamma,\beta,\pi-\alpha) = [D^l_{m'm}(\alpha,\beta,\gamma)]^*. \tag{21}$$

Another elementary property of the generalized spherical harmonics is easily obtained from property (14) of the $Y_{lm}(\theta,\phi)$:

$$D^l_{mm'}(\alpha,\beta,\gamma) = (-1)^{m-m'}[D^l_{-m,-m'}(\alpha,\beta,\gamma)]^*. \tag{22}$$

6. Addition theorem. We present a useful relation for spherical harmonics, which is known as the addition theorem. To obtain it, we consider two arbitrary vectors $\mathbf{r}_1$ and $\mathbf{r}_2$ whose directions are specified by the spherical coordinates (θ_1,ϕ_1) and (θ_2,ϕ_2). Let the angle between the vectors be ω. According to (20) and (19) we have

$$Y_{lm'}(\theta'_1,\phi'_1) = \sum_m (D^l_{mm'})^* Y_{lm}(\theta_1,\phi_1), \tag{23}$$

$$Y_{lm}(\theta_2,\phi_2) = \sum_{m'} D^l_{mm'} Y_{lm'}(\theta'_2,\phi'_2). \tag{24}$$

As the result of a rotation of the coordinate system let the direction of the z' axis coincide with that of the radius vector $\mathbf{r}_2$. Then $\theta'_1 = \omega$, $\theta'_2 = 0$.

We set $m' = 0$ in (23). Since by virtue of (11)

$$Y_{l0}(\theta_1', \phi_1') = \sqrt{\frac{2l+1}{4\pi}} P_l(\cos\omega),$$

we have

$$\sqrt{\frac{2l+1}{4\pi}} P_l(\cos\omega) = \sum_m (D_{m0}^l)^* Y_{lm}(\theta_1, \phi_1). \tag{23a}$$

According to (7), at $\theta_2' = 0$ we have $Y_{lm'}(0, \phi_2') = 0$ if $m' \neq 0$. Therefore, by (11) and (5.12), formula (24) takes the form

$$Y_{lm}(\theta_2, \phi_2) = D_{m0}^l Y_{l0}(0, \phi_2) = D_{m0}^l \sqrt{\frac{2l+1}{4\pi}}. \tag{24a}$$

Comparing (23a) and (24a) yields

$$P_l(\cos\omega) = \frac{4\pi}{2l+1} \sum_{m=-l}^{l} Y_{lm}(\theta_1, \phi_1) Y_{lm}^*(\theta_2, \phi_2). \tag{25}$$

Relation (25) is known as the *addition theorem for spherical harmonics*. It has numerous applications, for example in the theory of atomic spectra. Formula (25) is very often applied in order to expand $1/|\mathbf{r}_1 - \mathbf{r}_2|$ in a series of the spherical harmonics $Y_{lm}(\theta_1, \phi_1)$ and $Y_{lm}(\theta_2, \phi_2)$. Since (see (5.14))

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \frac{r_<^l}{r_>^{l+1}} P_l(\cos\omega),$$

we find from the addition theorem that

$$\frac{1}{|\mathbf{r}_1 - \mathbf{r}_2|} = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{4\pi}{2l+1} \frac{r_<^l}{r_>^{l+1}} Y_{lm}(\theta_1, \phi_1) Y_{lm}^*(\theta_1, \phi_2). \tag{26}$$

Here $r_< = \min(r_1, r_2)$ and $r_> = \max(r_1, r_2)$.

Example 1. Consider the potential

$$u(\mathbf{r}) = \int_V \frac{\rho(\mathbf{r}')}{|\mathbf{r} - \mathbf{r}'|} d\tau', \tag{27}$$

of a distribution of electric charge of density $\rho(\mathbf{r})$ inside a volume V. To calculate the potential $u(\mathbf{r})$ at great distances from V we need its expansion in powers of $1/r$, taking the origin inside V. Using (26) with $\mathbf{r}_1 = r$, $\mathbf{r}_2 = r'$ and $r > r'$, we can represent (24) in the form

$$u(\mathbf{r}) = \sum_{l=0}^{\infty} \sum_{m=-l}^{l} \frac{Q_{lm}}{r^{l+1}} Y_{lm}(\theta, \phi), \tag{28}$$

where

$$Q_{lm} = \frac{4\pi}{2l+1} \int_V (r')^l \rho(\mathbf{r}') Y_{lm}(\theta', \phi') d\tau'. \tag{29}$$

Formula (28) is known as the *multipole expansion of the potential.*

If V is a sphere $0 < r' < a$ and $\rho(\mathbf{r}') = \rho(r')$, the integral (29) is easily evaluated: $Q_{lm} = \sqrt{4\pi} Q \delta_{l0} \delta_{m0}$, where Q is the total charge. In this case, as one would expect, $u(\mathbf{r}) = Q/r$.

