Summary:
- We calculate the eigenfunctions and eigenvalues of the Laplacian on the unit cube.
- We then give examples of how to use these eigenfunctions and eigenvalues to solve Possion's equation and the heat equation on this cube.

[NOTE. These lecture notes do not cover all of the material discussed in lecture but are rather of a summary form, intended to indicate the main points related to problems in rectangular coordinates and also to give the two examples. They will be supplemented later by additional information, particularly concerning the eigenfunctions of the Laplacian in cylindrical coordinates.]

EIGENFUNCTIONS AND EIGENVALUES OF THE LAPLACIAN ON THE UNIT CUBE. Throughout the rest of these lecture notes we shall denote the unit cube in $\mathbf{R}^3$ by

$$Q = \{(x, y, z)|0 \leq x, y, z \leq 1\}.$$

Now consider the following problem: determine all functions $u : Q \to \mathbf{R}$ not identically zero and all real numbers λ such that

$$\nabla^2 u = \lambda u, \quad u|_{\partial Q} = 0.$$

We attempt to solve this by applying separation of variables. Thus let $u = X(x)Y(y)Z(z)$; substituting this into the equation $\nabla^2 u = \lambda u$ and dividing through by u, we obtain

$$\frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = \lambda.$$

We see from this that all three of the quantities $\frac{X''}{X}$, $\frac{Y''}{Y}$ and $\frac{Z''}{Z}$ must be constants. The next step is clearly to try to determine whether they are positive or negative. This is determined by the boundary conditions. In our case, the boundary conditions give

$$u|_{x=0,1} = u|_{y=0,1} = u_{z=0,1} = 0;$$

in terms of X, Y, and Z, these become

$$X(0) = X(1) = 0, \quad Y(0) = Y(1) = 0, \quad Z(0) = Z(1) = 0.$$

Thus we see that each of the functions X, Y and Z must be oscillatory, meaning that each of $\frac{X''}{X}$, $\frac{Y''}{Y}$ and $\frac{Z''}{Z}$ must be negative. Let us work with X first. We may write $\frac{X''}{X} = -\mu^2$, where at this point all we know is that $\mu \in \mathbf{R}$ (and we may take $\mu > 0$: $\mu \neq 0$ since the only solution if $\mu = 0$ that satisfies the boundary conditions would be $X = 0$ which would give $u = 0$). Thus

$$X = a \cos \mu x + b \sin \mu x;$$

$X(0) = 0$ gives $a = 0$, while $X(1) = 0$ then gives (since $b \neq 0$ as $b = 0$ implies that $X = 0$, hence $u = 0$) $\mu = \ell\pi$, $\ell \in \mathbf{Z}$, $\ell > 0$. Similarly, we find that

$$Y = \sin m\pi y, \quad Z = \sin n\pi z,$$

$m, n \in \mathbf{Z}$, $m, n > 0$. Thus we have for u

$$u = \sin \ell\pi x \sin m\pi y \sin n\pi z,$$

$\ell, m, n \in \mathbf{Z}$, $\ell, m, n > 0$. The corresponding eigenvalue is clearly

$$\lambda = \frac{X''}{X} + \frac{Y''}{Y} + \frac{Z''}{Z} = -\ell^2\pi^2 - m^2\pi^2 - n^2\pi^2 = -\pi^2 \left(\ell^2 + m^2 + n^2\right).$$

We shall denote the above function by $\mathbf{e}_{\ell mn}(x, y, z)$ and the above eigenvalue (if needed) by $-\lambda_{\ell mn}^2$ (changing the notation slightly); thus we have

$$\mathbf{e}_{\ell mn}(x, y, z) = \sin \ell\pi x \sin m\pi y \sin n\pi z, \quad -\lambda_{\ell mn}^2 = -\pi^2\left(\ell^2 + m^2 + n^2\right).$$

Here we have $\ell, m, n \in \mathbf{Z}, \ell, m, n > 0$.

Let us pause to consider the properties of the set of eigenfunctions here. We note that the set $\{\sin \ell\pi x | \ell \in \mathbf{Z}, \ell > 0\}$ is complete on $[0, 1]$, and similarly for the sets $\{\sin m\pi y | m \in \mathbf{Z}, m > 0\}$ and $\{\sin n\pi z | n \in \mathbf{Z}, n > 0\}$. Now let $f : Q \to \mathbf{R}$ be any suitably well-behaved (for example, piecewise continuous) function on Q. Then we may expand successively as follows:

