11 More ordinary differential equations

11.1 Second order ordinary differential equations

Second order differential equations are central to the modeling of physical systems. While first order ordinary differential equations model processes with exponentially growing or diminishing observables, second order ordinary differential equations can be used to model a variety of phenomena including oscillatory motion. This section explores the general form of second order ordinary differential equations and diverse nature of the solutions.

11.1.1 General features of second order ordinary differential equations

In Chapter 10 we considered the first order ordinary differential equation

$$\frac{d}{dx}y(x) = ay(x)$$

We found the solution $y(x)$ must be a function of the form $y(x) = c_1\,e^{ax}$ where c_1 is a constant, since the first derivative of the exponential function is proportional to the function itself. Similarly, the equation

$$\frac{d}{dx}y(x) = -ay(x)$$

will have a solution of the form $y(x) = c_1\,e^{-ax}$. In each case, the constant coefficient c_1 is determined by a boundary condition.

Let's apply the same approach to the solution of the second order ordinary differential equation

$$\frac{d^2}{dx^2}y(x) = a^2y(x) \tag{11.1}$$

where $a > 0$ and real. In this case, we seek a function $y(x)$ with second derivative proportional to a positive constant times the function itself. The exponential functions $c_1\,e^{ax}$ and $c_2\,e^{-ax}$ with real arguments possess that essential property, yielding the solution

$$y(x) = c_1\,e^{ax} + c_2\,e^{-ax}$$

where c_1 and c_2 are constant coefficients.[1]

[1] Since $y_1(x) = c_1\,e^{\alpha x}$ and $y_2(x) = c_2\,e^{-\alpha x}$ are each solutions to the linear second order differential equation, Equation 11.1, it follows that the linear *superposition* $y(x) = y_1(x) + y_2(x)$ is also a solution.

Now consider the equation

$$\frac{d^2}{dx^2}y(x) = -a^2\, y(x) \tag{11.2}$$

We seek a function $y(x)$ with a second derivative equal to a negative constant times the function itself. The exponential functions $c_1\, e^{iax}$ and $c_2\, e^{-iax}$ with imaginary arguments have that property.[2] As such, we can write the solution $y(x) = c_1\, e^{iax} + c_2\, e^{-iax}$ where the coefficients c_1 and c_2 are determined by the boundary conditions.

[2] We could equivalently propose solutions of the from $c_1' \cos(ax)$ and $c_2' \sin(ax)$.

Now consider the homogeneous linear second order ordinary differential equation

$$\frac{d^2}{dx^2}y(x) + b\,\frac{d}{dx}y(x) + c\,y(x) = 0 \tag{11.3}$$

with constant coefficients b and c. We propose the *ansatz*

$$y(x) = e^{\alpha x}$$

where α is a *complex number*. Inserting this form for $y(x)$, we find

$$\frac{d^2}{dx^2}e^{\alpha x} + b\,\frac{d}{dx}e^{\alpha x} + c\,e^{\alpha x} = \alpha^2 e^{\alpha x} + b\,\alpha e^{\alpha x} + c\,e^{\alpha x} = 0$$

Ignoring the *trivial solution* $e^{\alpha x} = 0$, we arrive at the result[3]

[3] A *trivial solution* is a formal solution to the problem from which we learn nothing.

$$\alpha^2 + b\alpha + c = 0 \tag{11.4}$$

This is known as the *auxiliary equation*. This quadratic equation in the variable α has two roots, $\alpha_\pm$, defined by the *quadratic formula*

$$\alpha_\pm = \frac{-b \pm \sqrt{b^2 - 4c}}{2}$$

Returning to our *ansatz*, we observe that both $c_1 e^{\alpha_+ x}$ and $c_2 e^{\alpha_- x}$ are solutions to Equation 11.3, where c_1 and c_2 are constant coefficients. As such, we write the general solution to Equation 11.3 as

$$y(x) = c_1\, e^{\alpha_+ x} + c_2\, e^{\alpha_- x} \tag{11.5}$$

where the constant coefficients c_1 and c_2 are determined by the *boundary conditions* typically defined in terms of the value of the function, $y(0)$, and its derivative, $y'(0)$.

11.1.2 *Qualitative theory of second order ordinary differential equations*

Our observations above can be summarized as follows. For the second order differential equation

$$\frac{d^2}{dx^2}y(x) + b\,\frac{d}{dx}y(x) + c\,y(x) = 0$$

there is a general solution of the form

$$y(x) = c_1\, e^{\alpha_+ x} + c_2\, e^{\alpha_- x}$$

where the constants $\alpha_\pm$ are the roots of the auxiliary equation

$$\alpha^2 + b\alpha + c = 0$$

defined by the quadratic formula

$$\alpha_\pm = \frac{-b \pm \sqrt{b^2 - 4c}}{2}$$

The nature of the solution $y(x)$ is determined by the roots $\alpha_\pm$, which may be real, imaginary, complex, or degenerate (double) roots, depending on the particular values of the parameters b and c. Figure 11.1 shows the bc-parameter space divided into the four regimes.

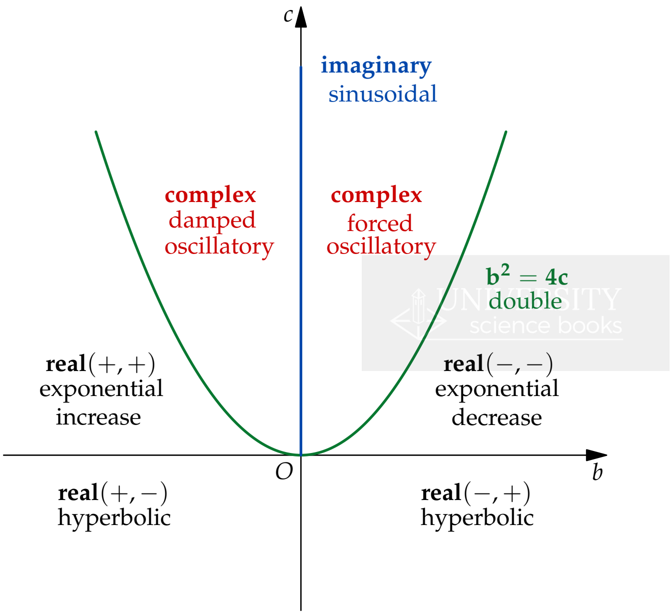


Figure 11.1: The nature of roots of the auxiliary equation as a function of the parameters b and c. Double roots are found on the parabola defined by $b^2 = 4c$ (thick green). Complex roots are found atop the parabolic curve for $c > b^2/4$. Purely imaginary roots occupy a surface normal to the bc-plane (thick blue). In this projection, imaginary roots are restricted to the positive c-axis. Below the parabolic curve the roots are real, forming exponential or hyperbolic functions.

When $b^2 > 4c$, the roots $\alpha_\pm$ are real. The solution $y(x)$ is exponentially increasing or decreasing with increasing x. Real roots support solutions involving exponentially decaying or growing functions of the kind found in physical kinetics, capturing the behavior of populations or concentrations that grow or diminish exponentially in time.

When $b = 0$, the roots $\alpha_\pm$ are imaginary. The solution $y(x)$ is a purely oscillatory function of x. Imaginary roots support solutions involving oscillatory functions of the kind used to model a vibrating mass on a spring and waves found in the study of quantum theory.

When $b^2 < 4c$, the roots $\alpha_\pm$ are complex. The solution $y(x)$ oscillates with an amplitude that exponentially increases or decreases with increasing x. Complex roots capture damped oscillatory motion as found an oscillator feeling the effects of friction that gradually attenuate the amplitude of motion. Solutions with complex roots are also used to model propagating electromagnetic waves.

When $b^2 = 4c$, we find the special case of double roots where $\alpha_+ = \alpha_- = -b/2$. Double roots are a special coincidence in the values of the b and c parameters that we do not expect to find in nature. Examples of the various kinds of qualitative behavior resulting from Equation 11.3 are presented below in Figure 11.2.

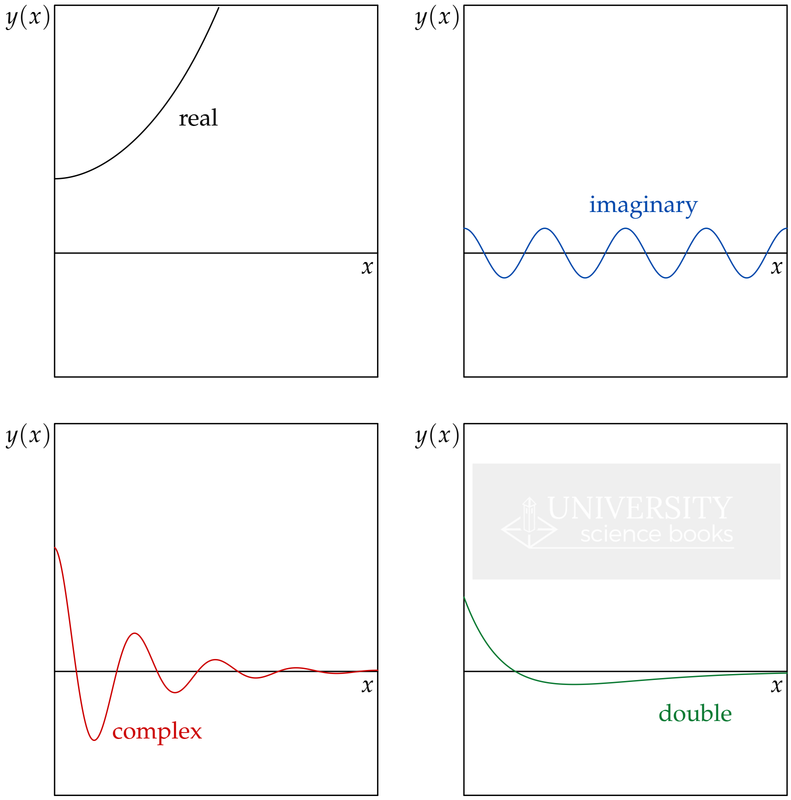


Figure 11.2: The nature of the roots of the auxiliary equation, Equation 11.4, determine the character of the solution to Equation 11.3. Examples of solutions with real roots (upper left), imaginary roots (upper right), complex roots (lower left), and double roots (lower right).

In summary, our analysis demonstrates that Equation 11.3 can be used to model a wide variety of physical phenomena.

$$\frac{d^2}{dx^2}y(x) + b\,\frac{d}{dx}y(x) + c\,y(x) = 0$$

The particular choice of parameters b and c lead to roots

$$\alpha_\pm = \frac{-b \pm \sqrt{b^2 - 4c}}{2}$$

that determine the nature of the solution

$$y(x) = c_1\,e^{\alpha_+ x} + c_2\,e^{\alpha_- x}$$

In the next section, we explore the solution of the homogeneous linear second order ordinary differential equation, Equation 11.3, for a variety of examples relevant to modeling processes in the physical sciences.

11.2 Applications of second order differential equations

SECOND ORDER DIFFERENTIAL EQUATIONS with constant coefficients yield solutions exhibiting a wide range of behavior, including exponential growth or decay, sinusoidal oscillation, and exponentially attenuated oscillation. This section explores applications exhibiting the variety of behavior found in solutions of second order ordinary differential equations.

11.2.1 *Survey of second order ordinary differential equations*

In this section, we explore specific examples of differential equations representing domains with real roots, imaginary roots, complex roots, and double roots. In doing so, we will appreciate how this variety of solutions can be used to model a remarkable diversity of physical systems.

Case #1: real roots

When the coefficients b and c are such that $b^2 > 4c$, the roots

$$\alpha_\pm = \frac{-b \pm \sqrt{b^2 - 4c}}{2}$$

are real. For the case $c = 0$, there will be one zero root and one non-zero root equal to $-b$, leading to a solution of the form

$$y(x) = c_1 + c_2\, \mathrm{e}^{-bx}$$

For the more general case of $c \neq 0$ and $b^2 > 4c$, the roots of the auxiliary equation $\alpha_\pm$ are real and the solution $y(x)$ will have exponentially divergent behavior as a function of x.

When the coefficients c_1 and c_2 are of the same sign, the solution $y(x)$ has the character of a *hyperbolic cosine* (see Figure 11.3, red line). In contrast, when the coefficients c_1 and c_2 are of opposite sign, the general solution has the character of a *hyperbolic sine* (see Figure 11.3, black line). In each case, the solution $y(x)$ diverges with increasing x. Exponential growth of this kind is observed in population growth as observed in Chapter 10.

