SEPARATION OF VARIABLES METHOD

Separation of variables is a method for solving partial differential equations — such as Laplace, Poisson, or Schrödinger equations — is volumes whose boundaries line up with the coordinate surfaces. For example, a rectangular box in Cartesian coordinates (x,y,z), the space outside a sphere in spherical coordinates (r,θ,ϕ), or a cylindrical cavity in cylindrical coordinates (ρ,ϕ,z). In these notes I focus on the Laplace equation — solving the electrostatic boundary problem in a suitable volume $\mathcal{V}$, with no charges inside $\mathcal{V}$ but unknown charges outside $\mathcal{V}$ or on its surface.

The basic idea of the separation of variables method is to look for the solutions (of the Laplace equation subject to non-trivial boundary conditions) in the product form

$$\begin{aligned} \Phi(x,y,z) &= f(x)g(y)h(z), && \text{(1.a)}\\ \text{or } \Phi(r,\theta,\phi) &= f(r)g(\theta)h(\phi), && \text{(1.b)}\\ \text{or } \Phi(\rho,\phi,z) &= f(\rho)g(\phi)h(z). && \text{(1.c)} \end{aligned}$$

More generally, one starts by looking for infinite series of such product solutions to the Laplace equation subject to the *homogeneous* boundary conditions (such as $\Phi = 0$ at some boundaries), and then looks for the linear combination of such product solutions that would also satisfy the remaining non-homogeneous boundary conditions (such as $\Phi(\mathbf{x}) =$ given $\Phi_b(\mathbf{x})$ at the remaining boundaries).

But instead of developing a general theory of the separation-of-variables method, I am going to explain it by giving a few specific examples.

A 2D Cartesian Coordinate Example

Let's start with an effectively 2D problem where the potential $\Phi(x,y,z)$ depends on the x and y coordinates but does not depend on the z. Specifically, consider an infinite slot

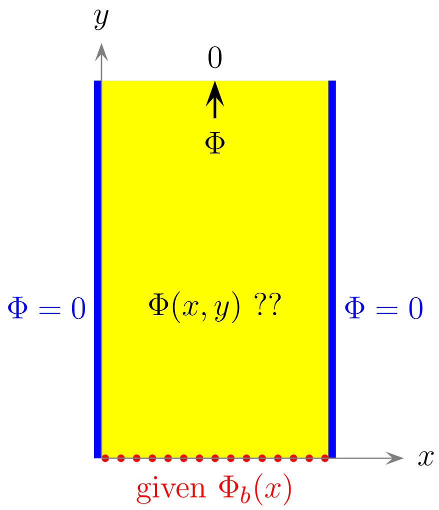
$$0 \le x \le a, \quad 0 \le y < \infty, \quad -\infty < z < +\infty \tag{2}$$

between 2 conducting and grounded walls (where $\Phi = 0$) at $x = 0$ and at $x = a$. There are no electric charges within the slot, but there are some unknown charges outside the slot, and also unknown surface charges on the wall. On the other hand, somebody have measured the potential at the front boundary $y = 0$ of the slot and found that it depends only on the x coordinate across the slot but not on the vertical z coordinate,

$$@y = 0, \quad \Phi(x, 0, z) \;=\; \text{known } \Phi_b(x \text{ only}). \tag{3}$$

And since the slot's geometry is symmetries WRT translations in the z direction, we presume the potential inside the slot to also be independent on z.

Mathematically, this gives us a 2D boundary problem inside the yellow semi-infinite strip $0 \leq x \leq a$, $0 \leq y < \infty$ on the following diagram:



(4)

Specifically, we looking for $\Phi(x, y)$ which obeys:

$$\begin{aligned}
&[1] & \triangle_{2d}\Phi \;&=\; \frac{\partial^2\Phi}{\partial x^2} + \frac{\partial^2\Phi}{\partial y^2} \;=\; 0,\\
&[2] & @x = 0 \text{ and } @x = a : \Phi \;&=\; 0, \quad \text{and for } y \to +\infty : \Phi \to 0\\
&[3] & \Phi(x, y = 0) \;&=\; \text{given } \Phi_b(x).
\end{aligned}$$

In the separation-of-variables method, we start by focusing on the homogeneous conditions [1] and [2] — but not the inhomogeneous condition [3] — and look for the solutions of the product form

$$\Phi(x,y) \;=\; f(x)\times g(y). \tag{5}$$

For a potential of this form, its 2D Laplacian is

$$\triangle_{2d}\Phi(x,y) \;=\; f''(x)g(y) \;+\; f(x)g''(y), \tag{6}$$

hence

$$\frac{\triangle_{2d}\Phi}{\Phi} \;=\; \frac{f''(x)}{f(x)} \;+\; \frac{g''(y)}{g(y)}\,. \tag{7}$$

Consequently, the Laplace equation for the potential requires

$$\frac{f''(x)}{f(x)} \;+\; \frac{g''(y)}{g(y)} \;=\; 0 \quad \forall x,y, \tag{8}$$

and since the first term on the LHS here depends only on x while the second term depends only on y, the only way they can add up to zero for all x and y if both terms are constants. Thus,

$$\left.\begin{aligned} \frac{f''(x)}{f(x)} &= -C, \\ \frac{g''(y)}{g(y)} &= +C, \end{aligned}\right\} \quad \text{for the same constant } C. \tag{9}$$

At the same time, the homogeneous boundary conditions [2] translate into conditions for the $f(x)$ and $g(y)$ as

$$\begin{aligned} f(x=0) \;=\; f(x=a) &\;=\; 0, \\ \lim_{y\to+\infty} g(y) &\;=\; 0. \end{aligned} \tag{10}$$

