Physics 464/511   Lecture F   Fall, 2016

Because we seem to live in a three dimensional space with physical laws which are rotationally and translationally symmetric, we are often concerned with the dynamics of a scalar field $\psi(\mathbf{x}, t)$ described by a Lagrangian density $\mathcal{L}(\mathbf{x}, t)$ which depends on $\psi(\mathbf{x}, t)$ and $\dot\psi(\mathbf{x}, t) = d\psi(\mathbf{x}, t)/dt$, but there must also be something which connects ψ at different points, or else each point would evolve independently of all the others, which is not the common situation. Now all fundamental physics is local, so coupling between points can only come from a derivative term, so $\mathcal{L}$ will also depend on $\vec\nabla\psi$, and as $\mathcal{L}$ is a rotationally invariant scalar, not a vector, it most likely occurs as $(\vec\nabla\psi)^2$. To derive the equations of motion by considering a variation $\delta\psi$ in $L = \int_V \mathcal{L}$, this gives a term

$$\int_V (\vec\nabla\psi) \cdot \vec\nabla\delta\psi = \int_V \vec\nabla \cdot \left(\delta\psi\vec\nabla\psi \right) - \int_V \delta\psi\nabla^2\psi,$$

and as the first term is the integral of a divergence and by Gauss equal to a surface integral, it may be discarded[1], and we get a $\nabla^2\psi$ term in the equation of motion. (This is analogous to what happens to the $\frac{1}{2}m(\dot x)^2$ term in H in particle dynamics, giving $m\ddot x$ term in the equation of motion.)

So whatever the motivation, we are presented with many equations involving the Laplacian ∇^2, such as

Poisson's equation	$\nabla^2\psi = f(\mathbf{x})$
Helmholtz equation	$\nabla^2\psi + k^2\psi = 0$
Wave equation	$c^2\nabla^2\psi - \dfrac{\partial^2\psi}{\partial t^2} = 0$
Schrödinger equation	$i\hbar\dfrac{\partial}{\partial t}\psi = \left(-\dfrac{\hbar^2}{2m}\nabla^2 + V(\mathbf{x}, t) \right)\psi$
Diffusion (constant coefficient D)	$\dfrac{\partial\psi}{\partial t} = D\nabla^2\psi$

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[1]In the variation, we are supposed to keep $\delta\psi = 0$ for the initial and final states, and we may also assume it vanishes on the spatial boundary of our region, if it exists (Dirichlet boundary conditions), or as $|\vec r| \to \infty$.

Poisson's equation is Laplace's ($\nabla^2\psi = 0$) with a source added. We often consider adding sources to Helmholtz' equation and the wave equation as well.

So there is no doubt that it would be very useful to have a good method of dealing with (inhomogenous) linear partial differential equations where the differentials are in ∇^2.

Now homogeneous linear equations have the advantage that solutions form a vector space, so particular solutions can be arbitrarily added. In many interesting situations it is possible to write down a complete set of particular solutions, so that any solution lies in an (infinite dimensional) vector space with basis given by that set. In the case of inhomogeneous equations, *i.e.* equations which have a source term such as f in the Poisson equation, if we can write the source as a sum of terms for which we can find solutions, the full solution is just the sum of these. Also, if we have found one solution to the inhomogeneous equation and the general solution of the homogeneous one, the most general solution of the inhomogeneous equation is the one we have plus an arbitrary homogeneous equation solution.

Now one way to solve a linear partial differential equation, probably the most common analytic one, is by separation of variables.   That is, we may be able find a set of curvilinear coordinates q^j describing our space, for which the *ansatz* $\psi(q^1, q^2, q^3) = Q_1(q^1)Q_2(q^2)Q_3(q^3)$, when plugged into the partial differential equation, separates into ordinary differential equations for the three functions Q_j. Generally this decomposition involves some constants which couple the ordinary equations to each other, becoming parameters in the ordinary differential equations. Then the solutions may form a complete set of functions when the parameters are varied.

Whether this is a useful expansion or not depends on two things:

- whether the differential equation, acting on the product, is simplified, falling into separable ordinary differential equations.

- whether the boundary conditions, expressed in these variables, are simple.

Simple essentially means that it doesn't mix terms in the sum.