Example 2. Let us use (25) to solve the *first interior boundary value problem (Dirichlet problem) for Laplace's equation in a spherical region*:

$$\Delta u = 0, \quad u(r, \theta, \phi)|_{r=a} = f(\theta, \phi).$$

We look for a solution by separation of variables in the form of a series of spherical harmonics $r^l Y_{lm}(\theta, \phi)$:

$$u(r, \theta, \phi) = \sum_{l,m} C_{lm} \left(\frac{r}{a}\right)^l Y_{lm}(\theta, \phi). \tag{30}$$

The coefficients C_{lm} are obtained from the boundary conditions on $r = a$ and the orthogonality of the functions $Y_{lm}(\theta, \phi)$. Then

$$C_{lm} = \int f(\theta', \phi') Y^*_{lm}(\theta', \phi') d\Omega'.$$

The solution (30) can also be represented as an integral. To obtain this, we substitute the expression for C_{lm} into (30), interchange summation and integration, and then carry out the summation on m by means of the addition formula:

$$\begin{aligned} u(r, \theta, \phi) &= \int d\Omega' f(\theta', \phi') \left[\sum_{l,m} \left(\frac{r}{a}\right)^l Y_{lm}(\theta, \phi) Y^*_{lm}(\theta', \phi') \right] \\ &= \int d\Omega' f(\theta', \phi') \left[\sum_l \frac{2l+1}{4\pi} \left(\frac{r}{a}\right)^l P_l(\mu) \right]. \end{aligned}$$

Here μ is the cosine of the angle between the directions (θ, ϕ) and (θ', ϕ'):

$$\mu = \cos\theta\cos\theta' + \sin\theta\sin\theta'\cos(\phi - \phi').$$

To carry out the summation on l, we use the generating function of the Legendre polynomials:

$$\sum_{l=0}^{\infty} t^l P_l(\mu) = \frac{1}{\sqrt{1 - 2t\mu + t^2}}.$$

Since

$$\begin{aligned}\sum_l (2l+1) t^l P_l(\mu) &= 2\sqrt{t} \sum_l \left(l + \frac{1}{2}\right) t^{l-1/2} P_l(\mu) \\ &= 2\sqrt{t}\frac{d}{dt}\left[\sqrt{t}\sum_l t^l P_l(\mu)\right] \\ &= 2\sqrt{t}\frac{d}{dt}\left(\frac{\sqrt{t}}{\sqrt{1 - 2t\mu + t^2}}\right) = \frac{1 - t^2}{(1 - 2t\mu + t^2)^{3/2}}\end{aligned}$$

we have

$$\sum_l (2l+1)\left(\frac{r}{a}\right)^l P_l(\mu) = \frac{1 - (r/a)^2}{[1 - 2\mu r/a + (r/a)^2]^{3/2}}$$

and consequently the solution of the first boundary value problem for Laplace's equation in a spherical region can be represented in the form

$$u(r, \theta, \phi) = \frac{1}{4\pi}\int d\Omega' f(\theta', \phi') \frac{1 - (r/a)^2}{[1 - 2\mu r/a + (r/a)^2]^{3/2}}.$$

7. Explicit expressions for generalized spherical harmonics. We now obtain explicit expressions for the functions $D^l_{mm'}(\alpha, \beta, \gamma)$. Let us perform two successive rotations determined by the parameters $\alpha_1, \beta_1, \gamma_1$ and $\alpha_2, \beta_2, \gamma_2$; let the equivalent single rotation be determined by the parameters α, β, γ. Furthermore let the first rotation transform the coordinates of some given vector from (θ, ϕ) to (θ_1, ϕ_1), and let the second rotation transform these coordinates to (θ', ϕ'). Then

$$\begin{aligned}Y_{lm}(\theta, \phi) &= \sum_{m_1} D^l_{mm_1}(\alpha_1, \beta_1, \gamma_1) Y_{lm_1}(\theta_1, \phi_1), \\ Y_{lm_1}(\theta_1, \phi_1) &= \sum_{m'} D^l_{m_1 m'}(\alpha_2, \beta_2, \gamma_2) Y_{lm'}(\theta', \phi').\end{aligned}$$

On the other hand,

$$Y_{lm}(\theta, \phi) = \sum_{m'} D^l_{mm'}(\alpha, \beta, \gamma) Y_{lm'}(\theta', \phi').$$

