Separation of Variables

Lecture 1

Physics 342
Quantum Mechanics I

Monday, January 25th, 2010

There are three basic mathematical tools we need, and then we can begin working on the physical implications of Schrödinger's equation, which will take up the rest of the semester. So we start with a review of: Linear Algebra, Separation of Variables (SOV), and Probability. There will be no particular completeness to our discussions – at this stage, I want to emphasize those aspects of each of these that will prove useful. Pitfalls and caveats will be addressed as we encounter them in actual problems (where they won't show up, so won't be addressed).

Try as one might, it is difficult to relate these three areas, so we will take each one in turn, starting from the most familiar, and working to the least (that's a matter of taste, so apologies in advance for the wrong ordering – in anticipation of our section on probability: How many different orderings of these three subjects are there? On average, then, how many people disagree with the current one?).

We will begin with separation of variables, a simple technique that you have used recently – we will review the basic electrostatic interest in these solutions, and do a few examples of SOV applied to PDE's other than Laplace's equation ($\nabla^2 V = 0$).

1.1 Separation for the Laplace Problem

Separation of variables refers to a class of techniques for probing solutions to partial differential equations (PDEs) by turning them into ordinary differential equations (ODEs). We generally rely on some notion of uniqueness[1] for

[1] Uniqueness implying both a solution to the PDE and satisfaction of some boundary conditions.

our PDE – then the logic of SOV rests on the notion that finding a solution, even by this somewhat limited technique, suffices.

There are two basic flavors of SOV, additive and multiplicative – in either case, the style of argument is the same, so we'll start with the algebraically simpler version.

1.1.1 Additive Separation

We take the Laplace problem: Find $V(x, y)$ satisfying $\nabla^2 V = 0$ on some region, with some specified boundary conditions (for example, in E&M, we would have an implicit $V \longrightarrow 0$ at spatial infinity condition, and maybe some conducting boundaries where we set $V = 0$). Working in two dimensions (for simplicity), we start with a separation *ansatz* – additive, in this case:

$$V(x, y) = V_x(x) + V_y(y), \tag{1.1}$$

then running this through the Laplacian gives:

$$\frac{d^2 V_x}{dx^2} + \frac{d^2 V_y}{dy^2} = 0. \tag{1.2}$$

Now for the standard argument: $V_x''(x)$ depends only on x just as $V_y''(y)$ depends only on y – they cannot be equal unless each is equal to a constant. Suppose we set $V_x'' = \alpha$, then we must have $V_y'' = -\alpha$. The solution to these ODEs is:

$$V_x(x) = \frac{1}{2}\,\alpha\, x^2 + \beta\, x + \delta \qquad V_y(y) = -\frac{1}{2}\,\alpha\, y^2 + \gamma\, y + \rho. \tag{1.3}$$

for arbitrary constants $(\beta, \delta, \gamma, \rho)$, to be used in imposing the boundary condition(s). The solution, for any α, can be written as:

$$V(x, y) = \frac{1}{2}\,\alpha\,(x^2 - y^2) + \beta\, x + \gamma\, y + \kappa \tag{1.4}$$

As far as electrostatics goes, this solution does not match our usual notion of potential – it doesn't die at spatial infinity. That's not always a deal-breaker, but it is true that additive separation is of limited utility in E&M (it plays a much larger role in, for example, Hamilton-Jacobi theory). Nevertheless, the pattern of: ansatz, argument, solution is the same as for the more immediately useful, and algebraically involved multiplicative separation.

