# Lecture 26: Separation of Variables and Solutions to Common ODEs

Reading:
Kreyszig Sections: 5.3, 5.5, 5.6 (pages177–180, 189–197, 198–202)

## Special Functions: Solutions to Common ODEs

Most calculators have a button that evaluates the eigensolution to the simple first-order ODE $dy/dt = \lambda y$. Also, most calculators have buttons that evaluate the eigensolutions to the simple second-order ODE: $d^2y/dt^2 = \lambda y$.

Of course, these are also just the exponential and trigonometric functions.

However, there are many more simple differential equations that follow from physical models and these also have known solutions that are not simple combinations of sines, cosines, and exponentials. The solutions to these differential equations are called *special functions.* MATHEMATICA® has an extensive list of special functions and these are collected in its help browser.

For example, the positions of a vibrating drum head are modeled with in cylindrical coordinates by Bessel's equation:

$$\begin{aligned} r^2\frac{d^2h}{dr^2} + r\frac{dh}{dr} + (k^2r^2 - m^2)h = 0 \\ \rho^2\frac{d^2h}{d\rho^2} + \rho\frac{dh}{d\rho} + (\rho^2 - m^2)h = 0 \end{aligned} \tag{26-1}$$

where in the second equation $\rho = kr$. The displacement of the drum is $h(r)$; $k$ is related to an inverse wavelength (e.g., the wavelength would be the radius of the drum divided by the number of maxima in the drum head shape) and $m$ is the mode (e.g., the number of maxima traversing the drum by $2\pi$ in a circular direction).

There two solutions to Bessel's equation and the general solution is the sum the two:

$$\begin{aligned} h(r) = C_1J_m(kr) + C_2Y_m(kr) \\ h(\rho) = C_1J_m(\rho) + C_2Y_m(\rho) \end{aligned} \tag{26-2}$$

where $J_m(x)$ is called (naturally enough) an *order-m Bessel function of the first kind* and $Y_m(x)$ is called (naturally enough) an *order-m Bessel function of the second kind.* These are analogous to the sines and cosines, but for a different ODE.

Another equation that appears in models of the angular deformations of body in a central force potentials (for example, the ion distribution about a fixed charge; or, the Schrödinger equation for the electron in a hydrogen atom) in spherical coordinates is Legendre's equation:

$$\begin{aligned} \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Xi}{d\theta}\right) + \left[\ell(\ell+1) - \frac{m^2}{\sin^2\theta}\right]\Xi = 0 \\ \frac{d}{d\mu}\left[(1-\mu^2)\frac{d\Xi}{d\theta}\right] + \left[\ell(\ell+1) - \frac{m^2}{1-\mu^2}\right]\Xi = 0 \end{aligned} \tag{26-3}$$

where $\mu \equiv \cos\theta$ so that $-1 \le \mu \le 1$. The value $\ell$ is related to the number of modes in the $\theta$ direction and $m$ is related to the number of modes in the $\phi$ direction.

Legendre's equation has two solutions:

$$\Xi(\mu) = C_1 P_{lm}(\mu) + C_2 Q_{lm}(\mu) \tag{26-4}$$

The eigensolution $P_{lm}(\mu)$ is called (again, naturally enough) *order m Legendre functions of the first kind* and $Q_{lm}(\mu)$ are called *order lm Legendre functions of the second kind.*

There are many other types of special functions.

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## Lecture 26 MATHEMATICA® Example 1

Visualizing special functions.

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The ODEs that produce Bessel, Legendre, LaGuerre, and Hypogeometric functions are solved and these special functions are visualized.

**1:** This is *Bessel's equation* for $y(x)$.

**3:** *MyPlotStyle* is a function to set `PlotStyle` for a given number of curves so that their colors are spread over `Hue` from red (0) to blue (0.66).

**4:** This will produce at plot of the zeroeth Bessel's function of the first kind ( `BesselJ`) and zeroeth Bessel's function of the second kind ( `BesselY`)/ solutions.

