

Special Functions: Legendre functions, Spherical Harmonics, and Bessel Functions

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There are several special functions that recur in many branches of physics. You are all familiar, at some level, with spherical harmonics, from angular momentum in quantum mechanics. The spherical harmonics, more generally, are important in problems with spherical symmetry. They occur in electricity and magnetism. They are important also in astrophysics and cosmology, where they play the role of sines and cosines in fourier expanding functions on the sky. Legendre polynomials and legendre functions more generally solve the θ equations. Bessel functions arise in problems with spherical symmetry, but actually occur also more broadly. In quantum mechanics, particular instances solve the free particle radial equation in spherical coordinates, and again in cosmology, they appear as solutions to a number of problems.

Start with Laplace's eqn. in spherical coordinates:

$$\frac{1}{r} \frac{\partial^2}{\partial r^2}(r\Phi) + \frac{1}{r^2 \sin \theta} \frac{\partial}{\partial \theta} \left(\sin \theta \frac{\partial \Phi}{\partial \theta} \right) + \frac{1}{r^2 \sin^2 \theta} \frac{\partial^2 \Phi}{\partial \phi^2} = 0. \quad (1)$$

Separate variables:

$$\Phi = \frac{u(r)}{r} P(\theta) Q(\phi). \quad (2)$$

Leads to

$$r^2 \sin^2 \theta \left[\frac{1}{u} \frac{d^2 u}{dr^2} + \frac{1}{r^2 \sin \theta P} \frac{d}{d\theta} \left(\sin \theta \frac{dP}{d\theta} \right) \right] + \frac{1}{Q} \frac{d^2 Q}{d\phi^2} = 0. \quad (3)$$

The last term must be a constant:

$$\frac{d^2 Q}{d\phi^2} = -m^2 Q \quad (4)$$

or

$$Q = e^{\pm im\phi}. \quad (5)$$

Singlevaluedness $\Rightarrow m$ integer.

Now want equations for P , u . Divide by $\sin^2 \theta$;

$$r^2 \frac{1}{u} \frac{d^2 u}{dr^2} + \frac{1}{\sin \theta P} \frac{d}{d\theta} \left(\sin \theta \frac{dP}{d\theta} \right) - \frac{m^2}{\sin^2 \theta} = 0, \quad (6)$$

Second and third terms are independent of r , so can again introduce separation constant:

$$\frac{d^2 u}{dr^2} - \ell(\ell + 1) \frac{u}{r^2} = 0 \quad (7)$$

and

$$\frac{1}{\sin \theta} \frac{d}{d\theta} \left(\sin \theta \frac{dP}{d\theta} \right) + \left[\ell(\ell + 1) - \frac{m^2}{\sin^2 \theta} \right] P = 0. \quad (8)$$

u eqn. has solutions r^a , with $a(a - 1) = \ell(\ell + 1)$. So

$$u = ar^{\ell+1} + Br^{-\ell}. \quad (9)$$

If solving equation in all of space, can reject solution singular at the origin.

For the equation for P , we first write

$$x = \cos \theta; \quad \frac{d}{d\theta} = -\frac{1}{\sin \theta} \frac{d}{d \cos \theta} \quad (10)$$

so the equation can be rewritten as:

$$\frac{d}{dx} \left[(1 - x^2) \frac{dP}{dx} \right] + \left[\ell(\ell + 1) - \frac{m^2}{1 - x^2} \right] P = 0. \quad (11)$$

The case $m = 0$ is known as the *ordinary Legendre differential equation*; the case of non-zero m is known as Legendre's equation. The solutions of the first are known as *Legendre polynomials*; of the second as *associated Legendre functions*.

Solution by series method

Starting with the ordinary Legendre equation:

$$\frac{d}{dx} \left[(1 - x^2) \frac{dP}{dx} \right] + \ell(\ell + 1)P = 0. \quad (12)$$

try a solution:

$$P(x) = x^\alpha \sum_{j=0}^{\infty} a_j x^j \quad (13)$$

Substituting and equating powers of x^j , gives the relation:

$$a_{j+2} = \frac{(\alpha + j)(\alpha + j + 1) - \ell(\ell + 1)}{(\alpha + j + 2)(\alpha + j + 1)} a_j. \quad (14)$$

In addition, either $a_0 = 0$, or $\alpha(\alpha - 1) = 0$, or $a_1 = 0$ or $(\alpha + 1)\alpha = 0$. As a result, the series consists either of even terms, starting with x^0 , or odd terms starting with x^1 . For j large,

$$\frac{a_{j+2}}{a_j} \rightarrow 1; \quad (15)$$

this is the same as the series for $\frac{1}{1-x^2}$, and so diverges as $x \rightarrow 1$. In order that the series converge over the whole angular range, we require that the series terminates, which occurs if ℓ is a positive integer.