Let's explore the solution of the second order ordinary differential equation

$$\frac{d^2}{dx^2}y(x) + \frac{d}{dx}y(x) - 2\,y(x) = 0 \tag{11.6}$$

with the boundary conditions $y(0) = 3$ and $y'(0) = 0$. We take the *ansatz*

$$y(x) = \mathrm{e}^{\alpha x}$$

and insert it into Equation 11.6 with the result

$$\frac{d^2}{dx^2}\mathrm{e}^{\alpha x} + \frac{d}{dx}\mathrm{e}^{\alpha x} - 2\,\mathrm{e}^{\alpha x} = \alpha^2\,\mathrm{e}^{\alpha x} + \alpha\,\mathrm{e}^{\alpha x} - 2\,\mathrm{e}^{\alpha x} = 0$$

leading to the auxiliary equation

$$\alpha^2 + \alpha - 2 = (\alpha - 1)(\alpha + 2) = 0$$

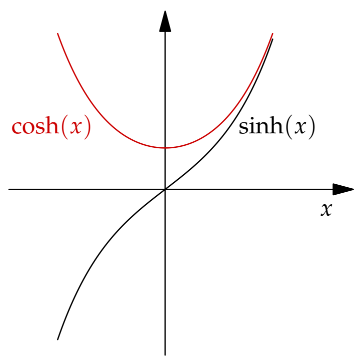


Figure 11.3: The hyperbolic functions $\sinh(x) = (\mathrm{e}^x - \mathrm{e}^{-x})/2$ (black line) and $\cosh(x) = (\mathrm{e}^x + \mathrm{e}^{-x})/2$ (red line).

This quadratic equation has real roots

$$\alpha_\pm = \begin{cases} 1 \\ -2 \end{cases}$$

leading to the general solution defined by Equation 11.5 as

$$y(x) = c_1\, e^{x} + c_2\, e^{-2x}$$

The coefficients c_1 and c_2 are determined by applying the boundary conditions

$$y(0) = c_1 + c_2 = 3$$

and

$$\left.\frac{dy}{dx}\right|_{x=0} = \left[c_1\, e^{x} - 2c_2\, e^{-2x}\right]_{x=0} = c_1 - 2c_2 = 0$$

We find $c_1 = 3 - c_2$ and $c_1 = 2c_2$ so that $c_1 = 2$ and $c_2 = 1$. The final solution to Equation 11.6 is

$$y(x) = 2\, e^{x} + \, e^{-2x} \qquad (11.7)$$

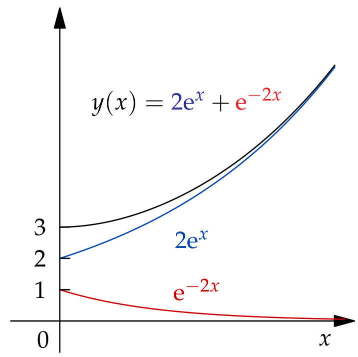


Figure 11.4: The function $y(x) = 2\exp(x) + \exp(-2x)$ (black) as a function of x. Shown for comparison are the two contributions forming the superposition $y(x)$, each of which is a solution to Equation 11.6.

This result is plotted in Figure 11.4. Note that we can validate our solution, Equation 11.7, by inserting it into the original differential equation, Equation 11.6, and proving the equality.

Case #2: imaginary roots

When the coefficients b and c are such that $b^2 < 4c$ and $b = 0$, the roots

$$\alpha_\pm = \pm i\sqrt{c}$$

are purely imaginary, leading to solutions of the form

$$y(x) = c_1\, e^{i\sqrt{c}x} + c_2\, e^{-i\sqrt{c}x} \qquad (11.8)$$

This solution appears to have real and imaginary parts. However, we expect the solution to be purely real. We will find the boundary conditions result in coefficients c_1 and c_2 that make the solution $y(x)$ purely real.

Recall that Euler's formula provides a connection between exponentials of imaginary arguments and the cosine and sine functions:

$$e^{ix} = \cos(x) + i\sin(x)$$

Using this identity, we can reformulate Equation 11.8 as

$$y(x) = c_1'\, \cos(\sqrt{c}x) + c_2'\, \sin(\sqrt{c}x)$$

where $c_1' = c_1 + c_2$ and $c_2' = i(c_1 - c_2)$. When the roots of the auxiliary equation are imaginary and the coefficients c_1 and c_2 are real, the resulting solution $y(x)$ is a real sinusoidal function of x.

Let's apply this method to solve the second order ordinary differential equation

$$\frac{d^2}{dx^2} y(x) + 9\, y(x) = 0 \qquad (11.9)$$

with the boundary conditions $y(0) = 1$ and $y'(0) = 6$. We take the *ansatz*

$$y(x) = e^{\alpha x}$$

and insert it into Equation 11.9 as

$$\frac{d^2}{dx^2} e^{\alpha x} + 9\, e^{\alpha x} = \alpha^2\, e^{\alpha x} + 9\, e^{\alpha x} = 0$$

leading to the auxiliary equation

$$\alpha^2 + 9 = (\alpha - 3i)(\alpha + 3i) = 0$$

This quadratic equation has imaginary roots

$$\alpha_\pm = \begin{cases} 3i \\ -3i \end{cases}$$

leading to the general solution defined by Equation 11.5:

$$y(x) = c_1' \cos(3x) + c_2' \sin(3x)$$

The coefficients c_1' and c_2' can be determined by applying the boundary conditions

$$y(0) = c_1' = 1$$

and

$$\left.\frac{dy}{dx}\right|_{x=0} = \left[-3c_1' \sin(3x) + 3c_2' \cos(3x)\right]_{x=0} = 3c_2' = 6$$

We find $c_1' = 1$ and $c_2' = 2$. The final solution to Equation 11.9 is

$$y(x) = \cos(3x) + 2\sin(3x) \tag{11.10}$$

This result is plotted in Figure 11.5. Note that we can validate our solution, Equation 11.10, by inserting it into the original differential equation, Equation 11.9, and proving the equality.

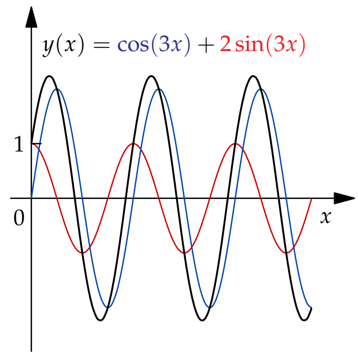


Figure 11.5: The solution to Equation 11.9 is the sinusoidal function $y(x) = 2\cos(3x) + \sin(3x)$ characterized by imaginary roots of the auxiliary equation and satisfying the boundary conditions $y(0) = 1$ and $y'(0) = 6$.

Case #3: complex roots

When the coefficients b and c are such that $b^2 < 4c$, the radical $\sqrt{b^2 - 4c}$ is imaginary. When $b \neq 0$, the roots

$$\alpha_\pm = \frac{-b \pm \sqrt{b^2 - 4c}}{2} = \frac{-b \pm \sqrt{c'}}{2}$$

are complex with real and imaginary parts. As a result, solutions are of the form

$$y(x) = c_1 \exp\left[-\frac{1}{2}\left(b - i\sqrt{c'}\right) x\right] + c_2 \exp\left[-\frac{1}{2}\left(b + i\sqrt{c'}\right) x\right]$$

where $c' = b^2 - 4c$. Pulling out the common exponential factor $e^{-bx/2}$ leads to

$$y(x) = e^{-bx/2}\left(c_1\, e^{i\sqrt{c'}x/2} + c_2\, e^{-i\sqrt{c'}x/2}\right)$$

Using Euler's formula, we can convert the sum of exponentials with imaginary arguments to sinusoidal functions with the result

$$y(x) = e^{-bx/2}\left[c_1' \cos\left(\sqrt{c'}x/2\right) + c_2' \sin\left(\sqrt{c'}x/2\right)\right]$$

where again $c_1' = c_1 + c_2$ and $c_2' = i(c_1 - c_2)$. The solutions $y(x)$ are exponentially decreasing (when $b > 0$) or increasing (when $b < 0$) sinusoidal functions.

Let's apply this method to solve the second order ordinary differential equation

$$\frac{d^2}{dx^2}y(x) + 2\frac{d}{dx}y(x) + 10\,y(x) = 0 \tag{11.11}$$

with the boundary conditions $y(0) = 1$ and $y'(0) = 0$. We take the *ansatz*

$$y(x) = e^{\alpha x}$$

and insert it into Equation 11.11 as

$$\frac{d^2}{dx^2}e^{\alpha x} + 2\frac{d}{dx}e^{\alpha x} + 10\,e^{\alpha x} = \alpha^2\,e^{\alpha x} + 2\,\alpha e^{\alpha x} + 10\,e^{\alpha x} = 0$$

leading to the auxiliary equation

$$\alpha^2 + 2\alpha + 10 = 0$$

This quadratic equation has complex roots[4]

$$\alpha_\pm = \begin{cases} -1 + 3i \\ -1 - 3i \end{cases}$$

leading to the general solution defined by Equation 11.5 as

$$y(x) = e^{-x}\left(c_1\,e^{3ix} + c_2\,e^{-3ix}\right)$$

and more conveniently written as

$$y(x) = e^{-x}\left[c_1' \cos(3x) + c_2' \sin(3x)\right]$$

The coefficients c_1' and c_2' can be determined by applying the boundary conditions

$$y(0) = c_1' = 1$$

and

$$\begin{aligned}\left.\frac{dy}{dx}\right|_{x=0} &= \Big[-e^{-x}\left[c_1' \cos(3x) + c_2' \sin(3x)\right] \\ &\quad + e^{-x}\left[-3c_1' \sin(3x) + 3c_2' \cos(3x)\right]\Big]_{x=0} \\ &= -c_1' + 3c_2' = 0\end{aligned}$$

We find $c_1' = 1$ and $c_2' = \frac{1}{3}$. The final solution to Equation 11.11 is

$$y(x) = e^{-x}\left[\cos(3x) + \frac{1}{3}\sin(3x)\right] \tag{11.12}$$

[4] Note that α_+ and α_- are complex conjugates so that $\alpha_+ = \alpha_-^*$.

This result is plotted in Figure 11.6 (black line). The solution exhibits oscillations that exponentially decay with increasing x. Note that we can validate our solution, Equation 11.12, by inserting it into the original differential equation, Equation 11.11, and proving the equality.

Now consider the second order ordinary differential equation

$$\frac{d^2}{dx^2}y(x) - 2\,\frac{d}{dx}y(x) + 10\,y(x) = 0 \qquad (11.13)$$

where we have changed the coefficient of the middle term from $b = 2$ in Equation 11.11 to $b = -2$. The roots of the auxiliary equation become

$$\alpha_{\pm} = \begin{cases} 1 + 3i \\ 1 - 3i \end{cases}$$

leading to the general solution

$$y(x) = e^{x}\left[c_1' \cos(3x) + c_2' \sin(3x)\right]$$

The decaying exponential in Equation 11.12 has been replaced with a growing exponential. Applying the boundary conditions $y(0) = 0$ and $y'(0) = 1/200$, the final result is

$$y(x) = \frac{1}{600}\, e^{x} \sin(3x)$$

as shown in Figure 11.6 (red line). The solution exhibits oscillations that exponentially grow in amplitude with increasing x.

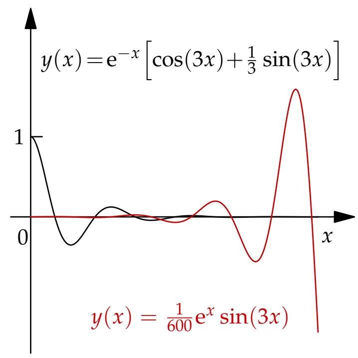


Figure 11.6: The solutions to Equations 11.11 and 11.13 are characterized by complex roots of the auxiliary equation resulting in sinusoidal functions with amplitudes that diminish (black line) or grow (red line) exponentially with increasing x.

Case #4: double roots

When the coefficients b and c are such that $b^2 = 4c$, the radical $\sqrt{b^2 - 4c}$ is zero and the two roots of the auxiliary equation are degenerate:

$$\alpha_{\pm} = \alpha = -\frac{b}{2}$$

This case is known as *double roots*. In the case of double roots, the solution takes the special form

$$y(x) = c_1\, e^{\alpha x} + c_2\, x e^{\alpha x}$$

Due to the degeneracy in the roots, each exponential varies at the same rate.