In particular, the $f(x)$ obeys the ordinary differential equation $f''(x) + Cf(x) = 0$, whose general solution is a combination of since and cosine waves (for $C > 0$) or hyperbolic sinh and cosh (for $C < 0$). However, the boundary conditions requiring nodes at both $x = 0$ and $x = a$

select the sine waves of particular wave numbers, specifically

$$f(x) \;=\; \sin\frac{n\pi x}{a} \tag{11}$$

for an *integer* $n = 1, 2, 3, \ldots$, and hence

$$C \;=\; +\left(\frac{n\pi}{a}\right)^2 \;>\; 0. \tag{12}$$

Consequently, the $g(y)$ function obeys $g''(y) = Cg(y)$ for a positive C, so the general solution is a combination of a sinh and a cosh, or equivalently

$$g(y) \;=\; A\times\exp\left(-\frac{n\pi y}{a}\right) \;+\; B\times\exp\left(+\frac{n\pi y}{a}\right). \tag{13}$$

However, the asymptotic condition $g \to 0$ for $y \to +\infty$ forces $B = 0$ so $g(y)$ is a decaying exponential only.

Altogether, a product solution to the conditions [1] and [2] has form

$$\Phi(x, y) \;=\; (\text{const})\times\sin\frac{n\pi x}{a}\times\exp\left(-\frac{n\pi y}{a}\right) \tag{14}$$

for an integer $n = 1, 2, 3, \ldots$. Note an infinite series of such solutions. And since the conditions [1] and [2] are homogeneous, and linear combination of their solutions is also a solution. Consequently, the more general solutions to the conditions [1] and [2] have form

$$\Phi(x, y) \;=\; \sum_{n=1}^{\infty} A_n\times\sin\frac{n\pi x}{a}\times\exp\left(-\frac{n\pi y}{a}\right) \tag{15}$$

for some real coefficients A_n. In fact *any* solution to the 2D Laplace equation [1] in the strip subject to the boundary conditions [2] can be written as a series (15) with some coefficients A_n. But for the sake of brevity, let me simply state this theorem but skip the proof.

Now let's go back to the complete boundary problem, including the inhomogeneous condition [3] — the known potential $\Phi_b(x)$ at the front boundary $y = 0$. It is this condition which determine the coefficients A_n in eq. (15). Indeed, for $y = 0$ all exponential factors in the series (15) become 1, thus

$$\Phi(x, y = 0) \;=\; \sum_{n=1}^{\infty} A_n \times \sin\frac{n\pi x}{a} \tag{16}$$

hence the boundary condition [3] becomes

$$\sum_{n=1}^{\infty} A_n \times \sin\frac{n\pi x}{a} \;=\; \text{given } \Phi_b(x). \tag{17}$$

In other words, the A_n are the Fourier coefficients of the given boundary potential $\Phi_b(x)$ expanded into the sine waves,

$$A_n \;=\; \frac{2}{a}\int_0^a dx\, \Phi_b(x) \times \sin\frac{n\pi x}{a}\,. \tag{18}$$

In particular, for a $\Phi_b(x)$ being a sine wave — or a combination of a few sine waves — there is only one — or only a few — non-zero coefficients A_n, so the series (15) becomes a finite sum.

For example, consider

$$\begin{aligned}\Phi_b(x) \;&=\; V_0 \times \sin^3\frac{\pi x}{a}\\ &=\; \frac{3V_0}{4} \times \sin\frac{\pi x}{a} \;-\; \frac{V_0}{4}\sin\frac{3\pi x}{a}\,.\end{aligned} \tag{19}$$

Comparing this boundary potential to the Fourier series (17), we immediately — without performing any integrals — identify

$$A_1 \;=\; \frac{3V_0}{4}\,, \quad A_3 \;=\; -\frac{V_0}{4}\,, \quad \text{all other } A_n \;=\; 0, \tag{20}$$

and therefore, in the interior of the slot

$$\Phi(x, y) \;=\; \frac{3V_0}{4} \times \sin\frac{\pi x}{a} \times \exp\left(-\frac{\pi y}{a}\right) \;-\; \frac{V_0}{4} \times \sin\frac{3\pi x}{a} \times \exp\left(-\frac{3\pi y}{a}\right). \tag{21}$$

For other kinds of boundary potentials $\Phi_b(x)$, the Fourier series (17) has an infinite number of terms, and the coefficients A_n obtain as Fourier integrals (18). For an example, suppose the from wall of the slot at $y=0$ is conducting but not grounded and insulated from the side walls at $x=0$ and $x=a$; instead, it's held a a constant but non-zero potential

$$\Phi_b(x) \;=\; V_0 \;\neq\; 0 \quad \text{(same at all } 0<x<a\text{)}. \tag{22}$$

In this case, the coefficients A_n obtain as

$$\begin{aligned} A_n \;&=\; \frac{2V_0}{a}\int\limits_0^a dx\,\sin\frac{n\pi x}{a} \;=\; \frac{2V_0}{n\pi}\int\limits_0^{n\pi} d\alpha\,\sin(\alpha) \\ &=\; \frac{2V_0}{n\pi}\Bigl(1\,-\,\cos(n\pi)\Bigr) \;=\; \frac{2V_0}{n\pi}\times\begin{cases} 2 & \text{for odd } n, \\ 0 & \text{for even } n. \end{cases} \end{aligned} \tag{23}$$