**6:** This is two-parameter form of *Ledendre's equation* for $y(x)$.

**8:** This is another form of Ledendre's equation for $y(x)$.

**14:** This will produce solutions to *Laguerres's equation* for $y(x)$.

```
Bessel's equation
1  BesselODE = x^2 y''[x] + x y'[x] + (x^2 - ν^2) y[x] == 0
2  DSolve[BesselODE, y[x], x]
3  MyPlotStyle[HowMany_Integer] :=
     Table[{Hue[0.66 * i / HowMany], Thickness[0.01]},
       {i, 0, HowMany}]
4  Plot[{BesselJ[0, x], BesselY[0, x]},
     {x, 0, 20}, PlotStyle → MyPlotStyle[2]]
5  Plot[{BesselJ[1 / 2, x], BesselY[1 / 2, x]},
     {x, 0, 20}, PlotStyle → MyPlotStyle[2]]
Legendre's equation
6  LegendreODE = (1 - x^2) y''[x] - 2 x y'[x] + (n (n + 1)) y[x] == 0
7  DSolve[LegendreODE, y[x], x]
8  AnotherFormLegendreODE =
     (1 - x^2) y''[x] - 2 x y'[x] + (n (n + 1) - m^2 / (1 - x^2)) y[x] == 0
9  DSolve[AnotherFormLegendreODE, y[x], x]
10 Plot[{LegendreP[0, x], LegendreQ[0, x]},
     {x, -1, 1}, PlotStyle → MyPlotStyle[2]]
11 Plot[{LegendreP[1, x], LegendreQ[1, x]},
     {x, -1, 1}, PlotStyle → MyPlotStyle[2]]
12 Plot[Evaluate[Table[LegendreP[i, x], {i, 0, 10}]],
     {x, -1, 1}, PlotStyle → MyPlotStyle[11]]
13 Plot[Evaluate[Table[LegendreQ[i, x], {i, 0, 10}]],
     {x, -1, 1}, PlotStyle → MyPlotStyle[11]]
Hypergeometric and Laguerre special functions
14 DSolve[x y''[x] + (q + 1 - x) y'[x] + p y[x] == 0, y[x], x]
15 Plot[LaguerreL[4, 1, x], {x, -5, 15}]
```

## Partial Differential Equations: Separation of Variables

Many *ordinary* differential equations that arise in practice derive from methods to solve *partial differential equations.*

In other words, the solution to the partial differential equation involving $c(x, y, z, t)$ and its partial derivatives with respect to $x$, $y$, $z$, and $t$ can sometimes be reduced to the solution of several ordinary differential equations.

In practice, most of the partial differential equations that can be solved analytically are solved by the *method of separation of variables.* Separation of variables works by isolating one of the variables

onto one side of equality—it is best described by simple example and here the one-dimensional wave-equation is a prototype. The wave-equation (e.g., the time ($t$)-dependent propagation of a scalar quantity ($h$) such as height, density, charge, etc. in a single direction $x$ is:

$$\frac{\partial^2 h(x,t)}{\partial t^2} = v^2 \frac{\partial^2 h(x,t)}{\partial x^2} \tag{26-5}$$

where $v$ is the phase-velocity $v = \omega/k$, $\omega$ is the angular frequency describing how rapidly the phase of the wave changes as it moves past a fixed position and $k = 2\pi/\lambda$ is the wave-number.

Consider a specific case in which waves are propogating in a guitar string of length $L$—this will give Dirichlet boundary conditions at the guitar's nut and saddle:

$$h(x=0,t) = 0 \qquad \text{and} \qquad h(x=L,t) = 0 \tag{26-6}$$

(two boundary conditions—one for each spatial derivative). The shape of plucked string gives the *initial condition*; for example, this could be modeled with a triangular shape:

$$h(x,t=0) = \begin{cases} Ax/\ell & 0 < x < \ell \\ A\frac{L-x}{L-\ell} & \ell < x < L \end{cases} \tag{26-7}$$

where the string is plucked at a position $x = \ell$ with a displacement $A$ at time $t = 0$.

The separation of variables method begins with the assumption that *the function can be factored into independent functions of the dependent variables.* For Eq. 26-5, this assumption is written as:

$$h(x,t) = \chi(x)\tau(t) \tag{26-8}$$

If this is inserted into Eq. 26-5, and both sides are divided by $v^2\chi(x)\tau(t)$ then

$$\frac{1}{v^2\tau(t)}\frac{d^2\tau(t)}{dt^2} = \frac{1}{\chi(x)}\frac{d^2\chi(x)}{dx^2} \tag{26-9}$$

Note that both sides of Eq. 26-9 depend on different variables and observe Fig. 26-28.