Let's prove this is true for the second order ordinary differential equation

$$\frac{d^2}{dx^2}y(x) + 2\frac{d}{dx}y(x) + y(x) = 0 \qquad (11.14)$$

with boundary conditions $y(0) = 1$ and $y'(0) = -3$. The solution to the corresponding auxiliary equation

$$\alpha^2 + 2\alpha + 1 = (\alpha + 1)(\alpha + 1) = 0$$

is the double root $\alpha = -1$ leading to the special solution

$$y(x) = c_1\, e^{-x} + c_2\, x e^{-x}$$

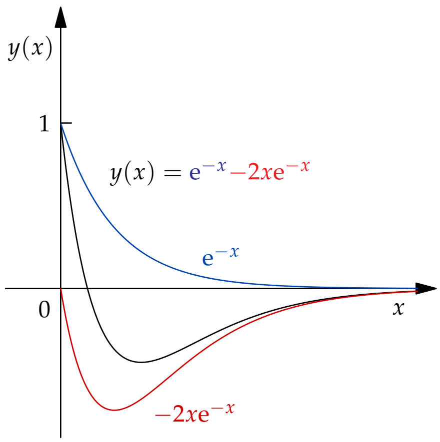


Figure 11.7: The solution for double roots $y(x) = \exp(-x) - 2x\exp(-x)$ (black) as a function of x. Shown for comparison are the two contributions forming $y(x)$ each of which is a solution to Equation 11.14.

Applying the boundary conditions

$$y(0) = c_1 = 1$$

and

$$\left.\frac{dy}{dx}\right|_{x=0} = \left[-c_1\,e^{-x} + c_2\,\left(e^{-x} - xe^{-x}\right)\right]_{x=0} = -c_1 + c_2 = -3$$

we find that $c_1 = 1$ and $c_2 = -2$. The final result is

$$y(x) = e^{-x} - 2\,xe^{-x} \tag{11.15}$$

as is shown in Figure 11.7. Checking our solution, we use $y'(x) = -3e^{-x} + 2xe^{-x}$ and $y''(x) = 5e^{-x} - 2xe^{-x}$. Inserting these relations into our original Equation 11.14 yields

$$\frac{d^2}{dx^2}y(x) + 2\frac{d}{dx}y(x) + y(x) = \left(5e^{-x} - 2\,xe^{-x}\right) + 2\,\left(-3e^{-x} + 2\,xe^{-x}\right) + \left(e^{-x} - 2\,xe^{-x}\right) = 0$$

validating our solution.

When we model a system using Equation 11.3 written

$$\frac{d^2}{dx^2}y(x) + b\,\frac{d}{dx}y(x) + c\,y(x) = 0$$

We expect the coefficients b and c to be real numbers defined by fundamental physical constants. The coincidence of having an auxiliary equation with the exact equality $b^2 = 4c$ is unlikely. As such, we do not expect to encounter double roots when when solving accurately parameterized models of physical systems.

In this section, we have developed a general method for the solution of linear second order ordinary differential equations with constant coefficients b and c, as in Equation 11.3. In the section that follows, we explore a more general class of second order ordinary differential equations, which will be applicable to cases where the coefficients $b(x)$ and $c(x)$ are functions of x.

11.3 Power series solutions to differential equations

MANY FIRST AND SECOND ORDER ORDINARY DIFFERENTIAL EQUATIONS yield solutions represented by common functions such as the exponential, sine and cosine, and hyperbolic sine and cosine. Our approach has been to make an educated guess, or *ansatz*, plug that in, and find a set of parameters representing a solution. However, it is possible to employ a more general approach to the solution of ordinary differential equations in which our *ansatz* is a power series representing continuous and differentiable functions normally encountered in modeling physical systems. In this section, we will explore this general and powerful approach to the solution of first and second order ordinary differential equations.

11.3.1 *Solving ordinary differential equations using power series*

Let's review our current ability to solve first and second order ordinary differential equations. We developed a general solution for homogeneous and non-homogeneous linear first order ordinary differential equations of the form

$$\frac{d}{dx}y(x) + q(x)y(x) = r(x)$$

and homogeneous linear second order ordinary differential equations with constant coefficients[5]

$$\frac{d^2}{dx^2}y(x) + b\frac{d}{dx}y(x) + c\,y(x) = 0$$

[5] While it is possible to form ordinary differential equations of arbitrary order, in the study of thermodynamics, quantum theory, and kinetics, we typically encounter first and second order equations.

However, we have no general solution for non-homogeneous linear second order ordinary differential equations of the form

$$\frac{d^2}{dx^2}y(x) + b(x)\frac{d}{dx}y(x) + c(x)\,y(x) + d(x) = 0$$

We also have no general solution for homogeneous linear second order ordinary differential equations where $d(x) = 0$ but the coefficients $b(x)$ and $c(x)$ depend on x.

How can we solve this more general differential equation when we cannot anticipate the specific form of our solution? We recall that most functions used to model physical properties can be expressed as a *power series*

$$y(x) = \sum_{n=0}^{\infty} a_n x^n$$

Depending on the specific set of coefficients $\{a_n\}$, the function $y(x)$ may be an exponential, sinusoid, damped sinusoid, polynomial, logarithm, or a variety of other functions. With this insight, we propose the power series as our *ansatz*, representing a general continuous and differentiable function. Inserting our proposed solution into the differential equation of interest, we solve for the coefficients $\{a_n\}$ defining our solution. Let's see how this works by solving two familiar ordinary differential equations using the power series method.

11.3.2 *Power series solutions for first order differential equations*

Let's apply this approach to solve the familiar first order ordinary differential equation

$$\frac{d}{dx}y(x) + y(x) = 0 \tag{11.16}$$

with the boundary condition $y(0) = 2$. As our *ansatz*, we propose the power series

$$y(x) = \sum_{n=0}^{\infty} a_n x^n \tag{11.17}$$

Inserting this proposed solution in Equation 11.16, we must evaluate the first derivative of $y(x)$ with respect to x as

$$\frac{d}{dx}y(x) = \frac{d}{dx}\sum_{n=0}^{\infty} a_n x^n = \sum_{n=0}^{\infty} a_n \left(\frac{d}{dx}x^n\right) = \sum_{n=0}^{\infty} a_n n x^{n-1}$$

Using this result in Equation 11.16, we find

$$\frac{d}{dx}y(x) + y(x) = \sum_{n=0}^{\infty} a_n n x^{n-1} + \sum_{n=0}^{\infty} a_n x^n = 0$$

To simplify this result, we must add the two power series together. To do that, we must form each series over the same range of n, with terms of a given n having the same power of x.

We are left to combine the two series. In the first series, the coefficient is proportional to n so that the $n = 0$ term is always zero. Removing the $n = 0$ term from the first series results in

$$\sum_{n=0}^{\infty} a_n n x^{n-1} \to \sum_{n=1}^{\infty} a_n n x^{n-1} = a_1 + 2a_2 x + 3a_3 x^2 + \ldots$$

where we have increased the lower end of the index n from 0 to 1. We are left to add the two series

$$\sum_{n=1}^{\infty} a_n n x^{n-1} + \sum_{n=0}^{\infty} a_n x^n = 0$$

This first power series starts from $n = 1$, but we would like this series to start from $n = 0$. To accomplish this, we shift the index $n \to n + 1$ with the result

$$\sum_{n=1}^{\infty} a_n n x^{n-1} \to \sum_{n=0}^{\infty} a_{n+1}(n+1)x^n = a_1 + 2a_2 x + 3a_3 x^2 + \ldots$$

Properly shifting the index in a power series can be tricky, but we will learn to do this with practice.[6]

Returning to our initial Equation 11.16, we insert our final form for the derivative of $y(x)$. We find

$$\begin{aligned}\frac{d}{dx}y(x) + y(x) &= \sum_{n=0}^{\infty} a_{n+1}(n+1)x^n + \sum_{n=0}^{\infty} a_n x^n \\ &= \sum_{n=0}^{\infty} \left[a_{n+1}(n+1) + a_n\right] x^n = 0 \qquad (11.18)\end{aligned}$$

[6] Equivalently, you can introduce a new index $n' = n - 1$, substituting $n \to n' + 1$. You can then rewrite the new index n' as n before combining the sums. Try both approaches and see what works best for you.

For Equation 11.18 to be true for all x, it must be that

$$a_{n+1}(n+1) + a_n = 0$$

for all values of n.This leads to the *recursion relation*. It tells us that

$$a_{n+1} = -\frac{a_n}{(n+1)} \qquad n = 0, 1, 2, \ldots$$

and can be used to recursively generate our coefficients (see Figure 11.8).[7]

[7] The negative sign in the recursion relation signals the fact that the coefficients lead to an alternating series.

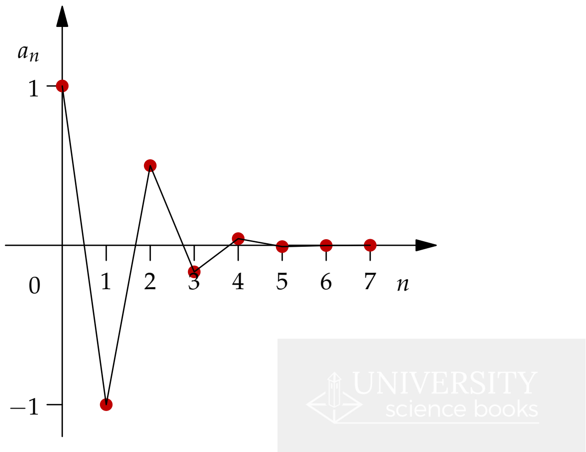


Figure 11.8: The power series coefficients $a_n = (-1)^n a_0/n!$ (red dots) for $a_0 = 1$.

We take our first coefficient to be a_0, a value we will determine later using our boundary conditions. We can generate the coefficient a_1 as

$$a_1 = -\frac{a_0}{0+1} = -a_0$$

where the negative sign in the recursion relation tells us that our solution for $y(x)$ will be an alternating series. We can continue to generate coefficients through recursion, including

$$a_2 = -\frac{a_1}{1+1} = -\frac{1}{2}a_1 = -\frac{1}{2}(-a_0) = \frac{1}{2}a_0$$

and

$$a_3 = -\frac{a_2}{2+1} = -\frac{1}{3}a_2 = -\frac{1}{3}\left(\frac{1}{2}a_0\right) = -\frac{1}{3\cdot 2}a_0$$

and so on. In general, we recognize that

$$a_n = (-1)^n \frac{1}{n!} a_0 \qquad n = 0, 1, 2, \ldots$$

Inserting this result for our coefficients in our original power series from Equation 11.17, we find

$$y(x) = \sum_{n=0}^{\infty} a_n x^n = \sum_{n=0}^{\infty} (-1)^n \frac{1}{n!} a_0 x^n = a_0 \sum_{n=0}^{\infty} (-1)^n \frac{1}{n!} x^n$$

We recognize this result as the power series of an exponential

$$e^{-x} = \sum_{n=0}^{\infty} (-1)^n \frac{1}{n!} x^n$$

so that

$$y(x) = a_0 e^{-x}$$

Applying our initial condition that $y(0) = 2$, we find $y(0) = a_0 = 2$, leading to our final solution to Equation 11.16

$$y(x) = 2e^{-x}$$

Our solution can be validated by inserting our result for $y(x)$ into Equation 11.16 and proving the equality

$$\frac{d}{dx} y(x) + y(x) = \frac{d}{dx} 2e^{-x} + 2e^{-x} = -2e^{-x} + 2e^{-x} = 0$$

11.3.3 Power series solutions for second order differential equations

Consider the second order ordinary differential equation

$$\frac{d^2}{dx^2} y(x) + y(x) = 0 \tag{11.19}$$

with the initial conditions $y(0) = 3$ and $y'(0) = 1$. As our *ansatz*, we propose

$$y(x) = \sum_{n=0}^{\infty} a_n x^n \tag{11.20}$$

Inserting this proposed solution in Equation 11.19, we must evaluate the second derivative of $y(x)$ with respect to x as

$$\frac{d^2}{dx^2} y(x) = \frac{d^2}{dx^2} \sum_{n=0}^{\infty} a_n x^n = \sum_{n=0}^{\infty} a_n \left(\frac{d^2}{dx^2} x^n \right) = \sum_{n=0}^{\infty} a_n n(n-1) x^{n-2}$$

Inserting this result in Equation 11.19, we find

$$\frac{d^2}{dx^2} y(x) + y(x) = \sum_{n=0}^{\infty} a_n n(n-1) x^{n-2} + \sum_{n=0}^{\infty} a_n x^n = 0$$

We are left to combine the two series. In the first series, the coefficient is proportional to $n(n-1)$ so that the $n = 0$ and $n = 1$ terms are always zero. Removing the $n = 0$ and $n = 1$ terms from the first series results in

$$\sum_{n=0}^{\infty} a_n n(n-1) x^{n-2} \to \sum_{n=2}^{\infty} a_n n(n-1) x^{n-2}$$

This leaves us with

$$\sum_{n=2}^{\infty} a_n n(n-1) x^{n-2} + \sum_{n=0}^{\infty} a_n x^n = 0$$

The first power series starts from $n = 2$, but we would like this series to start from $n = 0$ as we must eventually combine the first series with the second series that starts from $n = 0$. To accomplish this, we shift the index $n \to n+2$ by substituting $n \to n+2$, $n-1 \to n+1$, and $n-2 \to n$, with the result[8]

$$\sum_{n=2}^{\infty} a_n n(n-1)x^{n-2} \to \sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)x^n$$

[8] Equivalently, you can introduce a new index $n' = n-2$, substituting $n \to n'+2$. You can then rewrite the new index n' as n before combining the sums.