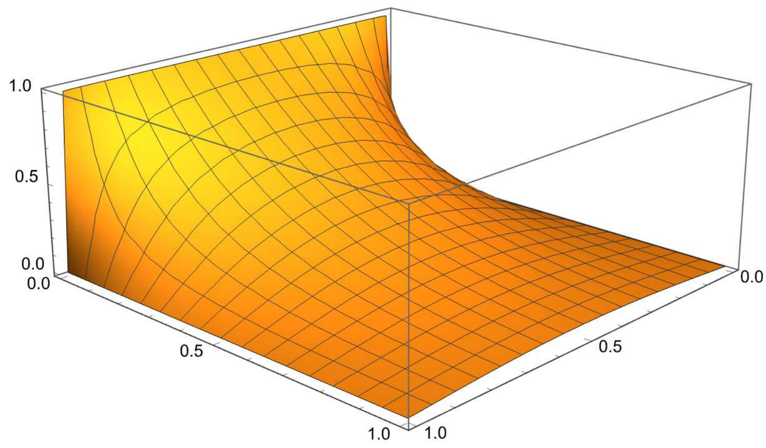
Consequently, inside the slot

$$\Phi(x,y) \;=\; \sum_{n=1,3,5,\ldots}^{\text{odd}\,n} \frac{4V_0}{n\pi}\times\sin\frac{n\pi x}{a}\times\exp\left(-\frac{n\pi y}{a}\right). \tag{24}$$

There happens to be an analytic formula for this infinite sum, namely

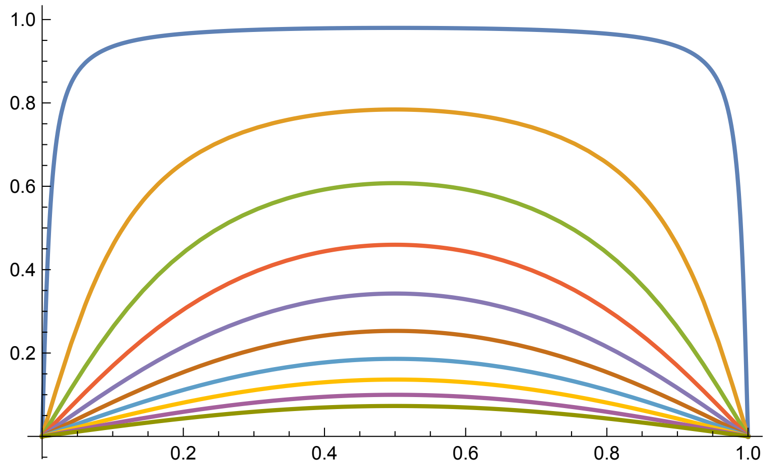
$$\Phi(x,y) \;=\; \frac{2V_0}{\pi}\,\arctan\left(\frac{\sin(\pi x/a)}{\sinh(\pi y/a)}\right), \tag{25}$$

but it's easier to understand the physical behavior of the potential (24) with a 3D plot:



(26)

And here are the cross-sectional profiles of $\Phi(x)$ at specific fixed y's, namely $(y/a)=0.01$, 0.11, 0.21, 0.31, 0.41, 0.51, 0.61, 0.71, 0.81, and 0.91:



(27)

As you can see, at small $y \ll a$ — near the front of the slot — the profile is almost constant like the $\Phi_b(x)$ except for the sharp bends down to zero at $x = 0$ and also at $x = a$. But as we go deeper into the slot — to larger y — we get lower and more rounded profiles with slower rises at the $x = 0$ and $x = a$ ends. And for larger y's — deeper and deeper into the slot — the profiles start looking just like the sine wave $\sin(\pi x/a)$ with smaller and smaller amplitudes.

The reason for this behavior becomes clear when we write the potential as the series (24): All the exponentials $\exp(-n\pi y/a)$ shrink with increasing y, but the exponentials with larger n shrink faster that the exponentials with smaller n. Consequently, for large y/a the leading $n = 1$ term completely dominates the potential, and we end up with

$$V \approx \frac{4V_0}{\pi} \times \exp(-\pi y/a) \times \sin(\pi x/a) \quad \text{for } y \gtrsim a, \tag{28}$$

a sine wave with a decreasing amplitude, exactly as we see on the plot (27).

A 3D Cartesian Coordinate Example

For a 3D example of the separation-of-variables method, consider a pipe with a rectangular $a\times b$ cross-section, but unlike a slot from the previous example, all 4 sides the pipe are conducting and grounded. On the other hand, the length of this pipe is infinite in only one direction, so in the obvious (x, y, z) coordinates, the interior of the pipe is limited to

$$0 < x < a, \quad 0 < y < b, \quad 0 < z < +\infty, \tag{29}$$

and the pipe has a rectangular opening at $z = 0$. Similar to the previous example, there are no electric charges inside the pipe but there unknown charges outside it and on the pipe's wall, and we are given the measured potential $\Phi_b(x, y, z = 0)$ across the pipe's opening; our task is to find the potential $\Phi(x, y, z)$ throughout the pipe's interior.