Exercise: Verify the recursion relation above. With the convention that $P(1) = 1$, determine the first three Legendre polynomials.

Properties of the Legendre Polynomials

$$P_\ell(x) = (-1)^\ell P_\ell(x). \quad (16)$$

Like $e^{ik \cdot x}$ in Fourier series, a complete, orthogonal set.

Orthogonality: Multiply Legendre's equation by $P_{\ell'}$ and integrate over x :

$$\int dx' P_{\ell'} \left[\frac{d}{dx} \left((1-x^2) \frac{dP_\ell}{dx} \right) + \ell(\ell+1)P_\ell \right] = 0. \quad (17)$$

Integrate by parts; then subtract the same equation with $\ell \leftrightarrow \ell'$. The surface term vanishes since $1-x^2=0$. Then, for $\ell \neq \ell'$,

$$\int_{-1}^1 dx P_\ell(x) P_{\ell'}(x) = 0. \quad (18)$$

We will do the case $\ell = \ell'$ (normalization) shortly.

Generating Function for the Legendre Polynomials

Just what it says: a way of generating the Legendre functions explicitly, without directly solving the differential equation. Start with the fact that

$$G(\vec{x}, \vec{x}') = \frac{1}{|\vec{x} - \vec{x}'|} \quad (19)$$

solves the Laplace equation, the angular part of which (ignoring ϕ) is Legendre's equation.

For $r' < r$, expand:

$$\begin{aligned} \frac{1}{|\vec{x} - \vec{x}'|} &= \frac{1}{(r^2 + r'^2 - 2rr' \cos \theta)^{1/2}} = \frac{1}{r} \frac{1}{(1 + \frac{r'^2}{r^2} - 2\frac{r'}{r} \cos \theta)^{1/2}} \quad (20) \\ &= \frac{1}{r} \sum_{\ell=0}^{\infty} \left(\frac{r'}{r}\right)^{\ell} A_{\ell}(\cos \theta). \end{aligned}$$

Note that the first term is the function $u(r)$. Claim is that $A_\ell = P_\ell$. Note for starters, that if A_ℓ satisfies the the condition $A_\ell(1) = 1$. The differential equation, in fact, follows by substituting the expansion. For any fixed ℓ , *because* u_ℓ satisfies our previous equation, A_ℓ must satisfy the P_ℓ equation. The expression, indeed, must hold for all θ and r , so it must hold term by term.

We can summarize:

$$g(t, x) = \frac{1}{(1 - 2xt + t^2)^{1/2}} = \sum_{\ell=0}^{\infty} P_{\ell}(x)t^{\ell}. \quad (21)$$

We can extract explicit form for the P_{ℓ} 's by extracting coefficient of t^{ℓ} : E.g.

$$P_0 = 1; \quad P_1 = x \quad (22)$$

We can extract explicit properties of P_{ℓ} 's by manipulating $g(t, x)$.

Normalization integral:

$$\int_{-1}^1 dx \frac{1}{1 - 2tx + t^2} = \int_{-1}^1 \left(\sum_{\ell=0}^{\infty} \right) \left(\sum_{\ell'=0}^{\infty} \right) P_{\ell}(x) P_{\ell'}(x) t^{\ell} t^{\ell'}. \quad (23)$$

Right hand side is

$$\int_{-1}^1 \sum P_{\ell}(x)^2 t^{2\ell}. \quad (24)$$

Left hand side is elementary:

$$\frac{1}{t} \ln\left(\frac{1+t}{1-t}\right). \quad (25)$$

Expand in powers of t , using

$$\log(1 + a) = \sum_{n=1}^{\infty} \frac{(-1)^{n+1}}{n} a^n. \quad (26)$$

So we have

$$\frac{1}{t} \log \left(\frac{1+t}{1-t} \right) = \frac{2}{t} \frac{t^{2n+1}}{2n+1}. \quad (27)$$

So

$$\int_{-1}^1 dx P_n^2 dx = \frac{2}{2n+1}. \quad (28)$$

Exercise: Differentiate g with respect to t and derive the recursion relation:

$$(2n+1)xP_n - (n+1)P_{n+1} - nP_{n-1} = 0. \quad (29)$$

Similarly, differentiate with respect to x :

$$\frac{dP_{\ell+1}}{dx} - \frac{dP_{\ell-1}}{dx} - (2\ell+1)P_{\ell} = 0. \quad (30)$$

Other recursion formulas, integral formulas, can be derived similarly (see, e.g., Arfken and Weber).