Returning to our initial equation, we find

$$\begin{aligned} \frac{d^2}{dx^2}y(x) + y(x) &= \sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)x^n + \sum_{n=0}^{\infty} a_n x^n \\ &= \sum_{n=0}^{\infty} \left[a_{n+2}(n+2)(n+1) + a_n\right] x^n = 0 \end{aligned}$$

This leads to the condition

$$a_{n+2}(n+2)(n+1) + a_n = 0$$

and the recursion relation

$$a_{n+2} = -\frac{1}{(n+2)(n+1)}a_n \qquad n = 0, 1, 2, \ldots$$

which we will use to generate the set of power series coefficients (see Figure 11.9).[9] The coefficients a_0 and a_1 will be determined through our boundary conditions. All other coefficients will be determined in terms of a_0 and a_1 through the recursion relation.

[9] Again, the negative sign in the recursion relation signals the fact that the coefficients lead to an alternating series.

The coefficients with even indices are

$$a_0 \qquad a_2 = -\frac{a_0}{2\cdot 1} \qquad a_4 = -\frac{a_2}{4\cdot 3} = \frac{a_0}{4!} \qquad a_6 = -\frac{a_4}{6\cdot 5} = -\frac{a_0}{6!}$$

and so on. As such, we find

$$a_{2n} = (-1)^n \frac{1}{(2n)!}a_0 \qquad n = 0, 1, 2, \ldots \tag{11.21}$$

The coefficients with odd indices are

$$a_1 \qquad a_3 = -\frac{a_1}{3\cdot 2} \qquad a_5 = -\frac{a_3}{5\cdot 4} = \frac{a_1}{5!} \qquad a_7 = -\frac{a_5}{7\cdot 6} = -\frac{a_1}{7!}$$

and so on, such that

$$a_{2n+1} = (-1)^n \frac{1}{(2n+1)!}a_1 \qquad n = 0, 1, 2, \ldots \tag{11.22}$$

As we have identified the coefficients, we can form a series solution for $y(x)$.

We will form two series, one for even powers of x and one for odd powers of x, and combine those results. Inserting Equation 11.21 for even powers of x in our original power series Equation 11.20 results in[10]

$$a_0 \sum_{n=0}^{\infty} (-1)^n \frac{1}{(2n)!}x^{2n}$$

[10] Note that the sum

$$\sum_{n=0}^{\infty} x^{2n}$$

contains only even powers of x.

Similarly, inserting Equation 11.22 for odd powers of x into our original

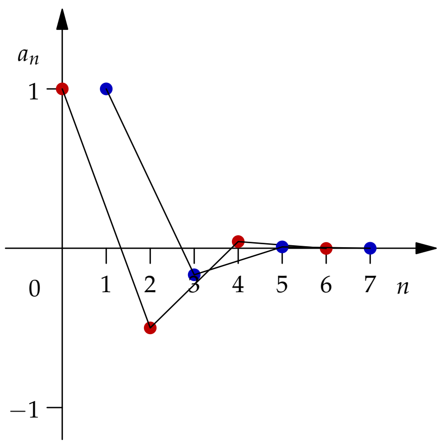


Figure 11.9: The power series coefficients $a_{2n} = (-1)^n a_0/(2n)!$ for even n and $a_0 = 1$ (red dots) and $a_{2n+1} = (-1)^n a_1/(2n+1)!$ for odd n and $a_1 = 1$ (blue dots).

power series Equation 11.20 results in the following power series

$$a_1 \sum_{n=0}^{\infty} (-1)^n \frac{1}{(2n+1)!} x^{2n+1}$$

Combining these results we arrive at the result

$$y(x) = a_0 \sum_{n=0}^{\infty} (-1)^n \frac{1}{(2n)!} x^{2n} + a_1 \sum_{n=0}^{\infty} (-1)^n \frac{1}{(2n+1)!} x^{2n+1}$$

Referring to our results for power series expansions of familiar functions explored in Chapter 7, including Equation 8.4 and Equation 8.3, we recognize that[11]

$$\cos(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n)!} x^{2n} \qquad \sin(x) = \sum_{n=0}^{\infty} \frac{(-1)^n}{(2n+1)!} x^{2n+1}$$

We can reformulate our result as

$$y(x) = a_0 \cos(x) + a_1 \sin(x)$$

Applying the boundary condition $y(0) = 3$ leads to $y(0) = a_0 = 3$, while the boundary condition $y'(0) = 1$ leads to $a_1 = 1$. Our final solution is

$$y(x) = 3\cos(x) + \sin(x)$$

which can be validated by inserting our result for $y(x)$ into Equation 11.19 and proving the equality.

We have used the power series method to derive again familiar solutions to first and second order ordinary differential equations. However, the power series method also provides a general means to solve more complicated ordinary differential equations that arise in the physical sciences. Specific examples of differential equations encountered in quantum theory, when modeling the translations of atoms and molecules, the vibrations of chemical bonds, the electronic properties of atoms, and the rotations of molecules, are explored in the complements.

[11] Note that the sum

$$\sum_{n=0}^{\infty} x^{2n+1}$$

contains only odd powers of x.

A$_{11}$ Quantum theory of a particle in a box

Consider the time-independent Schrödinger equation for a particle in one dimension:

$$-\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi(x) = E\psi(x) \tag{11.23}$$

where $\hbar = h/2\pi$, h is Planck's constant, m is the mass of the particle, E is the particle's energy, and $\psi(x)$ is the wave function describing the extent of the quantum particle along x. The particle is confined to a one-dimensional box defined by $0 \leq x \leq L$. The *boundary conditions* define the value of the wave function at the two ends of the box:

$$\psi(0) = \psi(L) = 0$$

We require two boundary conditions for any second order differential equation. Since we interpret the square of the wave function, $|\psi(x)|^2$, as a probability distribution, once we solve Equation 11.23 for $\psi(x)$, we will also impose the normalization condition

$$\int_0^L |\psi(x)|^2 dx = 1$$

This is a second order ordinary differential equation, and we can solve it using the methods developed in this chapter. We start by inserting $e^{\alpha x}$ for $\psi(x)$ in Equation 11.23 to find the auxiliary equation

$$-\frac{\hbar^2}{2m}\alpha^2 = E$$

As $E \geq 0$, we find the pure imaginary roots

$$\alpha_\pm = \pm i\sqrt{\frac{2mE}{\hbar^2}}$$

and expect an oscillatory solution (see Figure 11.5). The general solution can be written

$$\psi(x) = c_1 \ \exp\left(i\sqrt{\frac{2mE}{\hbar^2}}x\right) + c_2 \ \exp\left(-i\sqrt{\frac{2mE}{\hbar^2}}x\right)$$

We can determine the values of the coefficients c_1 and c_2 by applying the boundary conditions. Knowing that

$$\psi(0) = c_1 + c_2 = 0$$

tells us that $c_1 = -c_2$, so that

$$\psi(x) = c_1 \ \exp\left(i\sqrt{\frac{2mE}{\hbar^2}}x\right) - c_1 \ \exp\left(-i\sqrt{\frac{2mE}{\hbar^2}}x\right) = 2ic_1 \sin\left(\sqrt{\frac{2mE}{\hbar^2}}x\right)$$

where we have used the identity $\sin(x) = \frac{1}{2i}(e^{ix} - e^{-ix})$.

Knowing that

$$\psi(L) = 2ic_1 \sin\left(\sqrt{\frac{2mE}{\hbar^2}}L\right) = 0$$

it must be that

$$\sqrt{\frac{2mE}{\hbar^2}}L = n\pi \qquad n = 1,2,3,\ldots$$

This result provides us with a solution for the allowed values of the energy

$$E_n = \frac{n^2h^2}{8mL^2} \qquad n = 1,2,3,\ldots \tag{11.24}$$

We know the wave function is normalized such that

$$\int_0^L |\psi(x)|^2 dx = 1 = -4c_1{}^2 \int_0^L \sin^2\left(\frac{n\pi x}{L}\right) dx = -4c_1{}^2\,\frac{L}{2}$$

where the integral can be taken using the trigonometric half-angle identity $\sin^2(ax) = \frac{1}{2}(1-\cos(2ax))$, noting that the integral over the cosine term will be zero. This allows us to solve for the coefficient

$$c_1 = -\frac{i}{2}\sqrt{\frac{2}{L}}$$

As such, our final result for the solution to Equation 11.23 is

$$\psi_n(x) = \begin{cases} \sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right) & 0 \le x \le L \\ 0 & \text{everywhere else} \end{cases}$$

for $n = 1,2,3,\ldots$

Examples of the wave function $\psi_n(x)$ and the modulus squared of the wave function $|\psi_n(x)|^2$ are provided in Figure 11.10 and Figure 11.11 for $n = 1,2$, and 3. Note that each solution $\psi_n(x)$ has n half-oscillations in the box. As n increases, the number of half-oscillations increases, reflecting the increasing energy of the particle. Returning to Equation 11.23, we note that the second derivative of $\psi(x)$ is proportional to E. As E increases, the curvature of the wave function increases, reflected in an increasing number of oscillations in the box.

Finally, inserting our result for $\psi_n(x)$ into our original differential equation, we find

$$\begin{aligned} -\frac{\hbar^2}{2m}\frac{d^2}{dx^2}\psi_n(x) &= -\frac{\hbar^2}{2m}\left[-\left(\frac{n\pi}{L}\right)^2\sqrt{\frac{2}{L}}\sin\left(\frac{n\pi x}{L}\right)\right] \\ &= \frac{\hbar^2}{2m}\left(\frac{n\pi}{L}\right)^2\psi_n(x) = E_n\psi_n(x) \end{aligned}$$

The resulting allowed energies E_n for our particle in a box agree with those in Equation 11.24, validating our solution. This example demonstrates the effectiveness of our general approach to solving linear second order differential equations. Subsequent complements apply this approach to differential equations arising in classical theory of motion.

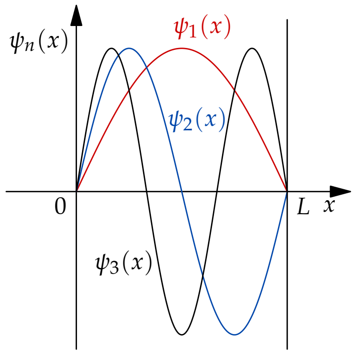


Figure 11.10: The wave function $\psi_n(x)$ for a particle confined to a box of length L. Three possible wave functions are shown for $n = 1,2$ and 3 corresponding to energies $E_1 = h^2/8mL^2$, $E_2 = 4h^2/8mL^2$, and $E_3 = 9h^2/8mL^2$.

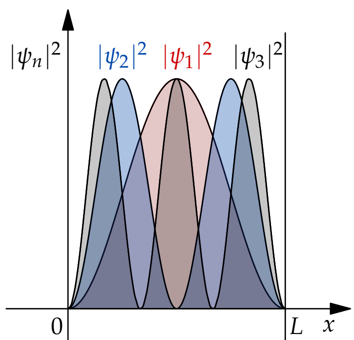


Figure 11.11: The modulus squared of the wave function $|\psi_n(x)|^2$ for a particle confined to a box of length L. Three possible wave functions are shown for $n = 1,2$ and 3. The area under each curve is unity making each $|\psi_n(x)|^2$ a normalized probability distribution.