Mathematically, we are looking at the potential $\Phi(x, y, z)$ in the region (29) which obeys the following conditions:

[1] Φ obeys the 3D Laplace equation, $\triangle\Phi(x, y, z) = 0$;

[2] Φ vanishes on the 4 grounded walls of the pipe,

$$\Phi(x, y, z) \;=\; 0 \text{ when } x = 0, \text{ or } x = a, \text{ or } y = 0, \text{ or } y = b, \tag{30}$$

and deep inside the pipe, the potential asymptotes to zero, $\Phi(x, y, z) \to 0$ for $z \to +\infty$;

[3] at the pipe's opening $z = 0$ the potential matches the given boundary potential,

$$\Phi(x, y, z = 0) \;=\; \text{given } \Phi_b(x, y). \tag{31}$$

Using the separation-of-variables method, we start by looking at the potentials of the form

$$\Phi(x, y, z) \;=\; f(x) \times g(y) \times h(z) \tag{32}$$

which obeys the Laplace equation [1] and the homogeneous boundary conditions [2] — but don't worry about the inhomogeneous condition [3]. Eventually, we shall find an infinite series of such solutions, and then we shall look for a linear combination of these solutions that happens to obey the condition [3].

So let's start with the Laplace equation. In 3D,

$$\begin{aligned}\triangle\Phi\ &=\ \frac{\partial^2\Phi}{\partial x^2}\ +\ \frac{\partial^2\Phi}{\partial y^2}\ +\ \frac{\partial^2\Phi}{\partial z^2}\\ &\qquad\langle\!\langle\,\text{for }\Phi\text{ as in eq. (32)}\,\rangle\!\rangle\\ &=\ f''(x)\times g(y)\times h(z)\ +\ f(x)\times g''(y)\times h(z)\ +\ f(x)\times g(y)\times h''(z),\end{aligned}\tag{33}$$

hence

$$\frac{\triangle\Phi}{\Phi}\ =\ \frac{f''(x)}{f(x)}\ +\ \frac{g''(y)}{g(y)}\ +\ \frac{h''(z)}{h(z)}\,,\tag{34}$$

and we want this expression to vanish for all x, y, z. But the first term here depends only on the x coordinate, the second — only on the y, and the third — only on the z, so the only way they can add up to zero for all independent x, y, z is if each one of these terms is a constant. Thus,

$$\begin{aligned}\frac{f''(x)}{f(x)}\ &=\ C_1\ =\ \text{const},\\ \frac{g''(y)}{g(y)}\ &=\ C_2\ =\ \text{const},\\ \frac{h''(z)}{h(z)}\ &=\ C_3\ =\ \text{const},\\ \text{and}\quad C_1\ +\ C_2\ +\ C_3\ &=\ 0.\end{aligned}\tag{35}$$

Next, the homogeneous boundary conditions [2] for the potential translate to the boundary conditions of the f, g, and h functions as

$$\begin{aligned}f(x=0)\ &=\ f(x=a)\ =\ 0,\\ g(y=0)\ &=\ g(y=b)\ =\ 0,\\ h(z)\ &\to 0\text{ for }z\to+\infty.\end{aligned}\tag{36}$$

Altogether, the $f(x)$ function obeys

$$f''(x)\ -\ C_1\times f(x)\ =\ 0,\quad f(0)\ =\ f(a)\ =\ 0,\tag{37}$$

exactly as in the previous 2D examples, so it has the same solutions:

$$f(x)\ =\ \sin\frac{m\pi x}{a}\,,\quad C_1\ =\ -(m\pi/a)^2\ <\ 0,\tag{38}$$

for an integer $m = 1, 2, 3, \ldots$. Likewise, the $g(y)$ function obeys similar conditions

$$g''(y) \;-\; C_2 \times g(y) \;=\; 0, \quad g(0) \;=\; g(b) \;=\; 0, \tag{39}$$

so it also has similar solutions:

$$g(y) \;=\; \sin\frac{n\pi y}{b}\,, \quad C_2 \;=\; -(n\pi/b)^2, \tag{40}$$

for an integer $n = 1, 2, 3, \ldots$. Note: the two integers m and n in eqs. (38) and (40) are completely independent from each other.

Now let's pick any particular positive integers m and n. For any choice of these integers, we have

$$C_3 \;=\; -C_1 \;-\; C_2 \;=\; +(m\pi/a)^2 \;+\; (n\pi/b)^2 \;>\; 0, \tag{41}$$

so let's define

$$\kappa_{m,n} \;\stackrel{\text{def}}{=}\; +\sqrt{C_3} \;=\; +\sqrt{(m\pi/a)^2 \,+\, (n\pi/b)^2}\,. \tag{42}$$

In terms of this $\kappa_{m,n}$, the conditions for the $h(z)$ function become

$$h''(z) \;-\; \kappa_{m,n}^2 \times h(z) \;=\; 0, \quad h(z) \;\to\; 0 \text{ for } z \to +\infty, \tag{43}$$

with the only solution to these conditions being

$$h(z) \;=\; \exp\bigl(-\kappa_{m,n} \times z\bigr). \tag{44}$$

Altogether, we see that all the product solutions to the conditions [1] and [2] for the potential inside the pipe have form

$$\Phi(x,y,z) \;=\; \text{const} \times \sin\frac{m\pi x}{a} \times \sin\frac{n\pi y}{b} \times \exp(-\kappa_{m,n} z) \tag{45}$$

for positive integers m and n. Similar to the 2D example we got an infinite but discrete set of solutions, although in the present 3D case we got a double series labeled by two independent integers m and n rather than a single series. And since the conditions [1] and [2] are linear and homogeneous, any linear combination of the product solutions (45) is also a solution, so a general non-product solution has form

$$\Phi(x,y,z) \;=\; \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} A_{m,n}\times\sin\frac{m\pi x}{a}\times\sin\frac{n\pi y}{b}\times\exp(-\kappa_{m,n}z) \qquad (46)$$

for some constant coefficients $A_{m,n}$. Again, a theorem says that *any* solution to [1] and [2] has form (46) for some real coefficients $A_{m,n}$, but for brevity's sake let me skip the proof of this theorem.