With these ingredients, we can expand any function of $\cos(\theta)$ (i.e. functions which are single-valued and otherwise well behaved as functions of θ) in terms of the Legendre polynomials.

$$f(\cos \theta) = \sum a_\ell P_\ell(\cos \theta) \quad (31)$$

with

$$a_\ell = \sqrt{\frac{2\ell + 1}{2}} \int_{-1}^1 f(x) P_\ell(x). \quad (32)$$

Associated Legendre Functions

Recall the more general differential equation:

$$(1 - x^2)v'' - 2xv' + \left[\ell(\ell + 1) - \frac{m^2}{1 - x^2} \right] v = 0. \quad (33)$$

This equation is solved by the *associated Legendre functions*:

$$P_\ell^m(x) = (-1)^m (1 - x^2)^{m/2} \frac{d^m}{dx^m} P_\ell(x). \quad (34)$$

The constant in front is conventional. That this solves the equation is shown by repeatedly differentiating Legendre's equation.

Exercise: Prove that the functions in eqn. 34 solve the full equation for positive m by repeated differentiation. For negative m , argue that the same is true by arguing that

$$P_\ell^{-m}(x) \propto P_\ell^m(x). \quad (35)$$

Not exercise: The normalization integral for the associated Legendre functions is:

$$\int_{-1}^1 P_{\ell'}^m(x) P_\ell^m(x) dx = \frac{2}{2\ell + 1} \frac{(\ell + m)!}{(\ell - m)!} \delta_{\ell\ell'}. \quad (36)$$

Spherical Harmonics

Solve the full θ, ϕ equations. Convention is to normalize to unity when integrated over the sphere.

$$Y_{\ell m}(\theta, \phi) = \sqrt{\frac{2\ell + 1}{4\pi} \frac{(\ell - m)!}{(\ell + m)!}} P_{\ell}^m(\cos \theta) e^{im\phi}. \quad (37)$$

Very useful is the *addition theorem*:

$$\frac{1}{|\vec{x} - \vec{x}'|} = 4\pi \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{\ell} \frac{1}{2\ell + 1} \left(\frac{r_{<}^{\ell}}{r_{>}^{\ell+1}} \right) Y_{\ell m}^*(\theta', \phi') Y_{\ell m}(\theta, \phi). \quad (38)$$

Bessel Functions

These arise frequently in problems with cylindrical symmetry. Consider separation of variables in cylindrical coordinates.

$$\frac{\partial^2 \Phi}{\partial \rho^2} + \frac{1}{\rho} \frac{\partial \Phi}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2 \Phi}{\partial \phi^2} + \frac{\partial^2 \Phi}{\partial z^2} = 0. \quad (39)$$

Take

$$\Phi = R(\rho)Q(\phi)Z(z). \quad (40)$$

Substitute in the differential equation and divide by RQZ to give

$$\frac{1}{R} \left(\frac{d^2 R}{d\rho^2} + \frac{1}{\rho} \frac{dR}{d\rho} \right) + \frac{1}{\rho^2 Q} \frac{d^2 Q}{d\phi^2} + \frac{1}{Z} \frac{d^2 Z}{dz^2} = 0. \quad (41)$$

So first we can take

$$\frac{1}{Z} \frac{d^2 Z}{dz^2} = k^2 \quad (42)$$

(k^2 positive, by assumption). Then multiply by ρ^2 to give:

$$\frac{1}{Q} \frac{d^2 Q}{d\phi^2} = -\nu^2. \quad (43)$$

This leaves the ρ equation:

$$\frac{d^2 R}{d\rho^2} + \frac{1}{\rho} \frac{dR}{d\rho} + \left(k^2 - \frac{\nu^2}{\rho^2} \right) R = 0. \quad (44)$$

From these equations we have:

$$Z = e^{\pm kz} \quad Q = e^{\pm i\nu\phi} \quad (45)$$

If the full range in azimuth is allowed, ν must be an integer. Setting $x = k\rho$ puts the radial equation in the standard form of Bessel's equation:

$$\frac{d^2 R}{dx^2} + \frac{1}{x} \frac{dR}{dx} + \left(1 - \frac{\nu^2}{x^2}\right) R = 0. \quad (46)$$