$$\begin{aligned}
f(x, y, z) &= \sum_{\ell=1}^{\infty} f_\ell(y, z) \sin \ell\pi x \\
&= \sum_{\ell=1}^{\infty} \left(\sum_{m=1}^{\infty} f_{\ell m}(z) \sin m\pi y \right) \sin \ell\pi x \\
&= \sum_{\ell=1}^{\infty} \left(\sum_{m=1}^{\infty} \left[\sum_{n=1}^{\infty} f_{\ell mn} \sin n\pi z \right] \sin m\pi y \right) \sin \ell\pi x \\
&= \sum_{\ell,m,n=1}^{\infty} f_{\ell mn} \sin \ell\pi x \sin m\pi y \sin n\pi z,
\end{aligned}$$

where

$$f_\ell(y, z) = 2\int_0^1 f(x, y, z) \sin \ell\pi x \, dx$$
$$f_{\ell m}(z) = 2\int_0^1 f_\ell(y, z) \sin m\pi y \, dy = 4\int_0^1 \int_0^1 f(x, y, z) \sin \ell\pi x \sin m\pi y \, dx \, dy$$
$$f_{\ell mn} = 2\int_0^1 f_{\ell m}(z) \sin n\pi z \, dz = 8\int_0^1 \int_0^1 \int_0^1 f(x, y, z) \sin \ell\pi x \sin m\pi y \sin n\pi z \, dx \, dy \, dz,$$

or in other words

$$f_{\ell mn} = \frac{(f, \mathbf{e}_{\ell mn})}{(\mathbf{e}_{\ell mn}, \mathbf{e}_{\ell mn})},$$

where we use the inner product

$$(f, g) = \iiint_Q f(x, y, z) \overline{g(x, y, z)} \, dV.$$

The foregoing is exactly what we would expect were the set $\{\mathbf{e}_{\ell mn}\}$ a complete orthogonal set on Q, and it turns out that this is the case. The foregoing is the closest we shall probably get to showing that the set is complete; orthogonality can be shewn as follows:

$$\begin{aligned}
(\mathbf{e}_{\ell mn}, \mathbf{e}_{\ell' m' n'}) &= \int_0^1 \int_0^1 \int_0^1 \mathbf{e}_{\ell mn}(x, y, z) \overline{\mathbf{e}_{\ell' m' n'}(x, y, z)} \, dV \\
&= \int_0^1 \int_0^1 \int_0^1 \sin \ell\pi x \sin m\pi y \sin n\pi z \sin \ell'\pi x \sin m'\pi y \sin n'\pi z \, dx \, dy \, dz \\
&= \int_0^1 \sin \ell\pi x \sin \ell'\pi x \, dx \int_0^1 \sin m\pi y \sin m'\pi y \, dy \int_0^1 \sin n\pi z \sin n'\pi z \, dz,
\end{aligned}$$

which is easily seen to be $\frac{1}{8}$ in case $\ell = \ell'$, $m = m'$, and $n = n'$, and to be zero if any of these equalities fails to hold. This means that the set $\{\mathbf{e}_{\ell mn}\}$ is orthogonal on Q, as claimed, with normalisation constant $\frac{1}{8}$ (in accord with the expansion formula above).

SOLVING POISSION'S EQUATION ON THE UNIT CUBE. The general idea behind this procedure has been explained already (see the notes for July 2 – 4). We shall illustrate it in this specific case with the following example.

Example. Solve the following problem on Q:

$$\nabla^2 u = (1-x^2)(1-y^2)(1-z^2), \quad u|_{\partial Q} = 0.$$

By our general method, the first step is to expand the right-hand side of the equation above in the above complete orthogonal set. To do this, we first calculate the following integral ($\ell \in \mathbf{Z}$, $\ell > 0$):

$$\begin{aligned}\int_0^1 (1-x^2)\sin \ell\pi x\,dx &= -(1-x^2)\frac{\cos \ell\pi x}{\ell\pi}\bigg|_0^1 - \int_0^1 (2x)\frac{\cos \ell\pi x}{\ell\pi}\,dx = \frac{1}{\ell\pi} - \frac{2}{\ell\pi}\int_0^1 x\cos \ell\pi x\,dx \\ &= \frac{1}{\ell\pi} - \frac{2}{\ell\pi}\left[x\frac{\sin \ell\pi x}{\ell\pi}\bigg|_0^1 - \int_0^1 \frac{\sin \ell\pi x}{\ell\pi}\,dx\right] \\ &= \frac{1}{\ell\pi} + \frac{2}{\ell^2\pi^2}\left(-\frac{\cos \ell\pi x}{\ell\pi}\bigg|_0^1\right) = \frac{1}{\ell\pi} + \frac{2}{\ell^3\pi^3}\left(1-(-1)^\ell\right).\end{aligned}$$