In particular, the solution for the full problem — including the inhomogeneous boundary condition at the $z = 0$ opening of the pipe — must have the form (46) for some coefficients $A_{m,n}$, and the values of such coefficients follow from the given boundary potential $V_b(x, y)$ at $z = 0$. To find these coefficient, let's evaluate eq. (46) for $z = 0$: Since $\exp(-\kappa_{m,n}z) = 1$ for $z = 0$ regardless of the value of $\kappa_{m,n}$, we get

$$\Phi(x,y,z=0) \;=\; \sum_{m=1}^{\infty}\sum_{n=1}^{\infty} A_{m,n}\times\sin\frac{m\pi x}{a}\times\sin\frac{n\pi y}{b} \;=\text{should be}=\; \text{given } \Phi_b(x,y). \qquad (47)$$

The double sum in this formula looks like a double Fourier expansion of $\Phi_b(x, y)$ into sine waves of x and of y, so the coefficients $A_{m,n}$ obtain from the corresponding Fourier integrals as

$$A_{m,n} \;=\; \frac{4}{ab}\int_0^a dx\int_0^b dy\,\Phi_b(x,y)\times\sin\frac{m\pi x}{a}\times\sin\frac{n\pi y}{b}\,. \qquad (48)$$

Example:

Suppose the pipe has a square cross-section $a \times a$ (thus $b = a$), and the boundary potential at the pipe's opening is a double-sine wave

$$\Phi_b(x,y) \;=\; V_0\times\sin\frac{3\pi x}{a}\times\sin\frac{4\pi y}{a}\,. \qquad (49)$$

In this case, we do not need to perform the integrals (48) to find the Fourier coefficients $A_{m,n}$.

Instead, we simply compare eq. (49) to the Fourier series (47):

$$\sum_{m=1}^{\infty}\sum_{n=1}^{\infty} A_{m,n}\times\sin\frac{m\pi x}{a}\times\sin\frac{n\pi y}{b} \;=\; V_0\times\sin\frac{3\pi x}{a}\times\sin\frac{4\pi y}{a}\,, \tag{50}$$

which immediately tells us that

$$A_{3,4} \;=\; V_0 \quad \text{while all other } A_{m,n} \;=\; 0. \tag{51}$$

Consequently, the double sum (46) for the potential inside the pipe has only one non-zero term, thus

$$V(x,y,z) \;=\; V_0\times\sin\frac{3\pi x}{a}\times\sin\frac{4\pi y}{a}\times\exp(-\kappa_{3,4}z), \tag{52}$$

where

$$\kappa_{3,4} \;=\; \sqrt{(3\pi/a)^2\,+\,(4\pi/a)^2} \;=\; (\pi/a)\times\sqrt{3^2+4^2} \;=\; (\pi/a)\times 5. \tag{53}$$

Altogether,

$$V(x,y,z) \;=\; V_0\times\sin\frac{3\pi x}{a}\times\sin\frac{4\pi y}{a}\times\exp\left(\frac{-5\pi z}{a}\right). \tag{54}$$

Separation of Variables in Spherical Coordinates

Boundary problems in volumes $\mathcal{V}$ with spherical or conical boundaries are often solved using separation of variables in spherical coordinates (r,θ,ϕ). In these notes we shall stick to the spherical boundaries only, so $\mathcal{V}$ can be a spherical cavity, or the space outside of a sphere, or a shell between two concentric spheres.

Let's start with a spherical cavity of radius R; there are no electric charges inside the cavity but there are some unknown charges outside the cavity and on its walls; and we happen to know the potential at the cavity's spherical boundary $r=R$. Thus, we seek the potential $\Phi(r,\theta,\phi)$ such that

[1] $$\triangle\Phi \;=\; 0,$$

[2] $$\Phi(r=R,\theta,\phi) \;=\; \text{given } \Phi_b(\theta,\phi).$$

In addition, there are pseudo-boundary conditions for the potential as a function $\Phi(r,\theta,\phi)$ of the spherical coordinates:

$$\begin{aligned}
\Phi \text{ is periodic in } \phi: \quad \Phi(r,\theta,\phi+2\pi) &= \Phi(r,\theta,\phi),\\
\Phi \text{ is finite and regular at the sphere's poles at } \theta=0 \text{ and } \theta=\pi,\\
\Phi \text{ is finite and regular at the coordinate center } r=0.
\end{aligned} \tag{[3]}$$

In the separation of variables method, we start by looking at product potentials

$$\Phi(r,\theta,\phi) \;=\; f(r)\times\mathcal{Y}(\theta,\phi) \tag{55}$$

that obey the Laplace equation [1] and the pseudo-boundary conditions [3], but put the outer boundary condition [2] aside for a moment. In spherical coordinates, the Laplace operator acts as

$$\triangle\Phi(r,\theta,\phi) \;=\; \frac{\partial^2\Phi}{\partial r^2} \;+\; \frac{2}{r}\frac{\partial\Phi}{\partial r} \;-\; \frac{1}{r^2}\mathbf{L}^2\Phi \tag{56}$$

where

$$\mathbf{L}^2 \;=\; -\frac{\partial^2}{\partial\theta^2} \;-\; \frac{1}{\tan\theta}\frac{\partial}{\partial\theta} \;-\; \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi^2} \tag{57}$$

is a differential operator in the angular coordinates (θ,ϕ). Its name $\mathbf{L}^2$ stems from it being the vector square of the first-order operator $\mathbf{L}=-i\mathbf{x}\times\nabla$, which you should recognize from the quantum mechanics class: $\mathbf{L}$ — or rather $\hbar\mathbf{L}$ — is the orbital angular momentum operator in the coordinate basis.