1.1.2 Multiplicative Separation

The difference here is in the starting ansatz – rather than additive single variable functions, we take the multiplicative combination:

$$V(x, y) = V_x(x)\, V_y(y), \tag{1.5}$$

then Laplace's equation becomes

$$\frac{d^2 V_x}{dx^2}\, V_y + V_x\, \frac{d^2 V_y}{dy^2} = 0, \tag{1.6}$$

and if we divide by $V(x, y)$ itself, we can write this in a form conducive to making the separation argument:

$$\frac{V_x''}{V_x} + \frac{V_y''}{V_y} = 0. \tag{1.7}$$

The first term depends only on x, the second only on y, so for a solution satisfying our functional assumptions, we must have both terms equal to a constant, call it α^2 (a convenient choice, as you will see in a moment) – for α complex. Then

$$\frac{V_x''}{V_x} = \alpha^2 = -\frac{V_y''}{V_y} \tag{1.8}$$

will certainly have $\nabla^2 V = 0$. The solutions here are familiar:

$$V_x = A\, e^{\alpha\, x} + B\, e^{-\alpha\, x} \qquad V_y = F\, e^{i\, \alpha\, y} + G\, e^{-i\, \alpha\, y}. \tag{1.9}$$

Now we see that for a generic complex number, both V_x and V_y will be combinations of growing and decaying exponentials, as well as oscillatory sines and cosines. For example, if α is real, V_x is growing and decaying, while V_y is pure sine and cosine. For $\alpha = i\, a$ with a real, the roles are reversed. In general, we use the boundary conditions to choose a convenient expression for α.

Example

Consider a pair of infinite, grounded conducting sheets separated a distance d with a conductor connecting the two sheets held at V_0 as shown in Figure 1.1. What is the potential in between the plates? We know that the potential satisfies Laplace's equation in the region between the plates (no charge in there), and the boundary conditions are clear:

$$V(x=0,y) = V(x=d,y) = 0 \qquad V(x,y=0) = V_0 \, \sin\left(\frac{2\,\pi\,x}{d}\right). \tag{1.10}$$

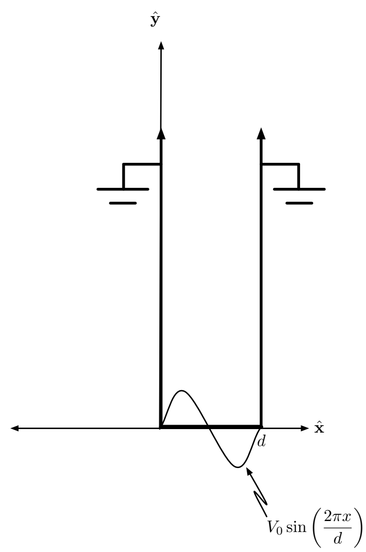


Figure 1.1: Two parallel plates separated by a distance d and held at $V=0$, the connecting plate is held at $V_0 \, \sin(2\,\pi\,x/d)$.

We know the solution will be of the form (1.9), but how to choose α and the constants (A,B,F,G)? There is an additional, implicit boundary condition – we'd like the potential to go to zero in the "open" spatial direction, $y \longrightarrow \infty$ – this tells us that we should set $\alpha = i\,a$ for $a \in \mathbb{R}$ to get growing and decaying exponentials for the $V_y(y)$ solution:

$$V_x = A\,e^{i\,a\,x} + B\,e^{-i\,a\,x} \qquad V_y = F\,e^{-a\,y} + G\,e^{a\,y} \tag{1.11}$$

and, furthermore, we should set $G=0$ to eliminate the growing exponential. By introducing $\tilde{A} = (A+B)$ and $\tilde{B} = i\,(A-B)$, we can write $V_x(x)$ in terms of sine and cosine. Our solution so far, then, is:

$$V_x = \tilde{A}\,\cos(a\,x) + \tilde{B}\,\sin(a\,x) \qquad V_y = F\,e^{-a\,y} \qquad V = V_x\,V_y. \tag{1.12}$$

Now for the rest of the boundary conditions: take $V_x(x=0) = 0$ – that tells us that $\tilde{A} = 0$. Our solution is now much simpler, the full potential has the

form
$$V = Q \sin(a\,x)\, e^{-a\,y} \tag{1.13}$$
where we have introduced yet another rewrite of combinations of constants ($Q = \tilde{A}\,F$). The boundary condition $V(x = d, y) = 0$ is interesting, this tells us that $\sin(a\,d) = 0$, not a statement about the obvious constant Q, but rather, a constraint on the allowed wavelengths:
$$\sin(a\,d) = 0 \longrightarrow a\,d = n\,\pi \tag{1.14}$$
for integer n. Then the only a's that satisfy the boundary condition are $a = \frac{n\,\pi}{d}$, still an infinite family, but labelled by the integer index n. So, we have
$$V_n(x, y) = Q_n \sin(n\,\pi\,x/d)\, e^{-n\,\pi\,y/d}, \tag{1.15}$$
and we put the subscript n here to remind us that any integer n provides a solution. This type of boundary condition, one that limits the allowed "wavelength", is what leads to the mathematical representation of quantization when applied to the separable solutions of Schrödinger's equation.