Thus we see that the expansion coefficients for the function $f = (1-x^2)(1-y^2)(1-z^2)$ are

$$\begin{aligned}f_{\ell mn} &= 8\int_0^1\int_0^1\int_0^1 (1-x^2)(1-y^2)(1-z^2)u_{\ell mn}\,dx\,dy\,dz \\ &= 8\int_0^1\int_0^1\int_0^1 (1-x^2)(1-y^2)(1-z^2)\sin \ell\pi x\sin m\pi y\sin n\pi z\,dx\,dy\,dz \\ &= 8\int_0^1 (1-x^2)\sin \ell\pi x\,dx\int_0^1 (1-y^2)\sin m\pi y\,dy\int_0^1 (1-z^2)\sin n\pi z\,dz \\ &= 8\left(\frac{1}{\ell\pi} + \frac{2}{\ell^3\pi^3}\left(1-(-1)^\ell\right)\right)\left(\frac{1}{m\pi} + \frac{2}{m^3\pi^3}\left(1-(-1)^m\right)\right)\left(\frac{1}{n\pi} + \frac{2}{n^3\pi^3}\left(1-(-1)^n\right)\right).\end{aligned}$$

Now suppose that u is a solution to the given problem, and let the expansion coefficients for u be $u_{\ell mn}$, so that

$$u = \sum_{\ell,m,n=1}^{\infty} u_{\ell mn}\sin \ell\pi x\sin m\pi y\sin n\pi z.$$

Substituting this into the equation $\nabla^2 u = (1-x^2)(1-y^2)(1-z^2)$, and assuming that we may differentiate term-by-term, we obtain

$$\begin{aligned}\nabla^2 u &= \sum_{\ell,m,n=1}^{\infty} u_{\ell mn}(-\lambda_{\ell mn}^2)\sin \ell\pi x\sin m\pi y\sin n\pi z \\ &= \sum_{\ell,m,n=1}^{\infty} 8\left(\frac{1}{\ell\pi} + \frac{2}{\ell^3\pi^3}\left(1-(-1)^\ell\right)\right)\left(\frac{1}{m\pi} + \frac{2}{m^3\pi^3}\left(1-(-1)^m\right)\right)\left(\frac{1}{n\pi} + \frac{2}{n^3\pi^3}\left(1-(-1)^n\right)\right) \\ &\qquad \cdot \sin \ell\pi x\sin m\pi y\sin n\pi z.\end{aligned}$$

Since $\{\sin \ell\pi x\sin m\pi y\sin n\pi z\}$ is a complete orthogonal set on Q, the coefficients in these two sums must be equal; thus we obtain

$$u_{\ell mn} = -\frac{8\left(\frac{1}{\ell\pi} + \frac{2}{\ell^3\pi^3}\left(1-(-1)^\ell\right)\right)\left(\frac{1}{m\pi} + \frac{2}{m^3\pi^3}\left(1-(-1)^m\right)\right)\left(\frac{1}{n\pi} + \frac{2}{n^3\pi^3}\left(1-(-1)^n\right)\right)}{\pi^2(\ell^2+m^2+n^2)},$$

whence finally we have the solution

$$u = \sum_{\ell,m,n=1}^{\infty} -\frac{8\left(\frac{1}{\ell\pi} + \frac{2}{\ell^3\pi^3}\left(1-(-1)^\ell\right)\right)\left(\frac{1}{m\pi} + \frac{2}{m^3\pi^3}\left(1-(-1)^m\right)\right)\left(\frac{1}{n\pi} + \frac{2}{n^3\pi^3}\left(1-(-1)^n\right)\right)}{\pi^2(\ell^2+m^2+n^2)} \cdot \sin \ell\pi x\sin m\pi y\sin n\pi z.$$

SOLVING THE HEAT EQUATION ON THE UNIT CUBE. We now consider a different problem which can also be treated using the above eigenfunctions for the Laplacian on the unit cube. We recall that early on in the course we derived the heat equation

$$\frac{\partial u}{\partial t} = \nabla^2 u,$$

which describes the time evolution of the temperature distribution of an object, and also other physical processes. We would like to learn how to solve this equation. First of all we must consider the question of what forms of initial or boundary data are appropriate. First we briefly recall what we know about ordinary differential equations: To solve a first-order ordinary differential equation, it suffices to know one piece of information, such as the value of the unknown function at some point (typically the initial point); to solve a second-order ordinary differential equation, we need to know two different pieces of information, such as the value of the function and its derivative at the initial point, or the value of the function at the end points. We have seen this latter situation play out in our study of Laplace's equation: in order to find a solution to Laplace's equation, we need to know something about the function on the boundary of the region we are considering; for example, its value over the whole boundary. (If we think back to the case of Laplace's equation on a cube, we see that this corresponds to the case in ordinary differential equations of giving the value of the function at the endpoints.) Now the heat equation is second-order in its spatial derivatives (just like Laplace's equation), but it is first-order in time. Thus we anticipate that we shall need to be given boundary data at each time of a sort similar to that we are given for Laplace's equation, while we also need to be given some kind of initial data. Since we are basically evolving the value of the function at each point in space, it seems reasonable to suspect that we may need to give as initial data the value of the function u at each point of Q, at some initial time (typically taken to be $t = 0$). We shall now give an example to indicate how this is done.