Back to the Laplace operator (56), when acting on the product potential (55) it yields

$$\triangle\big(f(r)\mathcal{Y}(\theta,\phi)\big) \;=\; f''(r)\times\mathcal{Y}(\theta,\phi) \;+\; \frac{2f'(r)}{r}\times\mathcal{Y}(\theta,\phi) \;-\; \frac{f(r)}{r^2}\times\mathbf{L}^2\mathcal{Y}(\theta,\phi), \tag{58}$$

hence

$$\frac{r^2\,\triangle\Phi}{\Phi} \;=\; \frac{r^2 f''(r)+2rf'(r)}{f(r)} \;-\; \frac{\mathbf{L}^2\mathcal{Y}(\theta,\phi)}{\mathcal{Y}(\theta,\phi)}\,. \tag{59}$$

For a potential obeying the Laplace equation this expression should vanish for all r,θ,ϕ, but since the first term on the RHS depends only on the radius r while the second term depends only on the angular coordinates, both terms must be constants. Thus,

$$r^2 f''(r) \;+\; 2rf'(r) \;=\; C\times f(r), \tag{60}$$

$$\mathbf{L}^2\mathcal{Y}(\theta,\phi) \;=\; C\times\mathcal{Y}(\theta,\phi), \tag{61}$$

for the same constant C.

The angular equation (61) is the eigenvalue/eigenstate equation for the $\mathbf{L}^2$ operator. Specifically, it's the eigenvalue/eigenstate equation in the space of functions that are periodic in ϕ and regular at the poles $\theta = 0$ and $\theta = \pi$. In principle, we should solve this equation using one more factorization $\mathcal{Y}(\theta,\phi) = g(\theta)\times h(\phi)$, turning the PDE (61) into ODEs for $g(\theta)$ and $h(\phi)$, and applying the pseudo-boundary conditions. But in the interest of brevity, let me skip all this process and simply use what you (should) already know from the quantum mechanics class: The spectrum of the orbital angular momentum² operator $\mathbf{L}^2$ comprises

$$C \;=\; \ell(\ell+1) \quad \text{for integer } \ell = 0, 1, 2, 3, \ldots. \tag{62}$$

And for each such ℓ, there are $2\ell + 1$ independent eigenstates $Y_{\ell,m}(\theta,\phi)$ called the spherical harmonics labeled by integer m running from $-\ell$ to $+\ell$ by 1. Here are some important features of the spherical harmonics:

- The $Y_{\ell,m}$ have form $Y_{\ell,m}(\theta,\phi) = (\text{const})\times P_{\ell(m)}(\cos\theta)\times\exp(im\phi)$ where the $P_{\ell(m)}(x)$ are called the *associate Legendre polynomials*, even though some of them are not really polynomials. Instead, $P_{\ell(m)}(\cos\theta) = (\sin\theta)^{|m|}\times$ degree $(\ell - |m|)$ polynomial of $\cos\theta$.
- For $m \neq 0$ the spherical harmonics are complex; by convention, $Y^*_{\ell,m} = (-1)^m Y_{\ell,-m}$. Also, all the harmonics with $m \neq 0$ vanish at the poles $\theta = 0$ and $\theta = \pi$.
- The only harmonics which do not vanish at the poles are the $Y_{\ell,0}$. These harmonics are independent of ϕ and are proportional to the regular Legendre polynomials $P_\ell(\cos\theta)$, but have different normalization: $Y_{\ell,0}(\theta,\cancel{\phi}) = \sqrt{(2\ell+1)/4\pi}\times P_\ell(\cos\theta)$.
- The spherical harmonics are orthogonal to each other and normalized to 1. That is

$$\iint Y^*_{\ell,m}(\theta,\phi)\,Y_{\ell',m'}(\theta,\phi)\,d^2\Omega(\theta,\phi) \;=\; \delta_{\ell,\ell'}\delta_{m,m'}\,. \tag{63}$$

- Any smooth, single-valued function $g(\theta,\phi)$ can be decomposed into a series of spherical harmonics,

$$g(\theta,\phi)\;=\;\sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}C_{\ell,m}Y_{\ell,m}(\theta,\phi)\quad\text{for}\quad C_{\ell,m}\;=\;\iint g(\theta,\phi)\,Y^*_{\ell,m}(\theta,\phi)\,d^2\Omega(\theta,\phi). \tag{64}$$

- Let $F(r,\theta,\phi)=r^\ell\times Y_{\ell,m}(\theta,\phi)$. Then in Cartesian coordinates, $F(x,y,z)$ is a homogeneous polynomial in x,y,z of degree ℓ. Moreover, $F(x,y,z)$ obeys the Laplace equation $\triangle F=0$.