If we combine these expansions, we obtain, by the linear independence of the spherical harmonics,

$$D^l_{mm'}(\alpha, \beta, \gamma) = \sum_{m_1} D^l_{mm_1}(\alpha_1, \beta_1, \gamma_1) D^l_{m_1 m'}(\alpha_2, \beta_2, \gamma_2),$$

i.e.

$$D(\alpha, \beta, \gamma) = D(\alpha_1, \beta_1, \gamma_1) D(\alpha_2, \beta_2, \gamma_2),$$

so that when two rotations are performed successively their matrices are multiplied in inverse order. There is a similar result for the effect of several rotations of the coordinate system. It follows from the definition of the Euler angles and the preceding considerations that in order to calculate the generalized spherical functions $D^l_{mm'}(\alpha, \beta, \gamma)$ we need only obtain expressions for them when the rotations are about the z and y axes. Let $C^l_{mm'}(\alpha)$ and $d^l_{mm'}(\beta)$ be the generalized spherical harmonics corresponding to a rotation through the angle α about the z axis and a rotation through the angle β about the y axis. Then we have

$$D^l_{mm'}(\alpha, \beta, \gamma) = \sum_{m_1 m_2} C^l_{mm_1}(\alpha) d^l_{m_1 m_2}(\beta) C^l_{m_2 m'}(\gamma).$$

We now look for explicit expressions for the functions $C^l_{mm'}(\alpha)$. Under a rotation through the angle α around the z axis, the spherical coordinates of a given vector become $\theta' = \theta$, $\phi' = \phi - \alpha$. Therefore

$$Y_{lm}(\theta, \phi) = Y_{lm}(\theta', \phi' + \alpha) = e^{im\alpha} Y_{lm}(\theta', \phi').$$

On the other hand,

$$Y_{lm}(\theta, \phi) = \sum_{m'} C^l_{mm'}(\alpha) Y_{lm'}(\theta', \phi').$$

Hence

$$C^l_{mm'}(\alpha) = e^{im\alpha} \delta_{mm'}$$

and consequently

$$D^l_{mm'}(\alpha, \beta, \gamma) = e^{i(m\alpha + m'\gamma)} d^l_{mm'}(\beta). \tag{31}$$

We now find the generalized spherical harmonics $d^l_{mm'}(\beta)$ corresponding to a rotation of the coordinate system through the angle β about the y axis. In this case

$$Y_{lm}(\theta,\phi) = \sum_{m'} d^l_{mm'}(\beta) Y_{lm'}(\theta',\phi'). \tag{32}$$

The new coordinates (x', y', z') are connected with the old coordinates (x, y, z) by

$$\begin{aligned} x &= x'\cos\beta + z'\sin\beta, \\ y &= y', \\ z &= z'\cos\beta - x'\sin\beta. \end{aligned}$$

Changing to spherical coordinates, we find the connection between (θ,ϕ) and (θ',ϕ'):

$$\begin{aligned} \sin\theta\cos\phi &= \sin\theta'\cos\phi'\cos\beta + \cos\theta'\sin\beta, \\ \sin\theta\sin\phi &= \sin\theta'\sin\phi', \\ \cos\theta &= \cos\theta'\cos\beta - \sin\theta'\cos\phi'\sin\beta. \end{aligned} \tag{33}$$

To determine $d^l_{mm'}(\beta)$ we find a differential relation between these functions. Since it is simplest to differentiate with respect to β and ϕ' on the right-hand side of (32), we consider this equation for a fixed θ', taking θ and ϕ as functions of β and ϕ'. Consequently

$$\begin{aligned} \frac{\partial Y_{lm}(\theta,\phi)}{\partial\beta} &= \frac{\partial Y_{lm}}{\partial\theta}\frac{\partial\theta}{\partial\beta} + \frac{\partial Y_{lm}}{\partial\phi}\frac{\partial\phi}{\partial\beta}, \\ \frac{\partial Y_{lm}(\theta,\phi)}{\partial\phi'} &= \frac{\partial Y_{lm}}{\partial\theta}\frac{\partial\theta}{\partial\phi'} + \frac{\partial Y_{lm}}{\partial\phi}\frac{\partial\phi}{\partial\phi'}. \end{aligned}$$

The derivatives $\partial\theta/\partial\beta, \partial\theta/\partial\phi', \partial\phi/\partial\beta$, and $\partial\phi/\partial\phi'$ are calculated by using (33). Differentiating the last of these equations yields

$$\frac{\partial\theta}{\partial\beta} = \cos\phi, \quad \frac{\partial\theta}{\partial\phi'} = -\sin\beta\sin\phi.$$

