Physics 116C

Helmholtz's and Laplace's Equations in Spherical Polar Coordinates: Spherical Harmonics and Spherical Bessel Functions

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I. HELMHOLTZ'S EQUATION

As discussed in class, when we solve the diffusion equation or wave equation by separating out the time dependence,

$$u(\vec{r}, t) = F(\vec{r})\, T(t)\,, \tag{1}$$

the part of the solution depending on spatial coordinates, $F(\vec{r})$, satisfies *Helmholtz's equation*

$$\boxed{\nabla^2 F + k^2 F = 0\,,} \tag{2}$$

where k^2 is a separation constant. In this handout we will find the solution of this equation in *spherical polar coordinates.* The radial part of the solution of this equation is, unfortunately, not discussed in the book, which is the reason for this handout.

Note, if $k = 0$, Eq. (2) becomes Laplace's equation $\nabla^2 F = 0$. We shall discuss explicitly the solution for this (important) case.

A. Reminder of the Solution in Circular Polars

Recall that the solution of Helmholtz's equation in *circular polars* (two dimensions) is

$$F(r, \theta) = \sum_k \sum_{n=0}^{\infty} J_n(kr)(A_{kn} \cos n\theta + B_{kn} \sin n\theta) \qquad \text{(2 dimensions)}, \tag{3}$$

where $J_n(kr)$ is a Bessel function, and we have ignored the second solution of Bessel's equation, the Neumann function[1] $N_n(kr)$, which diverges at the origin.

For the special case of $k = 0$ (Laplace's equation) you showed in the homework that the solution for the radial part is

$$R(r) = C_n r^n + D_n r^{-n}\,, \tag{4}$$

[1] The Neumann function is often called the "Bessel function of the second kind".

(for $n = 0$ the solution is $C_0 + D_0 \ln r$). The r^n solution in Eq. (4) arises as the limit of the $J_n(kr)$ solution in Eq. (3) for $k \to 0$, while the r^{-n} solution arises as the limit of the Neumann function $N_n(x)$ solution of Helmholtz's equation (not displayed in Eq. (3) which only includes the solution regular at the origin).

Since the solution of Helmholtz's equation in circular polars (two dimensions) involves Bessel functions, you might expect that some sort of Bessel functions will also be involved here in spherical polars (three dimensions). This is correct and in fact we will see that the solution involves *spherical* Bessel functions.

B. Separation of Variables in Spherical Polars

Now we set about finding the solution of Helmholtz's and Laplace's equation in *spherical polars.* In this coordinate system, Helmholtz's equation, Eq. (2), is

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial F}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial F}{\partial\theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 F}{\partial\phi^2} + k^2 F = 0\,. \tag{5}$$

To solve Eq. (5), we use the standard approach of separating the variables, i.e. we write

$$F(r,\theta,\phi) = R(r)\Theta(\theta)\Phi(\phi)\,. \tag{6}$$

We then multiply by $r^2/(R\Theta\Phi)$ which gives

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + k^2r^2 + \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) + \frac{1}{\Phi\sin^2\theta}\frac{d^2\Phi}{d\phi^2} = 0\,. \tag{7}$$

C. Angular Part

Multiplying Eq. (7) by $\sin^2\theta$, the last term, $\Phi^{-1}(d^2\Phi/d\phi^2)$, only involves ϕ (whereas the first two terms only depend on r and θ), and so must be a constant which we call $-m^2$, i.e.

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2\,. \tag{8}$$

The solution is clearly

$$\boxed{\Phi(\phi) = e^{im\phi}\,,} \tag{9}$$

with m an integer (in order that the solution is the same for ϕ and $\phi + 2\pi$). Substituting into Eq. (7) gives

$$\frac{1}{R}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + k^2r^2 + \frac{1}{\Theta\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right) - \frac{m^2}{\sin^2\theta} = 0\,. \tag{10}$$

The third and fourth terms in Eq. (10) are only a function of θ (whereas the first two only depend on r), and must therefore be a constant which, for reasons that will be clear later, we write as $l(l+1)$, i.e.

$$\frac{1}{\Theta \sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) - \frac{m^2}{\sin^2\theta} = -l(l+1)\,, \tag{11}$$

which can be written as

$$\frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta \frac{d\Theta}{d\theta}\right) + \left(l(l+1) - -\frac{m^2}{\sin^2\theta}\right)\Theta = 0. \tag{12}$$

With the substitution $x = \cos\theta$, Eq. (12) becomes

$$\boxed{\frac{d}{dx}\left[(1-x^2)\frac{d\Theta(x)}{dx}\right] + \left(l(l+1) - \frac{m^2}{1-x^2}\right)\Theta(x) = 0\,.} \tag{13}$$

Eq. (13) is the Associated Legendre equation, so the solution is

$$\boxed{\Theta(x) = \ P_l^m(x)} \quad (x = \cos\theta), \tag{14}$$

where the $P_l^m(\cos\theta)$ are *Associated Legendre Polynomials*, and, as shown in the book, we need $l = 0, 1, 2, \cdots$, and m runs over integer values from $-l$ to l. If l is not an integer one can show that the solution of Eq. (12) diverges for $\cos\theta = 1$ or -1 ($\theta = 0$ or π). Generally we require the solution to be finite in these limits, and this is the reason why we write the separation constant in Eq. (12) as $l(l+1)$ with l an integer.