Now consider the radial equation (60) for $C=\ell(\ell+1)$:

$$r^2\times f''(r)\;+\;2r\times f'(r)\;-\;\ell(\ell+1)f(r)\;=\;0. \tag{65}$$

This differential equation is invariant under rescaling of the radius, $r\to\text{const}\times r$, so let's look for the solutions $f(r)$ that are eigenstates of this symmetry, namely

$$f(r)\;=\;r^\alpha \tag{66}$$

for a constant power α. For such radial profiles

$$r\times f'(r)\;=\;\alpha\times r^\alpha,\qquad r^2\times f''(r)\;=\;\alpha(\alpha-1)\times r^\alpha, \tag{67}$$

hence eq. (65) becomes

$$\alpha(\alpha-1)\times r^\alpha\;+\;2\alpha\times r^\alpha\;-\;\ell(\ell+1)\times r^\alpha\;=\;\Big(\alpha(\alpha+1)\;-\;\ell(\ell+1)\Big)\times r^\alpha\;=\;0, \tag{68}$$

which makes $f(r)=r^\alpha$ a solution provided

$$\alpha(\alpha+1)\;-\;\ell(\ell+1)\;=\;0\quad\Longleftrightarrow\quad\alpha\;=\;+\ell\quad\text{or}\quad\alpha\;=\;-(\ell+1). \tag{69}$$

This, we have two independent solutions — r^ℓ and $r^{-\ell-1}$ — of the linear second-order equation (65), so a general solution is a linear combination

$$f(r)\;=\;(\text{const }A)\times r^\ell\;+\;(\text{const }B)\times\frac{1}{r^{\ell+1}}\,. \tag{70}$$

Altogether, a general product solution of the Laplace equation in the spherical coordinates has form

$$\Phi(r,\theta,\phi) \;=\; \left(A\times r^\ell\,+\,\frac{B}{r^{\ell+1}}\right)\times Y_{\ell,m}(\theta,\phi) \tag{71}$$

for some integer ℓ and m. And since the Laplace equation [1] and the pseudo-boundary conditions [3] for the spherical coordinates are all linear, any linear combination of the product solutions (71) —

$$\Phi(r,\theta,\phi) \;=\; \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell}\left(A_{\ell,m}\times r^\ell\,+\,\frac{B_{\ell,m}}{r^{\ell+1}}\right)\times Y_{\ell,m}(\theta,\phi) \tag{72}$$

is also a solution. Moreover, *any* solution of [1] and [3] has form (72) for some constant coefficients $A_{\ell,m}$ and $B_{\ell,m}$, but again I am going to skip the proof of this theorem.

Spherical Cavity

The values of the coefficients $A_{\ell,m}$ and $B_{\ell,m}$ for the specific solution of the complete boundary problem follow from the given boundary potential $\Phi_b(\theta,\phi)$ at the spherical boundary or boundaries. Let's start with a particularly simple case of $\mathcal{V}$ being a spherical cavity of radius R. In this case, there is only one spherical boundary at $r=R$ but there is also a pseudo-boundary at the coordinate center $r=0$. Since there are no electric charges inside the cavity — and in particular no charges at the center — the potential $\Phi(r,\theta,\phi)$ must be finite and regular at $r=0$. In terms of eq. (72), this means

$$\textbf{all }B_{\ell,m} \;=\; 0 \tag{73}$$

and therefore

$$\Phi(r,\theta,\phi) \;=\; \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} A_{\ell,m}\times r^\ell\times Y_{\ell,m}(\theta,\phi), \tag{74}$$

where the remaining coefficients $A_{\ell,m}$ follow from the given boundary potential at $r=R$. Indeed,

$$\Phi(r=R,\theta,\phi) \;=\; \sum_{\ell,m} A_{\ell,m}\times R^\ell\times Y_{\ell,m}(\theta,\phi) \;=\; \text{should be} \;=\; \text{given }\Phi_b(\theta,\phi), \tag{75}$$

and since the spherical harmonics form a complete orthonormal basis for functions of the angular coordinates, we have

$$\Phi_b(\theta,\phi) \;=\; \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} C_{\ell,m}Y_{\ell,m}(\theta,\phi) \quad\text{for}\quad C_{\ell,m} \;=\; \iint \Phi_b(\theta,\phi)\times Y^*_{\ell,m}(\theta,\phi)\,d^2\Omega(\theta,\phi). \qquad (64)$$

Comparing the last two formulae, we immediately see that

$$A_{\ell,m}\times R^\ell \;=\; C_{\ell,m} \qquad (76)$$

and hence

$$A_{\ell,m} \;=\; \frac{C_{\ell,m}}{R^\ell} \;=\frac{1}{R^\ell}\iint \Phi_b(\theta,\phi)\times Y^*_{\ell,m}(\theta,\phi)\,d^2\Omega(\theta,\phi). \qquad (77)$$

In particular, if the boundary potential $\Phi_b(\theta,\phi)$ happens to be a polynomial function of $\sin\theta e^{+i\phi}$, $\sin\theta e^{-i\phi}$, and $\cos\theta$, then it's a linear combination of a finite number of spherical harmonics with coefficient obtaining by inspection without any integrals. In such a case there are only a finite number of non-zero $A_{\ell,m}$ coefficients, and the series (74) has only a finite number of terms. But for more general boundary potentials, the series (64) and hence (74) do have infinitely many non-zero terms, and to obtain their coefficients we do have to evaluate the integrals (77).

Space Outside a Sphere

For a different example, let $\mathcal{V}$ span the whole space outside a sphere of radius R, with a known boundary potential $\Phi(r=R,\theta,\phi)=\Phi_b(\theta,\phi)$ on that sphere's surface. Again we have only one spherical boundary here, but we must supplement it with an asymptotic condition for the potential at $r\to\infty$. The simplest asymptotic condition is zero potential at infinity,

$$\lim_{r\to\infty}\Phi(r,\theta,\phi) \;=\; 0 \quad \forall\theta,\phi, \qquad (78)$$

which immediately requires all the $A_{\ell,m}$ coefficients in the series (15) to vanish. Hence,

$$\Phi(r,\theta,\phi) \;=\; \sum_{\ell,m}\frac{B_{\ell,m}}{r^{\ell+1}}\times Y_{\ell,m}(\theta,\phi), \qquad (79)$$

where the remaining coefficients $B_{\ell,m}$ follow from the boundary potential on the sphere's surface:

$$\Phi(r=R,\theta,\phi) \;=\; \sum_{\ell,m}\frac{B_{\ell,m}}{R^{\ell+1}}\times Y_{\ell,m}(\theta,\phi) \;=\; \text{should be} \;=\; \text{given }\Phi_b(\theta,\phi). \tag{80}$$