B_{11} Classical theory of motion of a harmonic oscillator

In Chapter 7 we found that a mass on a spring or a vibrating bond between two atoms can be modeled as a harmonic oscillator with potential energy

$$V(x) = \frac{1}{2}\kappa(x - x_0)^2$$

and force

$$F(x) = -\frac{dV}{dx} = -\kappa(x - x_0)$$

where x is the displacement of the oscillator from its mechanically stable position at x_0 and κ is the force constant. When $x > x_0$, the force acts in the negative direction to shorten the oscillator. When $x < x_0$, the force acts in the positive direction to extend the oscillator. And when $x = x_0$, the force is zero and the oscillator is in a state of *mechanical equilibrium*. These results are depicted in Figure 11.12.

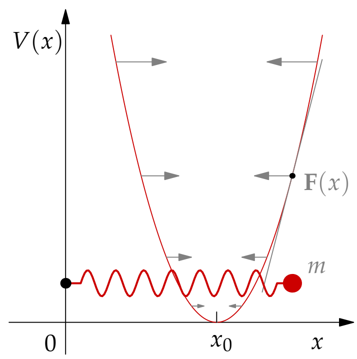


Figure 11.12: The quadratic potential energy function $V(x)$ and the corresponding force $\mathbf{F}(x)$.

The velocity is the rate of change in the position with respect to time:

$$v = \frac{dx}{dt}$$

The total energy of the oscillator is the sum of the kinetic energy and potential energy:

$$E = \frac{1}{2}mv^2 + \frac{1}{2}\kappa(x - x_0)^2$$

The total energy is constant in time.

The acceleration is the rate of change in the velocity with respect to time:

$$a = \frac{dv}{dt} = \frac{d^2x}{dt^2}$$

When a force acts on the oscillator, the mass accelerates according to Newton's equation of motion $ma = F$, or

$$m\frac{d^2x}{dt^2} = -\kappa(x - x_0)$$

where $\kappa > 0$ is the force constant. This is a linear second order ordinary differential equation. It can be solved to determine the position of the mass, $x(t)$, as a function of time.

We can reform the equation in terms of the variable $y(t) = x(t) - x_0$, representing the displacement of the oscillator from its equilibrium position:[12]

$$m\frac{d^2y}{dt^2} = -\kappa y$$

We would like to solve this equation to determine the position of the oscillator as a function of time $y(t)$. Substituting $e^{\alpha t}$ for $y(t)$ leads to

$$m\frac{d^2}{dt^2}e^{\alpha t} = m\alpha^2 e^{\alpha t} = -\kappa e^{\alpha t}$$

[12] Note that the velocity

$$v = \frac{dx}{dt} = \frac{d}{dt}(x - x_0) = \frac{dy}{dt}$$

and

$$a = \frac{d^2x}{dt^2} = \frac{d^2y}{dt^2}$$

for the acceleration are unchanged by this transformation.

which leads to the auxiliary equation

$$m\alpha^2 = -\kappa$$

with purely imaginary roots

$$\alpha_\pm = \pm i\sqrt{\frac{\kappa}{m}}$$

and the solution

$$y(t) = c_1 \exp\left(i\sqrt{\frac{\kappa}{m}}t\right) + c_2 \exp\left(-i\sqrt{\frac{\kappa}{m}}t\right)$$

The expression describes undamped oscillatory motion.

The time scale for the dynamics of the oscillator can be defined either by the *linear frequency* of motion

$$\nu = \frac{1}{2\pi}\sqrt{\frac{\kappa}{m}}$$

or equivalently by the *angular frequency*

$$\omega = \sqrt{\frac{\kappa}{m}} = 2\pi\nu$$

The period of oscillation is

$$T = \frac{1}{\nu} = \frac{2\pi}{\omega}$$

The larger the force constant, the higher the frequency of oscillation. The heavier the mass, the lower the frequency of oscillation.

With these definitions, we can reformulate $y(t) = x(t) - x_0$ as

$$y(t) = c_1 \exp(i\omega t) + c_2 \exp(-i\omega t)$$

We assume that at $t = 0$ the oscillator is displaced to y_0 and the velocity is zero

$$y(0) = y_0 \qquad v(0) = \left.\frac{dy}{dt}\right|_{t=0} = 0$$

As such, the initial total energy of the oscillator is $E(0) = \frac{1}{2}\kappa y_0^2$. Applying the initial condition for the velocity, we find

$$\begin{aligned}\left.\frac{dy}{dt}\right|_{t=0} &= \left[ic_1\omega e^{i\omega t} - ic_2\omega e^{-i\omega t}\right]_{t=0} \\ &= ic_1\omega - ic_2\omega = 0\end{aligned}$$

Accordingly, $c_1 = c_2$ so that

$$y(t) = c_1\left[\exp(i\omega) + \exp(-i\omega)\right] = 2c_1\cos(\omega t)$$

Applying the second initial condition, we find

$$y(0) = 2c_1\cos(\omega t)\Big|_{t=0} = 2c_1 = y_0$$

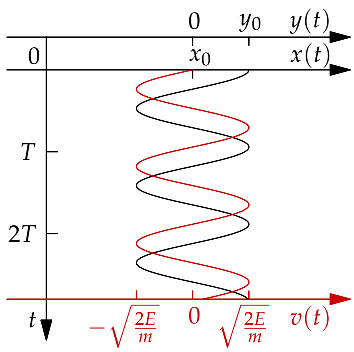


Figure 11.13: The trajectory of the harmonic oscillator shown in terms of the position, $x(t)$, the displaced coordinate, $y(t) = x(t) - x_0$, and the velocity, $v(t)$, as a function of t. The period of oscillation is $T = 2\pi/\omega$. The corresponding velocity oscillates between $\pm\sqrt{2E/m}$. Note that the velocity (red) is the derivative of the position (black) with respect to time.

so that the constant

$$c_1 = \frac{1}{2}y_0$$

Our final result for the position and velocity is

$$y(t) = y_0 \cos(\omega t) \qquad v(t) = \frac{dy}{dt} = -y_0\omega \sin(\omega t)$$

This result is depicted in Figure 11.13 which shows the position as a function of time in terms of $x(t)$ and $y(t)$ over three periods of oscillation $T = 2\pi/\omega$.

With a knowledge of the position and velocity of the oscillator as a function of time we can determine the total energy:

$$\begin{aligned} E(t) &= \frac{1}{2}mv(t)^2 + \frac{1}{2}\kappa y(t)^2 \\ &= \frac{1}{2}m\left(-y_0\omega \sin(\omega t)\right)^2 + \frac{1}{2}\kappa\left(y_0 \cos(\omega t)\right)^2 \\ &= \frac{1}{2}m\omega^2 y_0^2 \sin^2(\omega t) + \frac{1}{2}\kappa y_0^2 \cos^2(\omega t) \\ &= \frac{1}{2}\kappa y_0^2 \sin^2(\omega t) + \frac{1}{2}\kappa y_0^2 \cos^2(\omega t) \\ &= \frac{1}{2}\kappa y_0^2 \end{aligned}$$

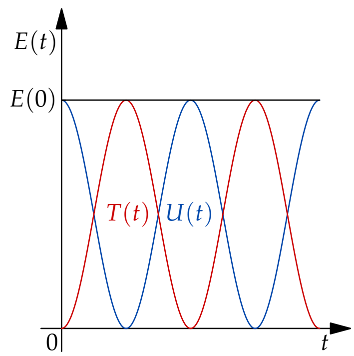


Figure 11.14: The kinetic energy, $T(t)$, potential energy, $U(t)$, and total energy $E(t) = T(t) + U(t)$ of the harmonic oscillator as a function of t. The total energy is conserved and is constant in time (black line).

During the vibration of the oscillator, the total energy is conserved and equals the initial energy:

$$E(t) = E(0) = \frac{1}{2}\kappa y_0^2$$

Figure 11.14 shows the complementary oscillations in the kinetic and potential energies. Potential energy is transformed to kinetic energy, and kinetic energy is transformed to potential energy in a repeating cycle, while the total energy remains constant.

It is interesting to consider the conservation of total energy

$$\frac{dE}{dt} = 0 = \frac{d}{dt}\left(\frac{1}{2}mv^2 + \frac{1}{2}\kappa(x - x_0)^2\right)$$

Evaluating the total time derivative leads to

$$\begin{aligned} \frac{d}{dt}\left(\frac{1}{2}mv^2 + \frac{1}{2}\kappa(x - x_0)^2\right) &= mv\frac{dv}{dt} + \kappa(x - x_0)\frac{dx}{dt} \\ &= mva + v\kappa(x - x_0) = 0 \end{aligned}$$

Canceling the common value of v, we find

$$ma + \kappa(x - x_0) = 0$$

or

$$ma = -\kappa(x - x_0) = F(x)$$

which is Newton's equation of motion. In this case of energy-conserving dynamics in one dimension, the conservation of energy implies Newton's equation of motion. This can be thought of as a special case of *Noether's theorem*.[13] The principle of conservation of energy (that the energy is constant

[13] Named for German mathematician *Emmy Noether* (1882-1935) whose work illuminated the relationship between conserved quantities, such as energy and angular momentum, and underlying symmetries of the system, such as time and rotation.

in time) is a consequence of an underlying symmetry, the invariance under translation in time. That is, when the time changes, the energy remains constant.

Finally, note that the position and velocity can also be written

$$y(t) = \sqrt{\frac{2E}{\kappa}}\cos(\omega t) \qquad v(t) = \frac{dy}{dt} = -\sqrt{\frac{2E}{m}}\sin(\omega t)$$

A slightly different set of equations defining the oscillator's motion are written in terms of the position and linear momentum $p(t) = mv(t)$:

$$y(t) = \sqrt{\frac{2E}{\kappa}}\cos(\omega t) \qquad p(t) = m\frac{dy}{dt} = -\sqrt{2mE}\sin(\omega t)$$

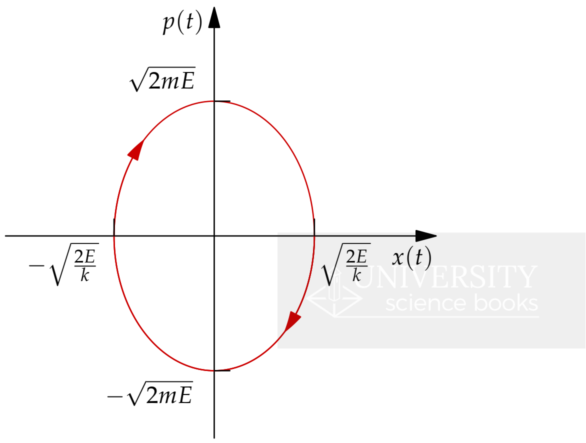


Figure 11.15: The motion of the harmonic oscillator defined by the position, $y(t)$, and momentum, $p(t)$, as a function of t. The elliptical curve is the phase portrait of the harmonic oscillator.

These equations define a trajectory on the yp-plane formed by the position, y, and the momentum, p. The yp-plane is called *phase space*. All possible states of the oscillator's dynamics are represented in this phase space of position and momentum. The constant total energy restricts the position and momentum to move in a cycle on an elliptical curve defined by[14]

$$E = \frac{\kappa}{2}y^2 + \frac{1}{2m}p^2$$

The elliptical curve defining the states visited in the oscillatory dynamics of the oscillator is called the *phase portrait*. Each total energy results in a unique phase portrait, an elliptical phase portrait that grows larger as the energy grows. This result is shown in Figure 11.15.

[14] The total energy of our oscillator is

$$E = \frac{\kappa}{2}y^2 + \frac{1}{2m}p^2$$

Dividing by E we find

$$1 = \frac{\kappa}{2E}y^2 + \frac{1}{2mE}p^2 = \frac{y^2}{a^2} + \frac{p^2}{b^2}$$

which is the equation of an ellipse where $a = \sqrt{\frac{2E}{\kappa}}$ and $b = \sqrt{2mE}$ (see Supplement S2).

C11 Classical theory of a damped harmonic oscillator

We found that a mass on a spring or a vibrating bond between two atoms can be modeled as a harmonic oscillator with potential energy

$$V(x) = \frac{1}{2}\kappa(x - x_0)^2$$

and corresponding force

$$F_{\text{spring}} = -\frac{dV}{dx} = -\kappa(x - x_0)$$

where x is the displacement of the oscillator from its mechanically stable position at x_0 and κ is the force constant. The corresponding velocity is the rate of change in the position with time, or

$$v = \frac{dx}{dt}$$

and the linear momentum is $p = mv$.