We have one boundary left – because Laplace's equation is a *linear* PDE, sums of solutions are still solutions, and we can make a general solution out of our n-indexed ones. Each term satisfies Laplace's equation and the boundary conditions at $x = 0, d$ and $y \longrightarrow \infty$, so the sum does as well:
$$V(x, y) = \sum_{n=1}^{\infty} Q_n \sin\left(\frac{n\,\pi\,x}{d}\right) e^{-\frac{n\,\pi\,y}{d}}. \tag{1.16}$$

As for the final boundary condition: $V(x, y = 0) = V_0 \sin(2\,\pi\,x/d)$, we can take $Q_n = 0$ for all n except for $n = 2$. We know that the solution is unique, so this is certainly valid. But it begs the question, what about a less well-adapted driving potential? That is a question for next time, as it is tied to the decomposition of functions in sin and cosine "bases", a linear algebra issue.

The final answer:
$$V(x, y) = V_0 \sin\left(\frac{2\,\pi\,x}{d}\right) e^{-\frac{2\,\pi\,y}{d}}. \tag{1.17}$$

This solution is just the potential at the $y = 0$ plate, decaying into the region between the plates – equal contours are shown in Figure 1.2.

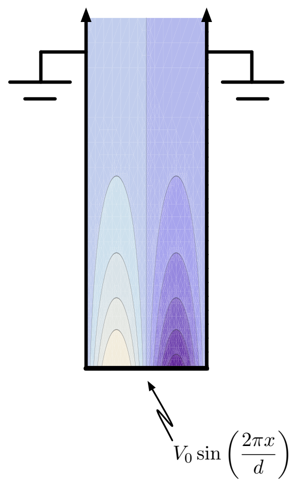


Figure 1.2: The potential between the plates for the setup shown in Figure 1.1.

There is not much more to say about separation of variables – the best approach is to do as many examples as you can get your hands on – that makes some of the choices that appear unmotivated at first (why should we make the integration constant α^2? Why do we pick the y solution to be growing and decaying?) more reasonable.

1.2 Separation for Other PDEs

We will be applying the SOV technique to Schrödinger's equation, and that is not going to be much different than the Laplacian example from E&M. The approach is independent of PDE, although the PDE must be linear (not strictly speaking true, but the superposition principle we invoked in writing (1.16) relied on linearity) – just to show some of the places where SOV comes up, we can look at the Helmholtz equation and the wave equation.

1.2.1 Helmholtz Equation

Suppose we consider the same problem as above, but for the Helmholtz PDE:

$$
\begin{gathered}
(\nabla^2 + \mu^2)\, V = 0 \\
V(x, y = 0, d) = 0 \quad V(x, y = 0) = V_0 \sin\left(\frac{2\,\pi\,x}{d}\right) \quad V(x, y \to \infty) \longrightarrow 0,
\end{gathered}
\tag{1.18}
$$

we are imagining a slight modification to electrostatics (actually amounts to a theory of electrostatics with a massive photon, but forget about that for now).