The derivatives $\partial\phi/\partial\beta$ and $\partial\phi/\partial\phi'$ are easily found by differentiating the second and first equations in (33):

$$\begin{aligned} \frac{\partial\phi}{\partial\beta} &= -\cot\theta\sin\phi, \\ \frac{\partial\phi}{\partial\phi'} &= -\sin\beta\cot\theta\cos\phi + \cos\beta. \end{aligned}$$

Hence

$$\frac{\partial Y_{lm}(\theta,\phi)}{\partial\beta} = \cos\phi\frac{\partial Y_{lm}(\theta,\phi)}{\partial\theta} - im\cot\theta\sin\phi\, Y_{lm}(\theta,\phi),$$

$$\frac{\partial Y_{lm}(\theta,\phi)}{\partial\phi'} = -\sin\beta\left[\sin\phi\frac{\partial Y_{lm}(\theta,\phi)}{\partial\theta} + im\cot\theta\cos\phi\, Y_{lm}(\theta,\phi)\right] + im\cos\beta\, Y_{lm}(\theta,\phi).$$

To calculate $\partial Y_{lm}(\theta,\phi)/\partial\theta$ we use the differentiation formula (15). Since (15) involves $e^{\pm i\phi}\partial Y_{lm}/\partial\theta$, and the expressions for $\partial Y_{lm}/\partial\beta$ and $\partial Y_{lm}/\partial\phi'$ involve $\cos\phi\cdot\partial Y_{lm}/\partial\theta$ and $\sin\phi\cdot\partial Y_{lm}/\partial\theta$, in order to use (15) we must first form the corresponding linear combinations of $\partial Y_{lm}/\partial\beta$ and $\partial Y_{lm}/\partial\phi'$. We have

$$\begin{aligned}\frac{\partial Y_{lm}(\theta,\phi)}{\partial\beta} &\mp \frac{i}{\sin\beta}\frac{\partial Y_{lm}(\theta,\phi)}{\partial\phi'} \\ &= e^{\pm i\phi}\left[\frac{\partial Y_{lm}}{\partial\theta} \mp m\cot\theta\, Y_{lm}\right] \pm m\cot\beta\, Y_{lm} \\ &= \mp\sqrt{l(l+1)-m(m\pm1)}\, Y_{l,m\pm1}(\theta,\phi) \pm m\cot\beta\, Y_{lm}(\theta,\phi).\end{aligned}$$

If we use the expansion (32) for $Y_{lm}(\theta,\phi)$ and $Y_{l,m\pm1}(\theta,\phi)$ and equate the coefficients of $Y_{lm'}(\theta',\phi')$ on the left-hand and right-hand sides of the equation, we obtain the required differential relation for $d^l_{mm'}(\beta)$:

$$\frac{d}{d\beta}d^l_{mm'} \pm \frac{m'-m\cos\beta}{\sin\beta}d^l_{mm'} = \mp\sqrt{l(l+1)-m(m\pm1)}\, d^l_{m\pm1,m'}. \tag{34}$$

Here we are to take $d^l_{\pm(l+1),m'}(\beta) = 0$. By using (34) and the condition $d^l_{mm'}(0) = \delta_{mm'}$, which follows from (32) for $\beta = 0$, we can determine the functions $d^l_{mm'}(\beta)$.

Let us rewrite (34) in a more compact form. If we multiply it by

$$\exp\left(\pm\int\frac{m'-m\cos\beta}{\sin\beta}d\beta\right) = (1-\cos\beta)^{\pm(m'-m)/2}(1+\cos\beta)^{\mp(m'+m)/2},$$

we obtain

$$\begin{aligned}\frac{d}{d\beta}&\left[(1-\cos\beta)^{\pm(m'-m)/2}(1+\cos\beta)^{\mp(m'+m)/2}d^l_{mm'}(\beta)\right] \\ &= \mp\sqrt{l(l+1)-m(m\pm1)}(1-\cos\beta)^{\pm(m'-m)/2} \\ &\quad\times(1+\cos\beta)^{\mp(m'+m)/2}d^l_{m\pm1,m'}(\beta).\end{aligned}\tag{35}$$

If we use the upper signs and take $m = l$, we find

$$(1-\cos\beta)^{(m'-l)/2}(1+\cos\beta)^{-(m'+l)/2}d^l_{lm'}(\beta) = \text{ const.}$$