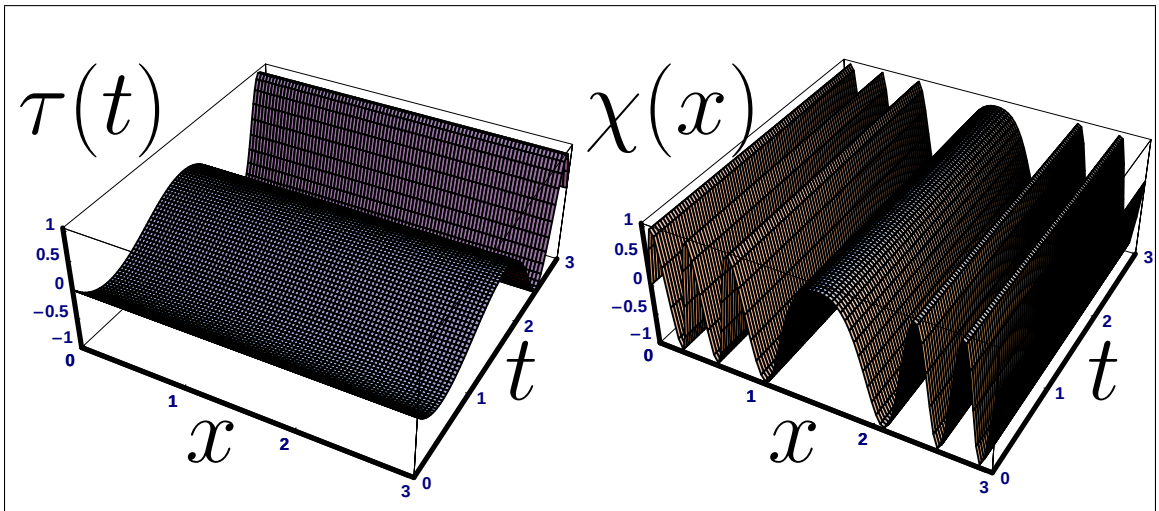


Figure 26-28: If two functions, $T(t)$ and $X(x)$, depend on different variables and are equal, then they can only be constant $\chi(x) = \tau(t) = \lambda$

Thus, both sides of Eq. 26-9 can be set equal to a *separation constant* $\lambda$:

$$\frac{1}{\chi(x)}\frac{d^2\chi}{dx^2} = \lambda \qquad \text{or} \qquad \frac{d^2\chi}{dx^2} - \lambda\chi = 0 \tag{26-10}$$

and

$$\frac{1}{v^2\tau(t)}\frac{d^2\tau}{dt^2} = \lambda \qquad \text{or} \qquad \frac{d^2\tau}{dt^2} - \lambda v^2\tau = 0 \tag{26-11}$$

For Eq. 26-10, the boundary conditions (Eq. 26-6) can also be written in terms of $\chi(x)$:

$$\chi(x=0) = 0 \qquad \text{and} \qquad \chi(x=L) = 0 \tag{26-12}$$

As advertised, ODEs are generated (Eqs. 26-10 and 26-11) in the process of solving the PDE 26-5. As only Eq. 26-10 has a boundary condition, it is solved first; in general its solution appears as:

$$\chi(x) = \begin{cases} A_+ \exp(\sqrt{\lambda}x) + B_+ \exp(-\sqrt{\lambda}x) \text{ 0.25in} & \text{if} \lambda > 0 \\ A_0 x + B_0 & \text{if} \lambda = 0 \\ A_- \cos(\sqrt{-\lambda}x) + B_- \sin(\sqrt{-\lambda}x) \text{ 0.25in} & \text{if} \lambda < 0 \end{cases} \tag{26-13}$$

The boundary conditions 26-12 place an initial restriction on the separation constant $\lambda > 0$ and specify that $\chi(x)$ must be a sum of sines and cosines. Furthermore, trying to solve Eqs. 26-12 at $x = 0$ shows that $A_- = 0$; at $x = L$, solutions must coincide with any of the *zeroes of the eigenfunction* $\sin(kx) = \sin(\sqrt{-\lambda}x)$, or

$$\lambda_n = \frac{-n^2\pi^2}{L^2} = -k_n^2 \quad n = 1, 2, 3, \ldots \tag{26-14}$$

The $\lambda_n$ (or equivalently the $k_n$) become *eigenvalues* of the ODE and generate an infinity of eigenfunctions with independent amplitudes $A_n$: $\chi_n(x) = A_n \sin(n\pi x/L)$.