First a word about notation. A solution to the heat equation on Q is a function of *four* variables, three spatial ones and one temporal one, which we denote as x, y, z and t, respectively, so that a solution is written $u = u(t, x, y, z)$. We assume further that we are interested in finding the function u for all positive times, given its value at $t = 0$; thus we solve the heat equation on the region $(0, +\infty) \times Q$.

Example. Solve the following problem on $(0, +\infty) \times Q$:

$$\frac{\partial u}{\partial t} = \nabla^2 u, \quad u|_{t=0} = xyz, \quad u|_{(0,+\infty)\times\partial Q} = 0.$$

(Here $u|_{t=0} = xyz$ is the initial data discussed above, while $u|_{(0,+\infty)\times\partial Q} = 0$ is the boundary data. Note that we do not need to give any 'boundary data' for the future in t; thus, if we consider $(0, +\infty) \times Q$ as a long rectangular prism, then we are given data only on the bottom and sides, not on the top. This is because the heat equation is only first-order in time.) For each t, we may expand the function $u(t, x, y, z)$ in the basis $\{\mathbf{e}_{\ell mn}\}$ as

$$u(t, x, y, z) = \sum_{\ell,m,n=1}^{\infty} u_{\ell mn}(t)\mathbf{e}_{\ell mn} = \sum_{\ell,m,n=1}^{\infty} u_{\ell mn}(t) \sin \ell\pi x \sin m\pi y \sin n\pi z.$$

Substituting this into the above equation, and assuming that we may differentiate term-by-term (and that the expansion coefficients $u_{\ell mn}(t)$ are differentiable), we obtain

$$u'_{\ell mn} = -\pi^2(\ell^2 + m^2 + n^2)u_{\ell mn}.$$

This equation can be solved easily to obtain

$$u_{\ell mn}(t) = u_{\ell mn}(0)e^{-\pi^2(\ell^2+m^2+n^2)t}$$

(that the multiplicative constant is in fact $u_{\ell mn}(0)$ may be seen by setting $t = 0$ in both sides of the above equation). Thus, to determine $u_{\ell mn}(t)$, and hence to determine the desired series expansion for u, it suffices to determine the expansion coefficients $u_{\ell mn}(0)$ for the initial data xyz. Now

$$\int_0^1 x \sin \ell\pi x\, dx = -x\frac{\cos \ell\pi x}{\ell\pi}\bigg|_0^1 + \frac{1}{\ell\pi}\int_0^1 \cos \ell\pi x\, dx = \frac{(-1)^{\ell+1}}{\ell\pi},$$

whence we see that the expansion coefficients $u_{\ell mn}(0)$ are

$$u_{\ell mn}(0) = 8\frac{(-1)^{\ell+1}}{\ell\pi}\frac{(-1)^{m+1}}{m\pi}\frac{(-1)^{n+1}}{n\pi} = -8\frac{(-1)^{\ell+m+n}}{\pi^3\ell mn},$$

so

$$u_{\ell mn}(t) = -8\frac{(-1)^{\ell+m+n}}{\pi^3\ell mn}e^{-\pi^2(\ell^2+m^2+n^2)t}$$

and the solution to our problem is

$$u(t,x,y,z) = \sum_{\ell,m,n=1}^{\infty} -8\frac{(-1)^{\ell+m+n}}{\pi^3\ell mn}e^{-\pi^2(\ell^2+m^2+n^2)t}\sin\ell\pi x\sin m\pi y\sin n\pi z.$$

A WORD ABOUT BOUNDARY CONDITIONS. So far we have considered various different kinds of boundary conditions without giving them names. Generally, the types of boundary conditions one considers for Laplace's equation (hence, for the spatial boundary conditions in the heat equation) on some region D are the following:

- Dirichlet: $u|_{\partial D} = f$.
- Neumann: $(\nabla u \cdot \mathbf{n})|_{\partial D} = g$.
- Robin: $(au + b\nabla u \cdot \mathbf{n})|_{\partial D} = h$.

Here $\mathbf{n}$ indicates the outer unit normal to the region D at its boundary.

One may also consider more general conditions (for example, Dirichlet over part of the boundary and Neumann over another part), which we may then term *mixed* boundary conditions.