13 SEPARATION OF VARIABLES

"Separation of variables" is a procedure which can turn a partial differential equation into a set of ordinary differential equations. The procedure only works in very special cases involving a high degree of symmetry. Remarkably, the procedure works for many important physics examples. Here, we will use the procedure on the Schrödinger equation in a central potential. Because there are several dimensions, the procedure requires a number of rounds, each consisting of the same set of six steps. In the first round, we will separate out an ordinary differential equation in the time variable.

Step 1: Write the partial differential equation in appropriate coordinate system. For Schrödinger's equation in any potential we have:

$$H_{\mathrm{op}}\Psi = i\hbar \frac{\partial \Psi}{\partial t} \tag{82}$$

Step 2: Assume that the solution Ψ can be written as the product of functions, at least one of which depends on only one variable, in this case t. The other function(s) must not depend at all on this variable, i.e. assume

$$\Psi(r, \theta, \phi, t) = \psi(r, \theta, \phi) T(t) \tag{83}$$

This is a very strong assumption. Not all solutions will be of this form. However, it turns out that all of the solutions can be written as linear combinations of solutions of this form. The study of when and why this works is called Sturm-Liouville theory.

Plug this assumed solution (83) into the partial differential equation (82). Because of the special form for Ψ, the partial derivatives each act on only one of the factors in Ψ.

$$(H_{\mathrm{op}}\psi)\, T = i\hbar\psi\, \frac{dT}{dt} \tag{84}$$

Any partial derivatives that act only on a function of a single variable may be rewritten as total derivatives.

Step 3: Divide by Ψ in the form of (83). Many, many students forget this step. Don't be one of them! The rest of the procedure doesn't work if you do.

$$\frac{1}{\psi}\,(H_{\mathrm{op}}\psi) = i\hbar \frac{dT}{dt}\frac{1}{T} \tag{85}$$

Step 4: Isolate **all** of the dependence on one coordinate on one side of the equation. Do as much algebra as you need to do to achieve this. In our example, notice that in (85), all of the t dependence is on the right-hand side of the equation while all of the dependence on the spatial variable is on the other side. In this case, the t dependence is already isolated, without any algebra on our part.

Step 5: Now imagine changing the isolated variable t by a small amount. In principle, the right-hand side of (85) could change, but nothing on the left-hand side would. (This argument is the magic of the separation of variables procedure–compare it to arguments about constants of the motion from classical mechanics.) Therefore, if the equation is to be true for all values of t, the particular combination of t dependence on the right-hand side must be constant. By convention, we call this constant E.

$$\frac{1}{\psi}\left(H_{\text{op}}\psi\right) = i\hbar\frac{dT}{dt}\frac{1}{T} \stackrel{\text{def}}{=} E \tag{86}$$

In this way we have broken our original partial differential equation up into a pair of equations, one of which is an ordinary differential equation involving only t, the other is a partial differential equation involving only the three spatial variables.

$$\frac{1}{\psi}H_{\text{op}}\psi = E \tag{87}$$

$$i\hbar\frac{dT}{dt}\frac{1}{T} = E \tag{88}$$

The separation constant E appears in both equations.

Step 6: Write each equation in standard form by multiplying each equation by its unknown function to clear it from the denominator.

$$H_{\text{op}}\psi = E\psi \tag{89}$$

$$\frac{dT}{dt} = -\tfrac{i}{\hbar}\,ET \tag{90}$$

Notice that (89) is an eigenvalue equation for the operator H_{op}. You may never have thought of the derivation of this "time independent version of the Schrödinger equation" from the Schrödinger equation as just a simple example of the separation of variables procedure. At the moment, the eigenvalue E could be anything. Much of the rest of the Paradigm will be directed toward finding the possible values of E!

Now we must repeat the steps until each of the variables has been separated out into its own ordinary differential equation. In the next round, we will isolate the r dependence.

Step 1: Since we want to isolate the r dependence, we must rewrite H_{op} to show the r dependence explicitly using (81)

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) - \frac{1}{\hbar^2 r^2}\,L^2_{\text{op}}\right]\psi + U(r)\psi = E\psi \tag{91}$$

Step 2: Assume $\psi(r,\theta,\phi) = R(r)Y(\theta,\phi)$.

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)Y - \frac{1}{\hbar^2 r^2}\,R(L^2_{\text{op}}Y)\right] + U(r)RY = ERY \tag{92}$$

Step 3:

$$-\frac{\hbar^2}{2\mu}\left[\frac{1}{r^2}\frac{d}{dr}\frac{1}{R}\left(r^2\frac{dR}{dr}\right)-\frac{1}{\hbar^2 r^2}\frac{1}{Y}(L_{\rm op}^2 Y)\right]+U(r)=E \tag{93}$$

Step 4: To isolate the r dependence we must first clear the r dependence from the angular term (involving angular derivatives in $L_{\rm op}$ and angular functions in Y). To do this, we need to multiply (93) by r^2 to clear this factor out of the denominators of the angular pieces. Further rearranging (93) to get all of the r dependence on the right-hand side, we obtain:

$$-\frac{1}{\hbar^2}\frac{1}{Y}(L_{\rm op}^2 Y)=-\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\frac{1}{R}-\frac{2\mu}{\hbar^2}(E-U(r))r^2 \tag{94}$$

Step 5: In this case, I have called the separation constant A.

$$-\frac{1}{\hbar^2}\frac{1}{Y}(L_{\rm op}^2 Y)=-\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)\frac{1}{R}-\frac{2\mu}{\hbar^2}(E-U(r))r^2\stackrel{\rm def}{=}A \tag{95}$$

In principle, A can be any complex number.

Step 6: Rearranging (95) slightly, we obtain the radial and angular equations in the more standard form:

$$\frac{d}{dr}\left(r^2\frac{dR}{dr}\right)+\frac{2\mu}{\hbar^2}(E-U(r))r^2\,R+AR=0 \tag{96}$$

$$L_{\rm op}^2 Y+\hbar^2 AY=0 \tag{97}$$

Notice that the only place that the central potential enters the set of differential equations is in the radial equation (96). (96) is not yet in the form of an eigenvalue equation since it contains two unknown constants E and A. (97) is an eigenvalue equation for the operator $L_{\rm op}^2$ with eigenvalue $\hbar^2 A$; it is independent of the form of the central potential.

In the last round, we must separate the θ dependence from the ϕ dependence. I will leave this as an important Practice Problem. The answer is:

$$\sin\theta\frac{d}{d\theta}\left(\sin\theta\frac{dP}{d\theta}\right)-A\sin^2\theta P-BP=0 \tag{98}$$

$$\frac{d^2\Phi}{d\phi^2}+B\Phi=0 \tag{99}$$

(99) is an eigenvalue equation for the operator $d^2/d\phi^2$ with eigenvalue B. (98) is not yet in the form of an eigenvalue equation since it contains two unknown constants A and B.

We started with a partial differential equation in four variables and we ended up with four ordinary differential equations (90), (96), (98), (99) by introducing **three** separation constants (E, A, and B). You should always get one fewer separation constant than the number of variables you started with; each separation constant should appear in two of the final set of equations.

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