The functions Θ and Φ are often combined into a spherical harmonic, $Y_l^m(\theta,\phi)$, where

$$\boxed{Y_l^m(\theta,\phi) = \text{const. } P_l^m(\cos\theta)\, e^{im\phi}\,,} \tag{15}$$

where "const." is a messy normalization constant, designed to get the right hand side of Eq. (16) below equal to unity when $l = l', m = m'$. The spherical harmonics are orthogonal and normalized, *i.e.*

$$\boxed{\int_0^{2\pi} d\phi \int_0^{\pi} d\theta\ \sin\theta\ Y_l^m(\theta,\phi)^\star\ Y_{l'}^{m'}(\theta,\phi) = \delta_{l,l'}\delta_{m,m'}\,.} \tag{16}$$

Note that since the spherical harmonics are complex we need to take the complex conjugate of one of them in this orthogonality-normalization relation.

The first few spherical harmonics are

$$
\begin{aligned}
Y_0^0(\theta,\phi) &= \sqrt{\frac{1}{4\pi}}, \\
Y_1^1(\theta,\phi) &= -\sqrt{\frac{3}{8\pi}}\sin\theta\, e^{i\phi}, \\
Y_1^1(\theta,\phi) &= \sqrt{\frac{3}{4\pi}}\cos\theta, \\
Y_1^{-1}(\theta,\phi) &= \sqrt{\frac{3}{8\pi}}\sin\theta\, e^{-i\phi}.
\end{aligned}
$$

Spherical harmonics arise in *many situations* in physics in which there is spherical symmetry. An important example is the solution of the Schrödinger equation in atomic physics.

For the case of $m = 0$, *i.e.* no dependence on the azimuthal angle ϕ, we have $\Phi(\phi) = 1$ and also $P_l^m(\cos\theta) = P_l(\cos\theta)$, where the $P_l(x)$ are *Legendre Polynomials.* Hence

$$
\boxed{Y_l^0(\theta,\phi) = \text{const. } P_l(\cos\theta)\,.} \tag{17}
$$

You will recall from earlier classes that the first three Legendre polynomials are

$$
\begin{aligned}
P_0(x) &= 1, \\
P_1(x) &= x, \\
P_2(x) &= \tfrac{1}{2}(3x^2 - 1).
\end{aligned}
$$

D. Radial Part

We now focus on the radial equation, which, from Eqs. (10) and (12), is

$$
\frac{d}{dr}\left(r^2\frac{dR}{dr}\right) + \left[k^2r^2 - l(l+1)\right]R = 0\,, \tag{18}
$$

or equivalently

$$
\boxed{r^2\frac{d^2R}{dr^2} + 2r\frac{dR}{dr} + \left[k^2r^2 - l(l+1)\right]R = 0\,.} \tag{19}
$$

It turns out to be useful to define a function $Z(r)$ by

$$
R(r) = \frac{Z(r)}{(kr)^{1/2}}\,. \tag{20}
$$

Substituting this into Eq. (19) we find that Z satisfies

$$
r^2\frac{d^2Z}{dr^2} + r\frac{dZ}{dr} + \left[k^2r^2 - (l+1/2)^2\right]Z = 0\,, \tag{21}
$$

which is Bessel's equation of order $l + 1/2$. The solutions are $J_{l+1/2}(kr)$ and $N_{l+1/2}(kr)$ which, together with the factor $(kr)^{-1/2}$ in Eq. (20), means that the solutions for $R(r)$ are the *spherical Bessel and Neumann functions*, $j_l(kr)$ and $n_l(kr)$ defined by

$$\boxed{j_l(x) = \sqrt{\frac{\pi}{2x}} J_{l+1/2}(x),} \qquad \boxed{n_l(x) = \sqrt{\frac{\pi}{2x}} N_{l+1/2}(x).} \tag{22}$$

From now one we will assume that the solution is finite at the origin, which rules out $n_l(kr)$, and so

$$\boxed{R(r) = j_l(kr)\,.} \tag{23}$$

Hence, the general solution of Helmholtz's equation which is regular at the origin is

$$\boxed{F(r, \theta, \phi) = \sum_k \sum_{l=0}^{\infty} \sum_{m=-l}^{l} a_{klm}\, j_l(kr)\, Y_l^m(\theta, \phi)\,,} \tag{24}$$

where the coefficients a_{klm} would be determined by boundary conditions. Eq. (24) is the solution of Helmholtz's equation in spherical polars (three dimensions) and is to be compared with the solution in circular polars (two dimensions) in Eq. (3).