First we'll find the ODE solutions to the Helmholtz PDE via $V(x, y) = V_x(x)\, V_y(y)$:

$$
\frac{V_x''}{V_x} + \frac{V_y''}{V_y} + \mu^2 = 0. \tag{1.19}
$$

We see immediately that we will again get oscillatory and exponential solutions, since we want the solution in the increasing y direction to decay, we'll call $\frac{V_y''}{V_y} = \alpha^2$, with α real. With the constant μ^2 in place, we don't need to set the x term equal to $-\alpha^2$, we have additional freedom. We know that the boundary conditions for x are easily imposed for sines, so set $\frac{V_x''}{V_x} = -\beta^2$ for β real. Then the constraint we must impose to solve the Helmholtz PDE is: $-\beta^2 + \alpha^2 + \mu^2 = 0$. Imposing the boundary conditions at $x = 0, d$ gives back $\beta = \frac{n\,\pi}{d}$ as before, so that

$$
V_x = A\, \sin\left(\frac{n\,\pi\,x}{d}\right). \tag{1.20}
$$

Now, for the V_y equation, we are given μ, and we have $\beta^2 = n^2\,\pi^2/d^2$, so the growing and decaying exponentials have the form:

$$
V_y = F\, e^{\sqrt{n^2\,\pi^2/d^2 - \mu^2}\, y} + G\, e^{-\sqrt{n^2\,\pi^2/d^2 - \mu^2}\, y}. \tag{1.21}
$$

There are interesting elements to this solution, most notably, a cutoff in n for which V_y is actually oscillatory ($n < \frac{\mu\,d}{\pi}$) – ignoring that for the moment, if we assume the above terms for V_y are indeed growing and decaying for $n = 2$, we have the solution:

$$
V(x, y) = V_0 \sin\left(\frac{2\,\pi\,x}{d}\right)\, e^{-\sqrt{4\,\pi^2/d^2 - \mu^2}\, y}, \tag{1.22}
$$

which just has a different fundamental decay length when compared to the Laplace form for electrostatics.

1.2.2 The Wave Equation

Separation of variables is not limited to purely spatial problems – we can mix in time. For the wave equation in one spatial dimension (call it x), defined in a medium with fundamental speed v, we have

$$-\frac{1}{v^2}\frac{\partial^2 u(x,t)}{\partial t^2}+\frac{\partial^2 u(x,t)}{\partial x^2}=0. \tag{1.23}$$

Take a multiplicative ansatz: $u(x,t)=u_x(x)\,u_t(t)$, then by the now familiar procedure of inputting and dividing by u:

$$-\frac{u_t''}{v^2\,u_t}+\frac{u_x''}{u_x}=0 \tag{1.24}$$

and again, setting both terms equal to a constant:

$$-\frac{u_t''}{v^2\,u_t}=\alpha^2 \qquad \frac{u_x''}{u_x}=-\alpha^2. \tag{1.25}$$

What is interesting here is that both the spatial solution u_x and the temporal u_t can be oscillatory – that is not true for the Laplace equation separable solutions we saw above. Without worrying about boundary conditions, we have the easy solution:

$$u_t=A\,\cos(\alpha\,v\,t) \qquad u_x=B\,\cos(\alpha\,x) \tag{1.26}$$

so we can write $u(x,t)=u_0\,\cos(\alpha\,x)\cos(\alpha\,v\,t)$ – of course, just as obvious is the solution $\hat{u}(x,t)=u_0\,\sin(\alpha\,x)\,\sin(\alpha\,v\,t)$. Since the wave equation is linear, the sum of these two solutions is also a solution, and it is an instructive one:

$$\begin{aligned} u(x,t)+\hat{u}(x,t) &= u_0\,(\cos(\alpha\,x)\,\cos(\alpha\,v\,t)+u_0\,\sin(\alpha\,x)\,\sin(\alpha\,v\,t)) \\ &= u_0\,\cos(\alpha\,(x-v\,t)), \end{aligned} \tag{1.27}$$

precisely a plane wave. Of course, in general, we would be given spatial boundary conditions and/or an initial waveform at $t=0$.