This infinity of eigenfunctions are needed to satisfy the initial conditions Eqs. 26-7, but first the solution to the second ODE 26-11 must be obtained for the *the restriced set of eigenvalues* for the separation constant:

$$\frac{d^2\tau}{dt^2} + \frac{n^2\pi^2}{L^2}v^2\tau = 0 \tag{26-15}$$

so that, in general,

$$\tau_n(t) = \mathcal{E}_n^\star \cos(\frac{n\pi vt}{L}) + \mathcal{O}_n^\star \sin(\frac{n\pi vt}{L}) \tag{26-16}$$

and therefore with Eq. 26-8, the superposition of all solutions is

$$\begin{aligned} h(x,t) &= \sum_{n=1}^{\infty} \tau_n(t)\chi_n(x) \\ &= \sum_{n=1}^{\infty} \left( \mathcal{E}_n \cos\frac{n\pi vt}{L} + \mathcal{O}_n \sin\frac{n\pi vt}{L} \right) \sin\frac{n\pi x}{L} \end{aligned} \tag{26-17}$$

And the initial conditions become

$$h(x,0) = \sum_{n=1}^{\infty} \tau_n(0)\chi_n(x) = \sum_{n=1}^{\infty} \mathcal{E}_n \sin\frac{n\pi x}{L} \tag{26-18}$$

(the sine (odd) coefficients are not needed in this case) and determination of the coefficients is reduced to the Fourier representation. For the initial conditions in Eq. 26-7, these can be computed using Eq. **??**:

$$\mathcal{E}_n = \frac{AL^2 \sin\frac{2\pi n\ell}{L}}{(2\pi n)^2 \ell(L-\ell)} \tag{26-19}$$

giving a solution:

$$h(x,t) = \sum_{n=1}^{\infty} \frac{AL^2 \sin\frac{2\pi n\ell}{L}}{(2\pi n)^2 \ell(L-\ell)} \cos\frac{n\pi vt}{L} \sin\frac{n\pi x}{L} \tag{26-20}$$

The Shrödinger equation for a central potential serves as a more involved example for the method of separation of variables and is provided in the following section.

## Special Functions in the Eigenfunctions of the Hydrogen Atom

The time-independent Shrödinger for the electron in a hydrogen atom is a partial differential equation involving three spatial variables. If the mass of the nucleus can be considered very large compared to that of an electron, then it is reasonable to fix the center of a spherical $1/r$–potential at the origin and use spherical coordinates $(r,\theta,\phi)$ to express the Shrödinger equation:[18]

$$\begin{aligned} \frac{\hbar^2}{2m_e}\nabla^2\psi + V\psi &= E\psi \\ \frac{\hbar^2}{2m_e}\left[\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right)+\frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial}{\partial\theta}\right)+\frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\phi^2}\right]\psi - \frac{Ze^2\psi}{\epsilon_o r} &= E\psi \end{aligned} \tag{26-21}$$

Here, $\phi$ wraps around like longitude and $\phi$ goes north and south from the equator ($\theta$=0) like latitude.

Because the potential depends only on $r$, the initial separation is between the radial and angular parts,

$$\psi(r,\theta,\phi) = \rho(r)Y(\theta,\phi) \tag{26-22}$$

which separates Eq. 26-21 into

$$\begin{aligned} &\frac{1}{\rho}\frac{d}{dr}\left(r^2\frac{d\rho}{dr}\right)+\frac{2m_e r^2}{\hbar^2}\left(E+\frac{Ze^2}{\epsilon_o r}\right) \\ &\quad =\frac{1}{Y}\left[\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}\right] \end{aligned} \tag{26-23}$$

Therefore, the two sides must be equal to a separation constant $\lambda$. The radial part becomes

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\rho}{dr}\right)+\left[\frac{2m_e}{\hbar^2}\left(E-\frac{Ze^2}{\epsilon_o r}\right)-\frac{\lambda}{r^2}\right]\rho = 0 \tag{26-24}$$

and the angular part becomes

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial Y}{\partial\theta}\right)+\frac{1}{\sin^2\theta}\frac{\partial^2 Y}{\partial\phi^2}+\lambda Y = 0 \tag{26-25}$$

Solutions to Eq. 26-25 are related to the *spherical harmonics* and can be derived through another separation of variables. Putting

$$Y(\theta,\phi) = \Theta(\theta)\Phi(\phi) \tag{26-26}$$

into Eq. 26-25 gives

$$\frac{1}{\Phi}\frac{d^2\Phi}{d\phi^2} = -m^2 = \frac{-\sin\theta}{\Theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)-\lambda\sin^2\theta \tag{26-27}$$

where the separation constant, $-m^2$, is explicitly set to a negative quantity reflecting that $\Phi$ must have periodic solutions, i.e., the two separated ODEs are:

$$\begin{aligned} 0 &= \frac{d^2\Phi}{d\phi^2}+m^2\Phi \\ 0 &= \frac{1}{\sin\theta}\frac{d}{d\theta}\left(\sin\theta\frac{d\Theta}{d\theta}\right)\left(\lambda-\frac{m^2}{\sin^2\theta}\right)\Theta \end{aligned} \tag{26-28}$$