Hence

$$d^l_{lm'}(\beta) = C_{lm'}(1-\cos\beta)^{(l-m')/2}(1+\cos\beta)^{(l+m')/2}$$

($C_{lm'}$ are constants). When $m < l$ the functions $d^l_{mm'}(\beta)$ can be expressed recursively in terms of $d^l_{lm'}(\beta)$ by taking the lower signs in (35). After the change of variable

$$x = \cos\beta, \quad v_{mm'}(x) = (1-x)^{(m-m')/2}(1+x)^{(m+m')/2}d^l_{mm'}(\beta),$$

we obtain

$$v_{m-1,m'} = -\frac{1}{\sqrt{l(l+1)-m(m-1)}}\frac{dv_{mm'}}{dx},$$

whence

$$v_{mm'} = (-1)^{l-m}\prod_{s=m+1}^{l}\frac{1}{\sqrt{l(l+1)-s(s-1)}}\frac{d^{l-m}}{dx^{l-m}}v_{lm'},$$

i.e.

$$\begin{aligned} d^l_{mm'}(\beta) = C_{lm'}&\frac{(-1)^{l-m}(1-x)^{(m'-m)/2}(1+x)^{-(m'+m)/2}}{\prod\limits_{s=m+1}^{l}\sqrt{l(l+1)-s(s-1)}} \\ &\times\frac{d^{l-m}}{dx^{l-m}}\left[(1-x)^{l-m'}(1+x)^{l+m'}\right]. \end{aligned} \tag{36}$$

To determine $C_{lm'}$ we use the equation $d^l_{m'm'}(0) = 1$. Carrying out the differentiations in (36) by Leibniz's rule, we obtain

$$d^l_{m'm'}(0) = C_{lm'}\frac{2^{-m'}2^{l+m'}(l-m')!}{\prod\limits_{s=m'+1}^{l}\sqrt{l(l+1)-s(s-1)}} = 1.$$

This yields

$$C_{lm'} = \frac{\prod\limits_{s=m'+1}^{l}\sqrt{l(l+1)-s(s-1)}}{2^l(l-m')!}.$$

Since

$$\prod_{s=m+1}^{l} [l(l+1) - s(s-1)] = \prod_{s=m+1}^{l} (l+s)(l-s+1) = \frac{(2l)!(l-m)!}{(l+m)!},$$

we finally obtain

$$\begin{aligned} d^l_{mm'}(\beta) &= \frac{(-1)^{l-m}}{2^l (l-m)!} \sqrt{\frac{(l+m)!(l-m)!}{(l+m')!(l-m')!}} \\ &\times (1-x)^{(m'-m)/2}(1+x)^{-(m'+m)/2} \frac{d^{l-m}}{dx^{l-m}} \left[(1-x)^{l-m'}(1+x)^{l+m'}\right]. \end{aligned} \tag{37}$$

Observe that the $d^l_{mm'}(\beta)$ are real. They can be expressed in terms of Jacobi polynomials:

$$\begin{aligned} d^l_{mm'}(\beta) &= \frac{1}{2^m} \sqrt{\frac{(l+m)!(l-m)!}{(l+m')!(l-m')!}} \\ &\times (1-x)^{(m-m')/2}(1+x)^{(m+m')/2} P^{(m-m',m+m')}_{l-m}(x), \end{aligned}$$

where $x = \cos\beta$. The $d^l_{mm'}(\beta)$ can be written in a different form by using the symmetry relations that follow from (21), (22), (31), and the fact that $d^l_{mm'}$ is real:

$$d^l_{mm'} = (-1)^{m-m'} d^l_{m'm}, \quad d^l_{mm'} = (-1)^{m-m'} d^l_{-m,-m'}. \tag{38}$$

By using (38) we can always ensure that

$$m - m' \geq 0, \quad m + m' \geq 0.$$

Comparing (37) for $m' = 0$ with (8), we have

$$d^l_{m0}(\beta) = \left(\frac{2}{2l+1}\right)^{1/2} \Theta_{lm}(x),$$

whence

$$\begin{aligned} D^l_{m0}(\alpha,\beta,\gamma) &= \left(\frac{4\pi}{2l+1}\right)^{1/2} Y_{lm}(\beta,\alpha), \\ D^l_{00}(\alpha,\beta,\gamma) &= P_l(\cos\beta). \end{aligned} \tag{39}$$

By using (21) we can obtain a similar equation

$$D^l_{0m}(\alpha,\beta,\gamma) = (-1)^m \left(\frac{4\pi}{2l+1}\right)^{1/2} Y_{lm}(\beta,\gamma).$$