1.2.3 Poisson's Equation

The utility of separation is not limited to source-free equations – consider Poisson's equation for electrostatic potential in the presence of source charge density ρ:

$$\nabla^2\,V=-\frac{\rho}{\epsilon_0}. \tag{1.28}$$

We must be given a ρ that is itself appropriately separable. The simplest possible such distribution would be a constant, but we can imagine more interesting charge distributions. As an example, suppose we are in spherical coordinates, and we have a spherically symmetric charge density: $\rho(r, \theta, \phi) = \rho(r)$, depending only on our distance from the origin. Poisson's equation becomes, in these variables

$$\left(\frac{1}{r^2} \frac{\partial}{\partial r} \left(r^2 \frac{\partial V}{\partial r} \right) + \frac{1}{r^2 \sin\theta} \frac{\partial}{\partial \theta} \left(\sin\theta \frac{\partial V}{\partial \theta} \right) + \frac{1}{r^2 \sin^2\theta} \frac{\partial^2 V}{\partial \phi^2} \right) V = -\frac{\rho(r)}{\epsilon_0}. \tag{1.29}$$

The separation ansatz now becomes $V(r, \theta, \phi) = V_r(r)\, V_\theta(\theta)\, V_\phi(\phi)$, and we can see what will happen – to satisfy the functional dependence assumption, we will have constant V_θ and V_ϕ, leaving us with just the radial ODE:

$$\frac{1}{r^2} \frac{d}{dr} \left(r^2 V_r' \right) = -\frac{\rho(r)}{\epsilon_0}. \tag{1.30}$$

Suppose we take $\rho(r) = \rho_0$ a constant, then the solution to the above is:

$$V_r(r) = \alpha + \frac{\beta}{r} - \frac{\rho_0\, r^2}{6\, \epsilon_0}. \tag{1.31}$$

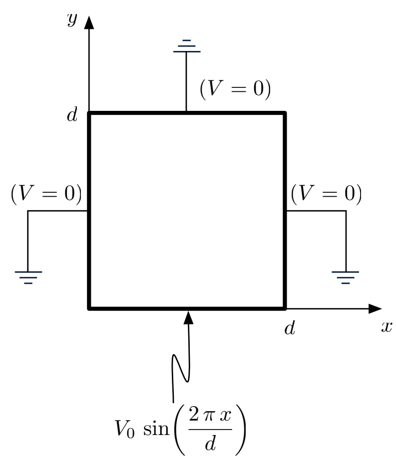
Notice that the first two terms are just solutions to $\nabla^2 V = 0$ (an overall constant and the potential outside a spherically symmetric distribution of charge) – if we are inside a uniformly charged sphere, with $r = 0$ included in the domain, then we must set $\beta = 0$. The constant α, of course, can be set to zero, and we are left with the usual potential for a uniformly charged sphere.

Homework

Reading: Griffiths "Introduction to Electrodynamics", pp. 127–136.

Problem 1.1

Solve Laplace's equation $\nabla^2 V = 0$ using separation: $V(x, y) = V_x(x)\, V_y(y)$ for the following two-dimensional boundary conditions: $V(0, y) = V(d, y) = 0$, $V(x, d) = 0$ and $V(x, 0) = V_0 \sin\left(\frac{2\pi x}{d}\right)$.



Physically, we are describing the electrostatic potential inside a square that has grounded lines on three sides, and a spatially-varying potential on the fourth side.

Problem 1.2

The heat equation in one (spatial) dimension reads

$$\frac{1}{k} \frac{\partial u(x, t)}{\partial t} = \frac{\partial^2 u(x, t)}{\partial x^2}, \tag{1.32}$$

where $u(x, t)$ is the temperature of an object with "thermal conductivity" k (a material property). For a complete solution, we must specify two boundary conditions (since this equation is second order in x) and an "initial" condition (the value of $u(x, t = 0)$, for example).

a. Using separation of variables: $u(x,t) = u_x(x)\, u_t(t)$, and separation constant $-\alpha^2$, write down the separated heat equation and solve for u_x and u_t.

b. Suppose we have a material that goes from $x = 0$ to $x = d$ – we set the temperature on both ends of the material to zero – i.e. $u(0,t) = u(d,t) = 0$. Initially, at time $t = 0$, we have temperature: $u(x,0) = u_0 \sin\left(\frac{\pi x}{d}\right)$. Using your separation solution, find the particular solution for this set of boundary and initial conditions.