We will need an example:

Consider the Helmholtz equation $\nabla^2\psi + k^2\psi = 0$ in cartesian coordinates

$q^i = x, y, z$, $Q_i = X, Y, Z$. Then

$$\frac{\partial^2 \psi}{\partial x^2} = \frac{d^2 X}{dx^2}(x) Y(y) Z(z),$$

and similarly for y and z, so

$$YZ \frac{d^2 X}{dx^2} + XZ \frac{d^2 Y}{dy^2} + XY \frac{d^2 Z}{dz^2} = -k^2 XYZ$$

or $\quad \underbrace{\frac{1}{X} \frac{d^2 X}{dx^2} + \frac{1}{Y} \frac{d^2 Y}{dy^2}}_{\text{not a function of } z} + \underbrace{\frac{1}{Z} \frac{d^2 Z}{dz^2}}_{\text{function only of } z} = -k^2,$

so $\dfrac{1}{Z} \dfrac{d^2 Z}{dz^2}$ must be a constant, say $-n^2$ (but n imaginary is okay), and similarly

$$\frac{1}{X} \frac{d^2 X}{dx^2} = -\ell^2, \qquad \frac{1}{Y} \frac{d^2 Y}{dy^2} = -m^2.$$

Now n, m and ℓ are, at this point, arbitrary constants, except that $n^2 + m^2 + \ell^2 = k^2$. As we will be summing over solutions, we may have a set of ℓ's, ℓ_j, and the individual equations $\dfrac{1}{X} \dfrac{d^2 X}{dx^2} = -\ell_j^2$ are trivial to solve:

$$
\begin{aligned}
X_j(x) &= a_j \cos \ell_j x + b_j \sin \ell_j x \\
\text{or} \qquad X_j(x) &= \text{Re } c_j e^{i\ell_j x}
\end{aligned}
$$

for example. The e^{ikx} solutions are a complete set, so any solution of Helmholtz's equation can be expanded in terms of the ones we just found by separation of variables. But the boundary conditions may be difficult to implement. In a rectangular box, the ℓ_j, m_j, n_j are determined (or rather restricted) by the boundary conditions. If, for example, the box is $[0, L_x] \times [0, L_y] \times [0, L_z]$ and has grounded walls on which $\psi = 0$, all the $a_i = 0$ and $\ell L_x = n_x \pi$, or $\ell = n_x \pi / L_x$ for n_x a positive integer, and similarly for Y and Z, $m = n_y \pi / L_y$ and $n = n_z \pi / L_z$, with $n_x, n_y, n_z \in \mathbb{Z}^+$. Thus there will only be solutions for certain values of k. For a cubic box, $L_x = L_y = L_z = L$, k^2 is a sum of three squares times π^2 / L^2.

   If, instead, our problem were in a spherical cavity, it would not be convenient to expand in this fashion. Instead, of course, one would try spherical

coordinates. More generally, we may consider trying an arbitrary orthogonal coordinate system, for which we have already found

$$\nabla^2 \psi = \frac{1}{h_1 h_2 h_3} \sum_i \frac{\partial}{\partial q^i} \left(\frac{h_1 h_2 h_3}{h_i^2} \frac{\partial \psi}{\partial q^i} \right).$$

If one tries to use $\psi = Q_1(q^1)Q_2(q^2)Q_3(q^3)$ and plug into Helmholtz's equation, you find

$$h_3^{-2} Q_3^{-1} Q_3'' + \frac{\partial}{\partial q^3}\left(\frac{h_1 h_2}{h_3} \right) \frac{1}{h_1 h_2 h_3} Q_3^{-1} Q_3' + (3 \leftrightarrow 1) + (3 \leftrightarrow 2) + k^2 = 0.$$

You might expect the conditions for separability would be that h_3^{-2} and $\frac{\partial}{\partial q^3}\left(\frac{h_1 h_2}{h_3} \right) \frac{1}{h_1 h_2 h_3}$ be independent of q^1 and q^2, and cyclic permutations thereof. But it's not that simple. In spherical coordinates with $q^1 = r$, $q^2 = \theta$ and $q^3 = \phi$, we have $h_1 = 1$, $h_2 = r$, $h_3 = r \sin \theta$, so h_3^{-2} is not independent of r or θ. But everything else is independent of ϕ, so the equation can be multiplied by h_3^2 to give $Q_3^{-1} Q_3'' = $ something independent of $q_3 = \phi$, but depending on none of the other variables either. So again it is a constant we will call $-m^2$, and $d^2 Q_3/d\phi^2 = -m^2 Q_3$. The solution is clearly $Q_3(\phi) = e^{im\phi}$.