To find these coefficients, we again expand the boundary potential into spherical harmonics

$$\Phi_b(\theta,\phi) \;=\; \sum_{\ell=0}^{\infty}\sum_{m=-\ell}^{+\ell} C_{\ell,m}Y_{\ell,m}(\theta,\phi) \quad\text{for}\quad C_{\ell,m} \;=\; \iint \Phi_b(\theta,\phi)\times Y^*_{\ell,m}(\theta,\phi)\,d^2\Omega(\theta,\phi), \tag{64}$$

and comparing the last two formulae we see that this time we need

$$B_{\ell,m} \;=\; R^{\ell+1}\times C_{\ell,m} \;=\; R^{\ell+1}\times\iint \Phi_b(\theta,\phi)\times Y^*_{\ell,m}(\theta,\phi)\,d^2\Omega(\theta,\phi). \tag{81}$$

But a different asymptotic condition at $r\to\infty$ may lead to a different solution with some of the $A_{\ell,m}\neq 0$ to make

$$\Phi(r,\theta,\phi) \;\xrightarrow[r\to\infty]{}\; \sum_{\ell,m} A_{\ell,m}r^{\ell}Y_{\ell,m}(\theta,\phi) \;=\; \text{should} \;=\; \text{given }\Phi_{\text{asymptotic}}(r,\theta,\phi). \tag{82}$$

For example, in problem 2(c) of the homework set#1, the asymptotic electric field is uniform $\mathbf{E}_0$. Assuming the direction of this asymptotic field is $+z$, this means

$$\Phi_{\text{asymptotic}}(x,y,z) \;=\; -E_0\times z, \tag{83}$$

or in spherical coordinates

$$\Phi_{\text{asymptotic}}(r,\theta,\phi) \;=\; -E_0\times r\times\cos\theta \;=\; -E_0\times r\times\sqrt{\frac{4\pi}{3}}Y_{1,0}(\theta,\phi). \tag{84}$$

Matching this asymptotics to eq. (82), we see that for this problem we need

$$A_{1,0} \;=\; -\sqrt{\frac{4\pi}{3}}\,E_0, \quad \text{while all other } A_{\ell,m} \;=\; 0. \tag{85}$$

As to the $B_{\ell,m}$ coefficients, they follow from the given boundary potential at $r=R$, but now you need to account $A_{1,0}\neq 0$ when calculating the $B_{\ell,m}$.

Spherical Shell

Finally consider a shell between two concentric spheres of radii $R_1 < R_2$. This time we don't have to worry about the limits $r \to 0$ or $r \to \infty$, but instead we have two boundary potentials

$$\Phi(r = R_1, \theta, \phi) \;=\; \Phi_{b1}(\theta, \phi) \quad \text{and} \quad \Phi(r = R_2, \theta, \phi) \;=\; \Phi_{b2}(\theta, \phi). \tag{86}$$

Let's expand both boundary potentials into spherical harmonics:

$$\begin{aligned} \Phi_{b1}(\theta, \phi) &= \sum_{\ell,m} C^{(1)}_{\ell,m} Y_{\ell,m}(\theta, \phi) \\ \text{for} \quad C^{(1)}_{\ell,m} &= \iint \Phi_{b1}(\theta, \phi) \times Y^*_{\ell,m}(\theta, \phi)\, d^2\Omega(\theta, \phi), \\ \Phi_{b2}(\theta, \phi) &= \sum_{\ell,m} C^{(2)}_{\ell,m} Y_{\ell,m}(\theta, \phi) \\ \text{for} \quad C^{(2)}_{\ell,m} &= \iint \Phi_{b2}(\theta, \phi) \times Y^*_{\ell,m}(\theta, \phi)\, d^2\Omega(\theta, \phi). \end{aligned} \tag{87}$$

Then matching these expansions to the expansion of the potential between the spheres

$$\Phi(r, \theta, \phi) \;=\; \sum_{\ell=0}^{\infty} \sum_{m=-\ell}^{+\ell} \left(A_{\ell,m} \times r^\ell \;+\; \frac{B_{\ell,m}}{r^{\ell+1}} \right) \times Y_{\ell,m}(\theta, \phi) \tag{72}$$

in the limiting cases of $r = R_1$ and $r = R_2$, we see that for each (ℓ, m) the coefficients $A_{\ell,m}$ and $B_{\ell,m}$ obtain from solving a couple of linear equations

$$\begin{cases} R_1^\ell \times A_{\ell,m} \;+\; \dfrac{1}{R_1^{\ell+1}} \times B_{\ell,m} \;=\; C^{(1)}_{\ell,m} \;=\; \displaystyle\iint \Phi_{b1}(\theta, \phi) \times Y^*_{\ell,m}(\theta, \phi)\, d^2\Omega(\theta, \phi), \\ R_2^\ell \times A_{\ell,m} \;+\; \dfrac{1}{R_2^{\ell+1}} \times B_{\ell,m} \;=\; C^{(2)}_{\ell,m} \;=\; \displaystyle\iint \Phi_{b2}(\theta, \phi) \times Y^*_{\ell,m}(\theta, \phi)\, d^2\Omega(\theta, \phi). \end{cases} \tag{88}$$