It turns out the spherical Bessel functions (i.e. Bessel functions of half-integer order, see Eq. (22)) are *simpler* than Bessel functions of integer order, because they are are related to trigonometric functions. For example, one has

$$j_0(x) = \frac{\sin x}{x}\,, \quad j_1(x) = \frac{\sin x}{x^2} - \frac{\cos x}{x}\,, \quad n_0(x) = -\frac{\cos x}{x}\,, \quad n_1(x) = -\frac{\sin x}{x} - \frac{\cos x}{x^2}\,. \tag{25}$$

Hence Eq. (24) is not quite as formidable as it may seem.

The only situations considered in detail in this course will be those in which there is no dependence on the azimuthal angle ϕ. In this case only the $m = 0$ terms contribute. For these, $Y_l^0(\theta, \phi) = \text{const.}\ P_l(\cos\theta)$, see Eq. (17), and so Eq. (24) simplifies to

$$\boxed{F(r, \theta) = \sum_k \sum_{l=0}^{\infty} a_{kl}\, j_l(kr)\, P_l(\cos\theta) \qquad \text{(azimuthal symmetry)}\,.} \tag{26}$$

E. Example with azimuthal symmetry: a plane wave

As a special case of Eq. (26), consider a plane wave traveling in the z direction (the direction of the polar axis). We know that in cartesian coordinates the spatial part of the amplitude of the wave is just $\exp(ikz)$, which we can also write as $\exp(ikr\cos\theta)$. Since the amplitude of the wave satisfies Helmholtz's equation (and there is no ϕ dependence), it must also be given by Eq. (26) (for the specified value of k), i.e.

$$e^{ikr\cos\theta} = \sum_{l=0}^{\infty} a_l \, j_l(kr) \, P_l(\cos\theta) \,, \tag{27}$$

for some choice of the a_l. In fact one can show that

$$a_l = (2l+1) \, i^l \,, \tag{28}$$

which gives

$$\boxed{e^{ikr\cos\theta} = \sum_{l=0}^{\infty} i^l \, (2l+1) \, j_l(kr) \, P_l(\cos\theta) \,,} \tag{29}$$

a result which is very important in "scattering theory" in quantum mechanics.

II. LAPLACE'S EQUATION

Finally we consider the special case of $k = 0$, *i.e.* Laplace's equation

$$\boxed{\nabla^2 F = 0 \,.}$$

A. Separation of variables

Separating the variables as above, the angular part of the solution is *still a spherical harmonic* $Y_l^m(\theta, \phi)$. The difference between the solution of Helmholtz's equation and Laplace's equation lies in the radial equation, which becomes

$$r^2 \frac{d^2 R}{dr^2} + 2r \frac{dR}{dr} - l(l+1)R = 0 \,.$$

As for the analogous case of circular polars, we can see by inspection that the solution just has a single power or r, *i.e.* $R(r) \propto r^\lambda$ for some value of λ. To determine λ we substitute r^λ in to the equation, which gives

$$\lambda(\lambda+1) - l(l+1) = 0 \,.$$

Factoring gives $(\lambda - l)(\lambda + l + 1) = 0$, so the two solutions of are

$$\lambda = l \text{ and } \lambda = -(l+1) \,.$$

If we specialize to the case of azimuthal symmetry for simplicity the general solution is

$$\boxed{F(r,\theta) = \sum_{l=0}^{\infty} \left(A_l r^l + \frac{B_l}{r^{l+1}} \right) P_l(\cos\theta) \,.} \tag{30}$$

The r^l term corresponds to the spherical Bessel function $j_l(kr)$ in Eq. (26) in the limit $k \to 0$, while the $r^{-(l+1)}$ term corresponds to the spherical Neumann function $n_l(kr)$ (not shown in Eq. (26) which only displays the solution of Helmholtz's equation regular at the origin) in the same limit.

Eq. (30) describes, for example, the electrostatic potential in regions of space where there is no charge. Coulomb's law, $F(r) \propto 1/r$ corresponds to the case of $l = 0$ (remember that $P_0(x) = 1$).

If the solution is valid in the region where $r \to \infty$ the A_l vanish since the potential should go to zero far away from any charges, and so

$$F(r,\theta) = \sum_{l=0}^{\infty} \frac{B_l}{r^{l+1}} P_l(\cos\theta) \,, \tag{31}$$

which is the *multipole expansion* that we discussed in the earlier part of the course.