This shows that we will have to play be ear which generalized coordinates are useful. But we have great faith that spherical ones must be, so if we write out the equation, plugging in h_i and $Q_3''/Q_3 = -m^2$, writting $Q_1 = R$ and $Q_2 = \Theta$, we find

$$\frac{R''}{R} + \left(\frac{\partial}{\partial r} r^2 \sin \theta \right) \frac{1}{r^2 \sin \theta} \frac{R'}{R} + \frac{1}{r^2} \frac{\Theta''}{\Theta} + \left(\frac{\partial}{\partial \theta} \sin \theta \right) \frac{1}{r^2 \sin \theta} \frac{\Theta'}{\Theta} - \frac{m^2}{r^2 \sin^2 \theta} + k^2 = 0.$$

the $\sin \theta$ cancels in the R'/R term, so if we multiply through by r^2, we find
$\frac{1}{\Theta}(\Theta'' + \cot \theta \, \Theta') - \frac{m^2}{\sin^2 \theta} = $ something independent of r but also depending only on r, and therefore constant, say Q, and we have

$$\frac{1}{\Theta}(\Theta'' + \cot \theta \, \Theta') - \frac{m^2}{\sin^2 \theta} = \text{const} = Q,$$
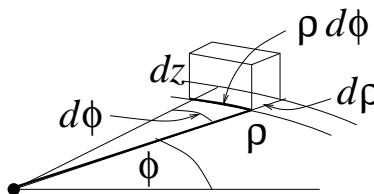
which then leaves
$$\frac{1}{R}\left(R'' + \frac{2}{r} R' \right) + \frac{Q}{r^2} + k^2 = 0.$$

We have therefore reduced the partial differential (Helmholtz) equation into three ordinary differential equations. We say that the laplacian is *separable* in spherical coordinates, just as in cartesian coordinates. The equation we get for $\Theta(\theta)$ is called the *associated Legendre equation*, which we will study in some detail later on. The equation for $R(r)$ is called the *spherical Bessel equation*.

    We would naturally use spherical coordinates if we were asking a question such as what frequency oscillations a spherical cavity of radius r_0 can sustain. Then we would impose on our equation a boundary condition $R(r_0) = 0$. But there are also boundary conditions on $\Theta(\theta)$ and $Q_3(\phi)$, due to the inherent meaning of the arguments. For Q_3, if the region of ϕ in question includes all of $[0, 2\pi]$, the condition is periodicity in ϕ with period 2π, $Q_3(\phi) = Q_3(\phi + 2\pi)$, which imposes the condition that m is an integer, or $m \in \mathbb{Z}$. For Θ, we will need to impose smoothness at $\theta = 0$ and $\theta = \pi$, where the $\cot \theta$ blows up. We shall see that this constrains the constant Q, and gives rise to the *associated Legendre polynomials*, and the "spherical harmonics", which are of crucial importance in quantum mechanics, particularly atomic and nuclear physics, and also in the multipole expansion in electrostatics or in electromagnetic radiation. We will consider these in more detail later.

    Another coordinate system we know will be important is the "circular cylindrical" or "cylindrical polar" coordinates ρ, ϕ, z, with

$$\rho = \sqrt{x^2 + y^2}, \quad x = \rho \cos \phi, \quad y = \rho \sin \phi.$$

We see $h_\rho = 1$, $h_\theta = \rho$, $h_z = 1$, so

$$\begin{aligned}
\nabla^2 &= \frac{1}{\rho} \left[\frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{\partial}{\partial \phi} \frac{1}{\rho} \frac{\partial}{\partial \phi} + \frac{\partial}{\partial z} \rho \frac{\partial}{\partial z} \right] \\
&= \frac{1}{\rho} \frac{\partial}{\partial \rho} \rho \frac{\partial}{\partial \rho} + \frac{1}{\rho^2} \frac{\partial^2}{\partial \phi^2} + \frac{\partial^2}{\partial z^2}.
\end{aligned}$$

If $\psi = R(\rho)\Phi(\phi)Z(z)$ and $(\nabla^2 + k^2)\psi = 0$, we have

$$\frac{1}{R} \frac{1}{\rho} \frac{d}{d\rho} \rho \frac{d}{d\rho} R(\rho) + \frac{1}{\rho^2 \Phi} \frac{d^2}{d\phi^2} \Phi + \frac{1}{Z} \frac{d^2}{dz^2} Z + k^2 = 0.$$

Only the third term could conceivably depend on z, so it must not, and $\frac{1}{Z} \frac{d^2}{dz^2} Z = -p^2$, a constant. Similarly only the second can depend on ϕ, so it

doesn't, and $\frac{1}{\Phi}\frac{d^2}{d\phi^2}\Phi = -m^2$. These have solutions which are sine waves or exponentials.

Finally

$$\left(\frac{1}{\rho}\frac{d}{d\rho}\rho\frac{d}{d\rho} - \frac{m^2}{\rho^2} + \gamma^2\right) R = 0$$

with $\gamma^2 = k^2 - p^2$. This is Bessel's equation.

Other coordinate systems are far less commonly used. They are, however, useful in special cases. For example, if you wanted to find the field of a long flat conductor of width w and negligible thickness, you would use elliptic cylindrical coordinates. Bipolar coordinates enable you to solve for the impedance of a pair of parallel wires such as the 300 Ω cable that used to connect your TV to the antenna. The rest of chapter 2 of the 2nd edition of Arfken is an exhaustive list. And you have a project to find another.