The first of these has the same form as Eq. 26-10 (solutions given by Eq. 26-13) but here the solutions will be written as

$$\Phi(\phi) = A_+ e^{\imath m\phi}+A_- e^{-\imath m\phi} \tag{26-29}$$

[18] To treat the hydrogen atom more accurately, the reduced mass $\tilde{m} = 1/(1/m+1/M)$, weighted coordinates $\tilde{x} = (mx_m+Mx_M)/M$ etc., and relative positions $\Delta x = x_m - x_M$, etc., would produce PDEs for the entire system and for the relative positions.

because the wavefunction is complex in general. Here, $m$, indicated how many maxima that the latitudinal part of $\phi$ will have, and the two different $A$ multiply wavefunctions that are out-of-phase by $\pi$. Either solution can be obtained by changing the sign of $m$, therefore in general

$$\Phi_m(\phi) = \frac{1}{\sqrt{2\pi}} e^{\imath m\phi} \qquad m = 0, \pm 1, \pm 2, \ldots \tag{26-30}$$

where the prefactor normalizes $\Phi$ so that $\int_0^{2\pi} \Phi_m \Phi_m^* d\phi = 1$.

The second of Eqs. 26-28 has the same form as Eq. 26-3 for which the relevant solution (because they are bounded) if an only if

$$\lambda = \ell(\ell+1) \quad \text{and} \quad |m| \leq \ell \quad \text{for} \quad \ell = 0, 1, 2, \ldots \tag{26-31}$$

Putting all of this together and normalizing, the spherical harmonic part of the H-atom orbital (Eq. 26-25) is:

$$Y_{\ell,m} = \sigma(m) \sqrt{\frac{2l+1}{4\pi} \frac{(\ell - |m|)!}{(\ell + |m|)!}} P_{\ell,m}(\cos\theta) e^{\imath m\phi} \tag{26-32}$$

where $\sigma(m) = 1$ if $m \leq 0$ or $m$ even, and $\sigma(m) = -1$ for odd-positive $m$.

Finally, for the radial part of the H-atom orbital (Eq. 26-24) with $\lambda = \ell(\ell+1)$ becomes an ODE in $r$:

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2 \frac{d\rho}{dr}\right) + \left[\frac{2m_e}{\hbar^2}\left(E - \frac{Ze^2}{\epsilon_o r}\right) - \frac{\ell(\ell+1)}{r^2}\right]\rho = 0 \tag{26-33}$$

where $E < 0$ defines a bound state.

This equation can also be solved analytically, and it has integer eigenvalues $n > \ell \geq |m|$:

$$\rho_{n,\ell}(r) = -\sqrt{\left(\frac{2Z}{na_0}\right)^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}} \exp(\frac{-Zr}{na_0}) \left(\frac{-2Zr}{na_0}\right)^\ell L_{n+1,2\ell+1}\left(\frac{2Zr}{na_0}\right) \tag{26-34}$$

where $a_0 = \hbar^2\epsilon_0/m_e e^2$ is the *Bohr radius* and the $L_{q,p}$ is yet another special function—c'est *LaGuerre polynomials*.

The Hydrogen orbitals are visualized in the following example.

## Lecture 26 MATHEMATICA® Example 2

Visualizing the Hydrogen atom eigenfunctions

Download notebooks, pdfs, or html from http://pruffle.mit.edu/3.016-2006.

This example is still in progress—it has not been check for accuracy yet.

**1:** This example will be completed at a later date.

Functions to display $\psi\psi^*$ will be developed.
Lengths will be normalized so that the Bohr radius is 1 and Z =

```
1  κ[n_] := κ[n] = 1/n
   A[n_, L_] := A[n, L] = Sqrt[Factorial[n - L - 1]/(2 n (Factorial[n + L])^3)]
   prefactor[n_, l_] := prefactor[n, l] = A[n, l] (2 κ[n])^(3/2)

2  spherefactor[l_, m_] :=
     spherefactor[l, m] = (2 l + 1)/(4 π) Factorial[l - m]/Factorial[l + m]

3  SquareRadialPart[n_, l_, ρ_] := (prefactor[n, l]
       Exp[-ρ] (2 ρ)^l LaguerreL[n - l - 1, 2 l + 1, 2 ρ])^2

4  SquareAngularPart[l_, m_, prob_, θ_, ϕ_] :=
     (*θ is longitude*)
     Module[{ctheta = Cos[θ], r},
       r = prob * (spherefactor[l, m] LegendreP[l, m, ctheta])^2;
       Return[{r Cos[ϕ] ctheta, r Sin[ϕ] ctheta, r Sin[θ]}]
     ]

5  << Graphics`FilledPlot`

6  << Graphics`ParametricPlot3D`
```