We can attempt a power series solution as before:

$$R(x) = x^\alpha \sum_{j=0}^{\infty} a_j x^j. \quad (47)$$

Substituting in the equation and rearranging terms gives:

$$\alpha = \pm\nu; \quad a_1 = 0. \quad (48)$$

We then have the recursion relation:

$$a_{2j} = -\frac{1}{4j(j+\alpha)} a_{2j-2} \quad (49)$$

which can be solved:

$$a_{2j} = \frac{(-1)^j a_0}{4^j j! (j+\alpha)(j+\alpha-1)\cdots(1+\alpha)}. \quad (50)$$

This can be written more concisely as:

$$a_{2j} = \frac{(-1)^j \Gamma(\alpha + 1)}{2^{2j} j! \Gamma(j + \alpha + 1)} a_0. \quad (51)$$

Convention:

$$a_0 = \frac{1}{2^\alpha \Gamma(\alpha + 1)}. \quad (52)$$

So two solutions:

$$J_{\pm\nu}(x) = \left(\frac{x}{2}\right)^{\pm\nu} \sum_{j=0}^{\infty} \frac{(-1)^j}{j! \Gamma(j \pm \nu + 1)} \left(\frac{x}{2}\right)^{2j} \quad (53)$$

If ν is not integer, these are two linearly independent solutions ("Bessel functions of the first kind"). If $\nu = m$, integer, the two solutions are not linearly independent (for $\nu = -m$, the *Gamma* function has poles for $j \leq m - 1$, so these terms vanish), and the rest is proportional to J_m).

Second solution can be taking to be ("Neumann function"):

$$N_\nu(x) = \frac{J_\nu(x) \cos(\nu\pi) - J_{-\nu}(x)}{\sin \nu\pi}. \quad (54)$$

For integer ν , this becomes:

$$N_\nu(x) = \frac{1}{\pi} \left[\frac{\partial J_\nu}{\partial \nu} - (-1)^\nu \frac{\partial J_{-\nu}}{\partial \nu} \right] \quad (55)$$

By directly differentiating Bessel's equation this can be shown to be a solution.

Asymptotic behavior:

- 1 Small x can be read off the series solution.
- 2 Large x requires more work, but it is easy to see that the solutions behave as $\frac{1}{\sqrt{x}} \cos(x + \delta)$.

$$J_\nu(x) \rightarrow \sqrt{\frac{2}{\pi x}} \cos\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right) \quad N_\nu(x) \rightarrow \sqrt{\frac{2}{\pi x}} \sin\left(x - \frac{\nu\pi}{2} - \frac{\pi}{4}\right). \quad (56)$$

Complete orthogonal sets:

Infinite numbers of roots, $J_\nu(x_{\nu m}) = 0$. $J_\nu(x_{\nu n}\rho/a)$ complete on interval $0 \leq \rho < a$. Similarly for derivatives of J .

Exercise: Verify the series expansion for the J_n 's.

Exercise: Verify that asymptotically the Bessel functions behave as $\frac{1}{\sqrt{x}} \cos(x + \delta)$. You don't have to determine δ .

Exercise: Verify directly from Bessel's equations that the functions are orthogonal for different n .

There are a variety of other functions defined in terms of J , N (Hankel functions; spherical Bessel functions, which we will encounter later). See Jackson, Arfken for definitions, basic properties.

For the J 's, there is also a generating function, analogous to that for the Bessel functions:

$$g(x, t) = e^{\frac{x}{2}(t-1/t)} = \sum_{n=-\infty}^{\infty} J_n(x)t^n. \quad (57)$$

Exercise: Verify, by comparing the series expression we derived earlier for J_n , and using $(-1)^n J_{-n} = J_n$. Differentiating with respect to t , verify the recursion formula:

$$J_{n+1} + J_{n-1} = \frac{2n}{x} J_n. \quad (58)$$

More on Spherical Harmonics

Connection to rotations: we have seen that Y_{00} is a scalar, and that the Y_{1m} 's are proportional to $x \pm iy$ and z . More generally, the $Y_{\ell m}$'s are irreducible tensors. To understand why this is the case, and how they transform under rotations, let's recall our discussion of rotations. Under an infinitesimal rotation, we saw that

$$\Delta x^i = \omega_j \epsilon_{ijk} x^k \quad (59)$$

where ω_j describes the infinitesimal rotation; its direction is the rotation axis, and its magnitude the angle of the rotation. So a function, $f(\vec{x})$, transforms as

$$\delta f(\vec{x}) = \omega_i \epsilon_{jik} \partial_j x^k f(\vec{x}). \quad (60)$$

This can be rewritten in terms of the usual angular momentum operator (without the \hbar), $L_i = -i\epsilon_{ijk}x_j\partial_k$:

$$f(\vec{f}) + \Delta f(\vec{x}) = (1 + i\vec{\omega} \cdot \vec{L})f(\vec{x}) \equiv U(\vec{\omega})f(\vec{x}). \quad (61)$$

Note that U is a unitary operator, $U^\dagger U = 1$.