The motion of this model oscillator is undamped in time. Once it begins to oscillate, it continues to oscillate with fixed frequency of motion and constant energy. However, physical oscillators such as a mass on a spring in the air or a vibrating molecule in a liquid will lose energy to the surroundings over time, damping the motion of the oscillator. To model this phenomenon, we introduce an additional force acting on the mass in the form of a frictional damping force

$$F_{\text{friction}} = -\gamma\frac{dx}{dt} = -\gamma v$$

where $\gamma \geq 0$ and the frictional force is proportional to the velocity. If the velocity is positive, the damping force is in the negative direction, slowing the oscillator. If the velocity is negative, the damping force is in the positive direction, slowing the oscillator. As such, the frictional force acts to reduce the speed, removing energy from the system and slowing the oscillator until the speed eventually reaches zero. This behavior is demonstrated in Figure 11.16 which can be compared with the motion of an undamped harmonic oscillator shown in Figure 11.13.

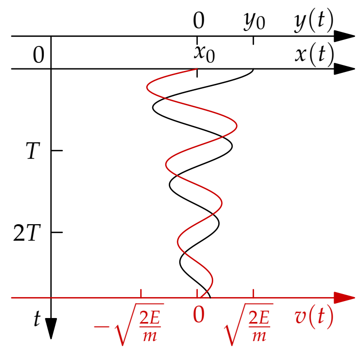


Figure 11.16: The trajectory of the damped harmonic oscillator shown in terms of the position, $x(t)$, the displaced coordinate, $y(t) = x(t) - x_0$, and the velocity, $v(t)$, as a function of t. The period of the undamped oscillator is $T = 2\pi/\omega$.

The acceleration is the rate of change in the velocity with time

$$a = \frac{dv}{dt} = \frac{d^2x}{dt^2}$$

The equation of motion for the oscillator is given by Newton's equation $F = ma$ where m is the mass and a is the acceleration:

$$m\frac{d^2x}{dt^2} = F_{\text{spring}} + F_{\text{friction}} = -\kappa(x - x_0) - \gamma\frac{dx}{dt}$$

We can reform the equation in terms of the variable $y = x - x_0$, representing the displacement of the oscillator from its equilibrium position

$$m\frac{d^2y}{dt^2} = -\kappa y - \gamma\frac{dy}{dt}$$

We would like to solve this equation to determine the displacement of the oscillator, $y(t)$, as a function of time. Substituting $e^{\alpha t}$ for $y(t)$ leads to

$$m\frac{d^2}{dt^2}e^{\alpha t} = -\kappa e^{\alpha t} - \gamma\frac{d}{dt}e^{\alpha t}$$

Evaluating the derivatives, we find

$$m\alpha^2 e^{\alpha t} = -\kappa e^{\alpha t} - \alpha\gamma e^{\alpha t}$$

which reduces to the auxiliary equation

$$\alpha^2 + \alpha\frac{\gamma}{m} + \frac{\kappa}{m} = 0$$

with roots

$$\alpha_\pm = \frac{1}{2}\left[-\frac{\gamma}{m} \pm \sqrt{\left(\frac{\gamma}{m}\right)^2 - \frac{4\kappa}{m}}\right] = -\frac{\gamma}{2m} \pm \sqrt{\left(\frac{\gamma}{2m}\right)^2 - \frac{\kappa}{m}}$$

This leads to the general solution for the displacement as a function of time, written

$$y(t) = c_1 e^{\alpha_+ t} + c_2 e^{\alpha_- t}$$

Let's consider the nature of the roots, $\alpha_\pm$, that can be purely imaginary, complex, or real depending on the magnitude of γ. In the case that $\gamma = 0$, there is no friction and we recover the pure imaginary roots

$$\alpha_\pm = \pm i\sqrt{\frac{\kappa}{m}} = \pm i\omega$$

associated with undamped oscillatory motion. In the case that $0 < \gamma < 2\kappa$, there is low friction and the roots will be complex, with real and imaginary terms

$$\alpha_\pm = -\frac{\gamma}{2m} \pm \sqrt{\left(\frac{\gamma}{2m}\right)^2 - \omega^2} = -\frac{\gamma}{2m} \pm i\omega'$$

where

$$\omega' = \sqrt{\omega^2 - \left(\frac{\gamma}{2m}\right)^2} = \omega\sqrt{1 - \left(\frac{\gamma}{2m\omega}\right)^2}$$

For these complex roots, there is an exponential damping term, with rate of damping $\gamma/2m$, and an oscillatory term, with frequency ω' shifted relative to the frequency of undamped motion. In this case, the motion of the oscillator is *underdamped* (see Figure 1.12). Finally, in the case that $\gamma \geq 2\kappa$, there is high friction and the roots are purely real:

$$\alpha_\pm = -\frac{\gamma}{2m} \pm \sqrt{\left(\frac{\gamma}{2m}\right)^2 - \omega^2}$$

In this case, the motion of the oscillator is *overdamped* (see Figure 1.12).

In each of the three cases, we can write

$$\alpha_\pm = \alpha_0 \pm \Delta\alpha$$

where

$$\alpha_0 = -\frac{\gamma}{2m} \qquad \Delta\alpha = \sqrt{\left(\frac{\gamma}{2m}\right)^2 - \omega^2}$$

and $\Delta\alpha$ may be real or imaginary.[15] With this notation, our solution takes the form

$$y(t) = c_1 e^{\alpha_+ t} + c_2 e^{\alpha_- t} = e^{\alpha_0 t}\left(c_1 e^{\Delta\alpha t} + c_2 e^{-\Delta\alpha t}\right)$$

[15] In the special case $\gamma = 2m\omega$ we find $\Delta\alpha = 0$, the double root $\alpha = -\gamma/2m$, and the solution

$$y(t) = c_1 e^{\alpha t} + c_2 t e^{\alpha t}$$

In the modeling of physical systems, it is possible but very improbable that the friction, frequency, and mass will exactly satisfy the equality $\gamma = 2m\omega$. As such, this special case will not be discussed in detail.

Considering the initial conditions

$$y(0) = y_0 \qquad \left.\frac{dy}{dt}\right|_{t=0} = 0$$

we find

$$y(0) = c_1 + c_2 = y_0$$

and

$$\begin{aligned}
\left.\frac{dy}{dt}\right|_{t=0} &= \frac{d}{dt}\left[e^{\alpha_0 t}\left(c_1 e^{\Delta\alpha t} + c_2 e^{-\Delta\alpha t}\right)\right] \\
&= \left[\alpha_0 e^{\alpha_0 t}\left(c_1 e^{\Delta\alpha t} + c_2 e^{-\Delta\alpha t}\right) + \Delta\alpha\, e^{\alpha_0 t}\left(c_1 e^{\Delta\alpha t} - c_2 e^{-\Delta\alpha t}\right)\right]_{t=0} \\
&= \alpha_0 (c_1 + c_2) + \Delta\alpha\,(c_1 - c_2) = 0
\end{aligned}$$

As such, $c_2 = y_0 - c_1$ and

$$c_1 = -\frac{(\alpha_0 - \Delta\alpha)y_0}{2\Delta\alpha} \qquad c_2 = \frac{(\alpha_0 + \Delta\alpha)y_0}{2\Delta\alpha}$$

Note that when $\gamma = 0$, $\alpha_0 = 0$ and we recover the coefficients expected for the harmonic oscillator in the absence of friction, where $c_1 = c_2 = y_0/2$. For the general case, we find

$$\begin{aligned}
y(t) &= y_0 e^{\alpha_0 t}\left[\cosh(\Delta\alpha t) - \frac{\alpha_0}{\Delta\alpha}\sinh(\Delta\alpha t)\right] \\
v(t) &= y_0 e^{\alpha_0 t}\left[-\frac{\omega^2}{\Delta\alpha}\sinh(\Delta\alpha t)\right]
\end{aligned}$$

where high friction leads to a real $\Delta\alpha$, real roots, and exponential damping. In contrast, low friction leads to an imaginary $\Delta\alpha$, complex roots, and an exponentially damped oscillator. We can also write the linear momentum as

$$p(t) = y_0 e^{\alpha_0 t}\left[-\frac{m\omega^2}{\Delta\alpha}\sinh(\Delta\alpha t)\right]$$

The solution is shown in Figure 11.16.

The total energy of the damped harmonic oscillator is defined

$$E(t) = \frac{1}{2}mv(t)^2 + \frac{1}{2}\kappa y(t)$$

An example of the time-dependence of $E(t)$ is shown in Figure 11.17 for an underdamped harmonic oscillator for which $0 < \gamma < 2m\omega$. For $\gamma > 0$, the vibration of the oscillator is damped and the total energy decreases monotonically from its initial value

$$E(0) = \frac{1}{2}\kappa y_0^2$$

When the kinetic energy reaches a maximum, the velocity is maximized as is the rate of frictional damping. This is reflected in the variation in the total energy, where periods of higher kinetic energy are also periods of greater energy loss. This leads to the stepping behavior observed in the total

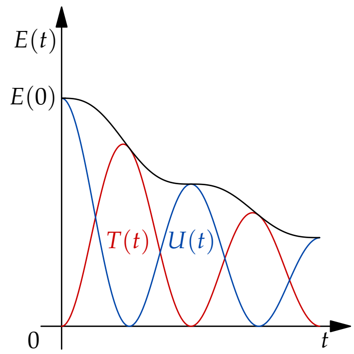


Figure 11.17: The kinetic energy, $T(t)$, potential energy, $U(t)$, and total energy $E(t) = T(t) + U(t)$ of the damped harmonic oscillator. The total energy is monotonically decreasing as a function of time (black line).

energy as a function of time. Compare this behavior to that of the undamped harmonic oscillator shown in Figure 11.14 where the trajectory performs a repeating elliptical orbit in phase space.

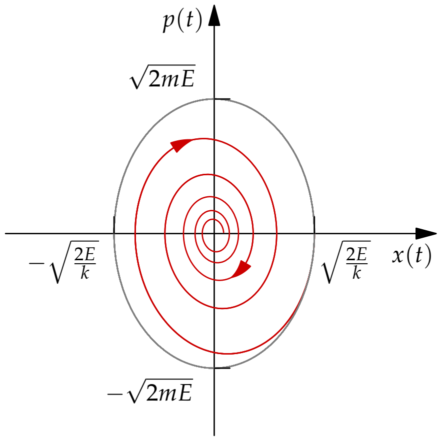


Figure 11.18: The phase portrait of the damped harmonic oscillator (red). The gray ellipse is formed by the values of position and momentum consistent with the initial energy $E(0)$. The continuous energy loss of the damped oscillator is reflected in the narrowing of the inward spiral with increasing time.

All possible states of the oscillator's dynamics are represented in this *phase space* of position and momentum. Our solutions for $y(t)$ and $p(t)$ define a trajectory on the yp-plane called the *phase portrait*. For an undamped harmonic oscillator, the position and momentum move in a repeating cycle restricted to an elliptical curve defined by the constant total energy

$$E(t) = \frac{\kappa}{2}y(t)^2 + \frac{1}{2m}p(t)^2 = E(0)$$

For a damped harmonic oscillator, the total energy of the oscillator decreases with time. As a result, the breadth of the elliptical path decreases with time leading to a phase portrait with the form of an inward elliptical spiral. This behavior is depicted in Figure 11.18 for a harmonic oscillator for which $0 < \gamma < 2m\omega$ and the motion is underdamped. This behavior can be compared to that of the undamped harmonic oscillator shown in Figure 11.15.

D_{11} Power series solutions to special equations in quantum theory

A number of special ordinary differential equations arise in the quantum theory of matter when solving the Schrödinger equation for electronic energy of a one electron atom or the rotations and vibrations of a diatomic molecule. These special differential equations may be solved using power series. In each case, the resulting power series represents a type of *special function* that finds wide use in the physical sciences.[16]

Special functions explored in this complement include the Hermite polynomials, found in the quantum theory of vibrational motion, the Laguerre polynomials, found in the quantum theory of the hydrogen atom, and the Legendre polynomials, found in the quantum theory of rotational motion and multipole expansions in the classical theory of electricity and magnetism.

[16] A classic reference for the properties of special functions is *Abramowitz and Stegun* or simply *AS* which still serves as a valuable compendium of special functions and their properties.