Now consider how the $Y_{\ell m}$'s transform. They are eigenfunctions of ℓ^2 , so

$$\delta Y_{\ell m} = i\vec{\omega} \cdot \vec{L} Y_{\ell m}. \quad (62)$$

Because \vec{L}^2 commutes with the components of \vec{L} , under rotations, ℓ doesn't change.

Because U is unitary:

$$\Delta(Y_{\ell m}^* Y_{\ell m}) = 0. \quad (63)$$

In other words, the spherical harmonics are transformed by unitary *matrices*. These *rotation matrices* you will encounter in your quantum mechanics course.

Proof of the Addition Theorem using unitarity of U :

$P_\ell(\gamma)$ can be expanded in either $Y_{\ell m}(\theta, \phi)$ or $Y_{\ell m}(\theta', \phi')$. Symmetry between θ and θ' implies that

$$P_\ell(\gamma) = \sum_{mm'} a_{mm'} Y_{\ell m}(\theta, \phi) Y_{\ell m'}^*(\theta', \phi'). \quad (64)$$

The first thing we can say is that $a_{mm'} = a_m \delta_{m,m'}$. This is because P is unchanged if we rotate both \vec{x} and \vec{x}' about the z axis. Actually, we can go further, using what we have just learned about the rotation properties of the $Y_{\ell m}$'s, and show that a_m is independent of m . This is because the sum on the right hand side must be invariant under *any* simultaneous rotation of \vec{x} and \vec{x}' . We have just learned that the $Y_{\ell m}$'s are transformed by a unitary matrix, and $Y_{\ell m}^* Y_{\ell m}$ is invariant.

All that is left, then, is to determine the constant. We can do this by taking $\theta' = \phi' = 0$. In this case, $\gamma = \theta$, and only the $m = 0$ term contributes in the sum. Recalling the connection between the Y 's and the P 's, gives $a = \frac{4\pi}{2^{\ell+1}}$, completing the proof of the theorem.

Multipole expansion

The representation of the Green's function in terms of spherical harmonics provides a very simple derivation of the multipole expansion, where each term clearly represents an irreducible tensor. Working in Cartesian coordinates is more awkward, but the same must apply. The monopole and dipole terms are simple. The quadrupole arises from the expansion of

$$\frac{1}{r(1 - \frac{\vec{x} \cdot \vec{x}'}{r^2} + \frac{\vec{x}'^2}{r^2})^{1/2}} \quad (65)$$

to second order in \vec{x}' . Using

$$\frac{1}{(1 + \epsilon)^{1/2}} \approx 1 - \frac{1}{2}\epsilon + \frac{3}{8}\epsilon^2 \quad (66)$$

we have

$$\Phi = \dots + \frac{1}{r^3} \int d^3x' \rho(\vec{x}') \left(-\frac{1}{2}\vec{x}'^2 + \frac{3}{2}(\vec{x} \cdot \vec{x}')^2 \right) \quad (67)$$

The last term can be written in terms of the quadrupole moment:

$$\Phi = \dots + \frac{1}{r^3} Q_{ij} x_i x_j \quad (68)$$

where

$$Q_{ij} = \int d^3x \rho(\vec{x}) \left(\frac{3}{2} x_i x_j - \frac{1}{2} \delta_{ij} x_i x_j \right). \quad (69)$$

Q is a traceless, symmetric tensor. It has five independent elements, like Y_{2m} , and is an irreducible representation of the rotation group.

Quick introduction to the Γ function

Devised as a generalization of the factorial.

$$\Gamma(z + 1) = z\Gamma(z) \quad \Gamma(1) = 1 \quad (70)$$

so

$$\Gamma(n + 1) = n!. \quad (71)$$

Beautiful analytic properties.

Integral representation:

$$\Gamma(z) = \int_0^{\infty} dt t^{z-1} e^{-t}. \quad (72)$$

Easily seen that eqns. 70 are satisfied.

Well behaved for $\text{Re } z > 0$. From the defining relation, simple poles at the integers. Defined for $\text{Re } z < 0$ by analytic continuation.

From the integral rep., can derive Stirling's formula, an estimate of the factorial for large n (asymptotic series)

$$\Gamma(p+1) \approx p^p e^{-p} \sqrt{2\pi p}. \quad (73)$$