Milton Abramowitz and Irene A. Stegun, editors. *Handbook of Mathematical Functions with Formulas, Graphs, and Mathematical Tables [1964]*. Dover Publications, first edition, 1972. ISBN 0-486-61272-4

Hermite's equation and Hermite polynomials

In the quantum theory of the harmonic oscillator, a special differential equation appears:

$$\frac{d^2}{dx^2}y(x) - 2x\frac{d}{dx}y(x) + 2\alpha y(x) = 0 \tag{11.25}$$

where α is a constant. This is known as *Hermite's equation*.[17] Proposing a power series solution of the form

[17] Named for French mathematician *Charles Hermite* (1822-1901).

$$y(x) = \sum_{n=0}^{\infty} a_n x^n$$

we find that Equation 11.25 can be written

$$\sum_{n=0}^{\infty} a_n n(n-1)x^{n-2} - 2x\sum_{n=0}^{\infty} a_n n x^{n-1} + 2\alpha\sum_{n=0}^{\infty} a_n x^n = 0 \tag{11.26}$$

In order to identify the recursion relation that defines the coefficients in our series, we must transform the first two series so that they can be combined with the third.

In the first series, the coefficients are proportional to $n(n-1)$, so that the $n = 0$ and $n = 1$ terms are always zero. Removing the $n = 0$ and $n = 1$ terms from the first series results in

$$\sum_{n=0}^{\infty} a_n n(n-1)x^{n-2} \to \sum_{n=2}^{\infty} a_n n(n-1)x^{n-2}$$

Now the series starts with $n = 2$, but we would like it to start from $n = 0$. As such, we shift the index by $n \to n+2$ so that[18]

[18] Equivalently, you can introduce a new index $n' = n - 2$, substituting $n \to n' + 2$. You can then rewrite the new index n' as n before combining the sums.

$$\sum_{n=2}^{\infty} a_n n(n-1)x^{n-2} \to \sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)x^n$$

For the second series, we simply absorb the factor of x in the sum, so that

$$-2x\sum_{n=0}^{\infty} a_n n x^{n-1} = -2\sum_{n=0}^{\infty} a_n n x^n$$

Inserting these results into Equation 11.26 leads to

$$\sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)x^n - 2\sum_{n=0}^{\infty} a_n n x^n + 2\alpha\sum_{n=0}^{\infty} a_n x^n = 0$$

Combining the sums, we find

$$\sum_{n=0}^{\infty} \left[a_{n+2}(n+2)(n+1) - 2a_n n + 2\alpha a_n\right] x^n = 0$$

and the condition

$$a_{n+2}(n+2)(n+1) - 2a_n n + 2\alpha a_n = 0$$

This condition can be used to derive a recursion relation relating a_{n+2} to a_n.

In particular, we find the recursion relation

$$a_{n+2} = -\frac{2(\alpha - n)}{(n+2)(n+1)}a_n$$

The even indices can be generated from a_0 as[19]

$$a_2 = -\frac{2\alpha}{2}a_0 \qquad a_4 = -\frac{2(\alpha-2)}{4\cdot 3}a_2 = \frac{2^2\alpha(\alpha-2)}{4!}a_0$$

leading to the following power series in even powers of x:

$$y_0(x) = a_0\left[1 - \frac{2\alpha}{2!}x^2 + \frac{2^2\alpha(\alpha-2)}{4!}x^4 - + \ldots\right]$$

The odd indices can be generated from a_1 as

$$a_3 = -\frac{2(\alpha-1)}{3\cdot 2}a_1 \quad a_5 = -\frac{2(\alpha-3)}{5\cdot 4}a_3 = \frac{2^2(\alpha-3)(\alpha-1)}{5!}a_1$$

leading to the following power series in odd powers of x:

$$y_1(x) = a_1\left[x - \frac{2(\alpha-1)}{3!}x^3 + \frac{2^2(\alpha-3)(\alpha-1)}{5!}x^5 - + \ldots\right]$$

The overall solution is written as a linear *superposition* of the two independent solutions $y_0(x)$ and $y_1(x)$. The remaining coefficients a_0 and a_1 are defined by the boundary conditions.

Let's examine the results for various values of the parameter α. We will find that the solutions to Hermite's equation form a series of polynomial equations known as the *Hermite polynomials*.[20] In defining the Hermite polynomials, it is helpful to consider the even power series, $y_0(x)$, and odd power series, $y_1(x)$, separately. When $\alpha = 0$, Hermite's equation is

$$\frac{d^2}{dx^2}y(x) - 2x\frac{d}{dx}y(x) = 0$$

with a solution defined by the even power series

$$y_0(x) = a_0$$

as all higher order terms contain a multiplicative factor of α and are therefore zero. This is the Hermite polynomial $H_0(x) = 1$ for $a_0 = 1$. For $\alpha = 1$, Hermite's equation is

$$\frac{d^2}{dx^2}y(x) - 2x\frac{d}{dx}y(x) + 2y(x) = 0$$

with a solution defined by the odd power series

$$y_1(x) = a_1 x$$

as all higher order terms in the series contain a multiplicative factor of $(\alpha - 1)$ and are zero. This is the Hermite polynomial $H_1(x) = 2x$ when $a_1 = 2$. When

[19] The negative sign in the recursion relation signals the fact that the coefficients lead to an alternating series.

[20] The Hermite polynomials were originally described by *Pierre-Simon Laplace* (1749-1827).

$\alpha = 2$, Hermite's equation is

$$\frac{d^2}{dx^2}y(x) - 2x\frac{d}{dx}y(x) + 4y(x) = 0$$

with a solution defined by the even power series

$$y_0(x) = a_0\left(1 - 2x^2\right)$$

which is the Hermite polynomial $H_2(x) = 4x - 2$ when $a_0 = -2$.

Repeating this process, we find that when $\alpha = 3$, the Hermite polynomial $H_3(x) = 8x^3 - 12x$ when $a_1 = -12$. When $\alpha = 4$, the Hermite polynomial $H_4(x) = 16x^4 - 48x^2 + 12$ when $a_0 = 12$. The first five Hermite polynomials are presented in Figure 11.19.

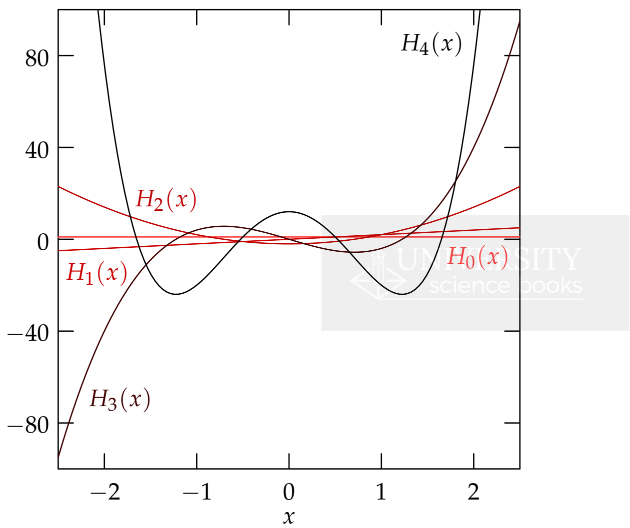


Figure 11.19: Variation in the first five Hermite polynomials $H_n(x)$ over the range $x \in [-2.5, 2.5]$.

Our success in solving Hermite's equation demonstrates the applicability of the power series method to the solution of linear second order differential equations with non-constant coefficients. The resulting solutions to Hermite's equation consist of an infinite number of Hermite polynomials. The Hermite polynomials possess special properties that will be explored in Chapter 13 in the complements.

Laguerre's equation and Laguerre polynomials

In the quantum theory of the one electron atom a special differential equation describes the radial dependence of the electron's wave function:

$$x\frac{d^2}{dx^2}y(x) - (1-x)\,\frac{d}{dx}y(x) + \alpha y(x) = 0 \tag{11.27}$$

where α is a constant. This is known as *Laguerre's equation*.[21] Proposing a power series solution

$$y(x) = \sum_{n=0}^{\infty} a_n x^n$$

[21] Named for French mathematician *Edmond Laguerre* (1834-1886).

we find that Equation 11.27 can be written

$$x \sum_{n=0}^{\infty} a_n n(n-1)x^{n-2} - (1-x) \sum_{n=0}^{\infty} a_n n x^{n-1} + \alpha \sum_{n=0}^{\infty} a_n x^n = 0 \tag{11.28}$$

We must transform the first two series so that they can be combined with the third.

In the first series, the coefficients are proportional to n, so the $n = 0$ term is always zero. Removing the $n = 0$ term from the first series and absorbing the factor of x leads to

$$x \sum_{n=0}^{\infty} a_n n(n-1)x^{n-2} \to \sum_{n=1}^{\infty} a_n n(n-1)x^{n-1}$$

Shifting the index by $n \to n+1$ results in[22]

$$\sum_{n=1}^{\infty} a_n n(n-1)x^{n-1} \to \sum_{n=0}^{\infty} a_{n+1}(n+1)n x^n$$

which is in the desired form in terms of the range of the index n and the sum over x^n, weighted by constant coefficients. We transform the second series by distributing the factor of $(1-x)$ resulting in two series

$$(1-x) \sum_{n=0}^{\infty} a_n n x^{n-1} = \sum_{n=0}^{\infty} a_n n x^{n-1} - \sum_{n=0}^{\infty} a_n n x^n$$

In the first series the coefficients are proportional to n so the $n = 0$ term is always zero. Removing the $n = 0$ term from the first series leads to

$$\sum_{n=0}^{\infty} a_n n x^{n-1} \to \sum_{n=1}^{\infty} a_n n x^{n-1}$$

Finally, shifting the index in the first series by $n \to n+1$ results in

$$\sum_{n=1}^{\infty} a_n n x^{n-1} \to \sum_{n=0}^{\infty} a_{n+1}(n+1)x^n$$

Inserting these results in Equation 11.28 leads to

$$\sum_{n=0}^{\infty} \left[a_{n+1}(n+1)n + a_{n+1}(n+1) - a_n n + \alpha a_n\right] x^n = 0$$

and the condition

$$a_{n+1}(n+1)n + a_{n+1}(n+1) - a_n n + \alpha a_n = 0$$

This leads to the recursion relation[23]

$$a_{n+1} = -\frac{\alpha - n}{(n+1)^2} a_n$$

The coefficients can be generated starting from a_0 as

$$a_1 = -\alpha a_0 \qquad a_2 = \frac{(\alpha-1)\alpha}{(2!)^2} a_0 \qquad a_3 = -\frac{(\alpha-2)(\alpha-1)\alpha}{(3!)^2} a_0$$

[22] Equivalently, you can introduce a new index $n' = n - 1$, substituting $n \to n' + 1$. You can then rewrite the new index n' as n before combining the sums.

[23] The negative sign in the recursion relation signals the fact that the coefficients lead to an alternating series.

leading to the power series solution

$$y(x) = a_0 \left[1 - \alpha x + \frac{(\alpha-1)\alpha}{(2!)^2}x^2 - \frac{(\alpha-2)(\alpha-1)\alpha}{(3!)^2}x^3 + - \ldots\right]$$

Let's examine our results for various values of the parameter α. We will find that the solutions to Laguerre's equation form a series of polynomial equations known as the *Laguerre polynomials*. When $\alpha = 0$, Laguerre's equation is

$$x\frac{d^2}{dx^2}y(x) - (1-x)\frac{d}{dx}y(x) = 0$$

with the solution

$$y(x) = a_0$$

as all higher order terms contain a multiplicative factor of α and are therefore zero. This is the Laguerre polynomial $L_0(x) = 1$ for $a_0 = 1$. For $\alpha = 1$, Laguerre's equation is

$$x\frac{d^2}{dx^2}y(x) - (1-x)\frac{d}{dx}y(x) + y(x) = 0$$

and the solution is

$$y(x) = a_0(1-x)$$

as all higher order terms in the series contain a multiplicative factor of $(\alpha - 1)$ and are zero. This is the Laguerre polynomial $L_1(x) = 1 - x$ when $a_0 = -1$.

Repeating this process for $\alpha = 2$, we find the Laguerre polynomial $L_2(x) = \frac{1}{2}\left(x^2 - 4x + 2\right)$ when $a_0 = 1$. When $\alpha = 3$, we find the Laguerre polynomial $L_3(x) = \frac{1}{6}\left(-x^3 + 9x^2 - 18x + 6\right)$ when $a_0 = 1$. The first four Laguerre polynomials are depicted in Figure 11.20.

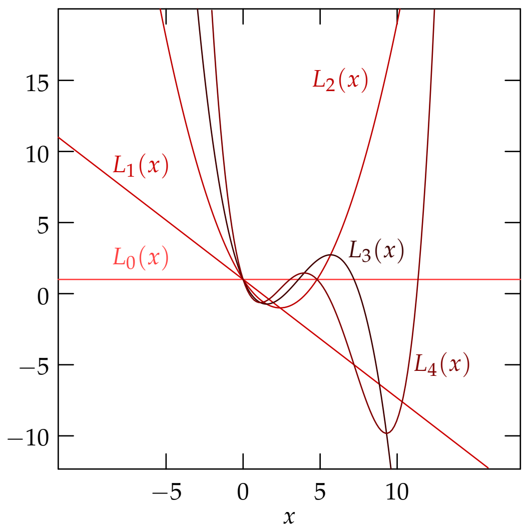


Figure 11.20: Variation in the first five Laguerre polynomials $L_n(x)$ over the range $x \in [-10, 15]$.

The Laguerre polynomials possess special properties that will be explored in Chapter 13 in the complements.

Legendre's equation and Legendre polynomials

In the quantum theory of rotational motion of a diatomic molecule, a special differential equation describes the rotational wave function:

$$(1-x^2)\frac{d^2}{dx^2}y(x) - 2x\frac{d}{dx}y(x) + l(l+1)y(x) = 0 \tag{11.29}$$

where l is a constant. This is known as *Legendre's equation*.[24] Proposing a power series solution

$$y(x) = \sum_{n=0}^{\infty} a_n x^n$$

we find that Equation 11.29 can be written

$$(1-x^2)\sum_{n=0}^{\infty} a_n n(n-1)x^{n-2} - 2x\sum_{n=0}^{\infty} a_n n x^{n-1} + l(l+1)\sum_{n=0}^{\infty} a_n x^n = 0 \tag{11.30}$$

We must transform the first two series so that they can be combined with the third.

We transform the first series by distributing the factor of $(1-x^2)$, resulting in two series

$$(1-x^2)\sum_{n=0}^{\infty} a_n n(n-1)x^{n-2} \to \sum_{n=0}^{\infty} a_n n(n-1)x^{n-2} - \sum_{n=0}^{\infty} a_n n(n-1)x^n$$

In the first series the coefficients are proportional to $n(n-1)$, so that the $n=0$ and $n=1$ terms are always zero. Removing the $n=0$ and $n=1$ terms from the first series results in

$$\sum_{n=0}^{\infty} a_n n(n-1)x^{n-2} \to \sum_{n=2}^{\infty} a_n n(n-1)x^{n-2}$$

Now the series starts with $n=2$ but we would like it to start from $n=0$. As such, we shift the index by $n \to n+2$ so that[25]

$$\sum_{n=2}^{\infty} a_n n(n-1)x^{n-2} \to \sum_{n=0}^{\infty} a_{n+2}(n+2)(n+1)x^n$$

For the second series in Equation 11.30, we absorb the factor of $-2x$, resulting in

$$-2x\sum_{n=0}^{\infty} a_n n x^{n-1} = -2\sum_{n=0}^{\infty} a_n n x^n$$

Inserting these results in Equation 11.30 leads to

$$\sum_{n=0}^{\infty}\Big[a_{n+2}(n+2)(n+1) - a_n n(n-1) - 2a_n n \\ + l(l+1)a_n\Big]x^n = 0$$

and the condition

$$a_{n+2}(n+2)(n+1) - a_n n(n-1) - 2a_n n + l(l+1)a_n = 0$$

[24] Named for French mathematician *Adrien-Marie Legendre* (1752-1833).

[25] Equivalently, you can introduce a new index $n' = n-2$, substituting $n \to n'+2$. You can then rewrite the new index n' as n before combining the sums.

We find the recursion relation

$$a_{n+2} = \frac{(n+1)n - l(l+1)}{(n+2)(n+1)} a_n = -\frac{[l + (n+1)]\,(l-n)}{(n+2)(n+1)} a_n$$

where the negative sign leads to an alternating series.

The even indices can be generated from a_0 as

$$a_2 = -\frac{(l+1)l}{2} a_0 = -\frac{(l+1)l}{2!} a_0$$
$$a_4 = -\frac{(l+3)(l-2)}{4 \cdot 3} a_2 = \frac{(l+3)(l-2)(l+1)l}{4!} a_0$$

and so on, leading to the following power series in even powers of x:

$$y_0(x) = a_0 \Big[1 - \frac{(l+1)l}{2!} x^2 + \frac{(l+3)(l-2)(l+1)l}{4!} x^4 - + \ldots \Big]$$

The odd indices can be generated from a_1 as

$$a_3 = -\frac{(l+2)(l-1)}{3 \cdot 2} a_1 = -\frac{(l+2)(l-1)}{3!} a_1$$
$$a_5 = -\frac{(l+4)(l-3)}{5 \cdot 4} a_3 = \frac{(l+4)(l-3)(l+2)(l-1)}{5!} a_1$$

and so on, leading to the following power series in odd powers of x:

$$y_1(x) = a_1 \Big[x - \frac{(l+2)(l-1)}{3!} x^3 + \frac{(l+4)(l-3)(l+2)(l-1)}{5!} x^5 - + \ldots \Big]$$

The overall solution is written as a linear *superposition* of the two independent solutions $y_0(x)$ and $y_1(x)$. The remaining coefficients a_0 and a_1 are defined by the boundary conditions.

Let's examine our results for various values of the parameter l. We will find that the solutions to Legendre's equation form a series of polynomial equations known as the *Legendre polynomials*. In defining the Legendre polynomials, it is helpful to consider the even power series, $y_0(x)$, and odd power series, $y_1(x)$, separately. When $l = 0$, Legendre's equation is

$$(1 - x^2) \frac{d^2}{dx^2} y(x) - 2x \frac{d}{dx} y(x) = 0$$

and the solution is

$$y(x) = a_0$$

as all higher order terms contain a multiplicative factor of l and are therefore zero. This is the Legendre polynomial $P_0(x) = 1$ for $a_0 = 1$. For $l = 1$, Legendre's equation is

$$(1 - x^2) \frac{d^2}{dx^2} y(x) - 2x \frac{d}{dx} y(x) + 2y(x) = 0$$

and the solution is

$$y(x) = a_1 x$$

as all higher order terms in the series contain a multiplicative factor of $(l-1)$ and are therefore zero. This the Legendre polynomial $P_1(x) = x$ when $a_1 = 1$. When $l = 2$, Legendre's equation is

$$(1-x^2)\frac{d^2}{dx^2}y(x) - 2x\frac{d}{dx}y(x) + 6y(x) = 0$$

and the solution is

$$y(x) = a_0\left(1 - 3x^2\right)$$

which is the Legendre polynomial $P_2(x) = \frac{1}{2}\left(3x^2 - 1\right)$ when $a_0 = -\frac{1}{2}$. When $l = 3$, Legendre's equation is

$$(1-x^2)\frac{d^2}{dx^2}y(x) - 2x\frac{d}{dx}y(x) + 12y(x) = 0$$

and the solution is

$$y(x) = a_1\left(x - \frac{5}{3}x^3\right)$$

which is the Legendre polynomial $P_3(x) = \frac{1}{2}\left(5x^3 - 3x\right)$ when $a_1 = -3$. The first four Legendre polynomials are depicted in Figure 11.21. The Legendre polynomials possess special properties that will be explored in Chapter 13 in the complements.

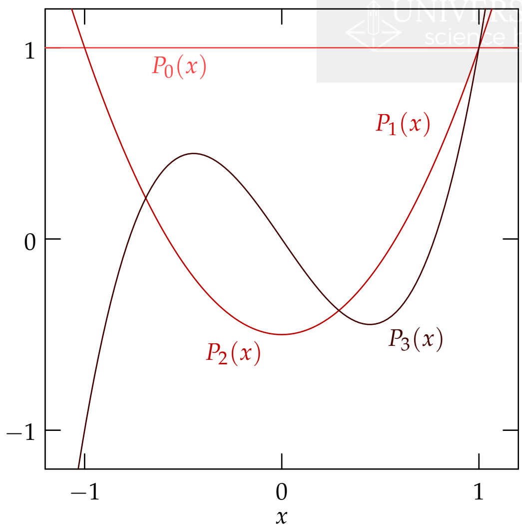


Figure 11.21: Variation in the first four Legendre polynomials $P_l(x)$ over the range $x \in [-1, 1]$.

The differential equations discussed in this complement play a special role in the quantum theory of atoms and molecules. We have found that differential equations can be solved using one or more *common functions* such as the exponentials and sinusoids.

The solution of these three differential equations using the power series method led to the discovery of three new special functions, the Hermite, Laguerre, and Legendre polynomials. It is good to remember that at one time the exponential function was a *special function* as well.[26] Through regular use, we come to regard special functions as common.

[26] The constant e, also known as *Euler's number* or *Napier's constant*, was not well defined until the late 17th century.

E_{11} End-of-chapter problems

> How can it be that mathematics, being after all a product of human thought independent of experience, is so admirably adapted to the objects of reality?
>
> Albert Einstein

Warm-ups

11.1 Consider the following second order ordinary differential equations.

(a) $\dfrac{d^2y(x)}{dx^2} - 4y(x) = 0$ (b) $\dfrac{d^2y(x)}{dx^2} + 2\,\dfrac{dy(x)}{dx} + 4y(x) = 0$

(c) $\dfrac{d^2y(x)}{dx^2} + 9y(x) = 0$ (d) $\dfrac{d^2y(x)}{dx^2} + 6\,\dfrac{dy(x)}{dx} = 0$

In each case, assume the solution $y(x) = \mathrm{e}^{\alpha x}$. Find the auxiliary equation and determine the two roots $\alpha_{\pm}$. Compose the overall solution

$$y(x) = c_1\,\mathrm{e}^{\alpha_+ x} + c_2\,\mathrm{e}^{\alpha_- x}$$

Apply the boundary conditions $y(0) = 0$ and $\left.\dfrac{dy(x)}{dx}\right|_{x=0} = 1$ to determine the coefficients c_1 and c_2.

11.2 Consider the linear second order differential equation

$$\frac{d^2y(x)}{dx^2} + 2\,\frac{dy(x)}{dx} + y(x) = 0$$

(a) Assume the solution $y(x) = \mathrm{e}^{\alpha x}$. Find the auxiliary equation and determine the roots $\alpha_{\pm}$. You should find double roots where $\alpha_+ = \alpha_- = \alpha$.

(b) Prove that

$$y(x) = c_1\,\mathrm{e}^{\alpha x} + c_2\,x\,\mathrm{e}^{\alpha x}$$

is a solution to the differential equation.

11.3 Consider the general second order ordinary differential equation

$$\frac{d^2y(x)}{dx^2} + a(x)\,\frac{dy(x)}{dx} + b(x)\,y(x) = 0$$

Prove that if $y_1(x)$ and $y_2(x)$ are each solutions to the differential equation, so is the linear superposition

$$y(x) = c_1\,y_1(x) + c_2\,y_2(x)$$

11.4 Reform the following sums so that the first term in the sum is $n = 0$

(a) $\displaystyle\sum_{n=2}^{\infty}(n-2)a_{n-2}x^n$ (b) $\displaystyle\sum_{n=2}^{\infty}n(n-1)a_n x^{n-2}$ (c) $\displaystyle\sum_{n=1}^{\infty}n a_n x^{n-1}$

11.5 Consider the following recursion relations where $n \geq 0$. In each case, derive a general expression for the coefficient a_n in terms of a_0.

(a) $a_{n+1} = -\dfrac{a_n}{(n+1)^2}$ (b) $a_{n+1} = \dfrac{n+2}{2(n+1)} a_n$ (c) $a_{n+1} = -\dfrac{2a_n}{n+1}$

11.6 Consider the second order differential equation

$$\frac{d^2}{dx^2} y(x) - y(x) = 0$$

(a) Find two linearly independent power series solutions of the form

$$\sum_{n=0}^{\infty} a_n x^n$$

Start by determining recursion relations for the coefficients a_n. You should find two recursion relations, one for n odd and one for n even.

(b) In each case, derive a general expression for a_n in terms of a_0 or a_1.

(c) Identify the common functions representing each series.

Homework exercises

11.7 The general solution for a homogeneous second order ordinary differential equation of the form

$$y(x) = c_1 \, e^{ibx} + c_2 \, e^{-ibx}$$

can be rewritten

$$y(x) = c_1{}' \cos(bx) + c_2{}' \sin(bx)$$

Derive expressions for $c_1{}'$ and $c_2{}'$ in terms of c_1 and c_2.

11.8 The position of an oscillator, $x(t)$, as a function of time, t, satisfies the second order differential equation

$$\frac{d^2 x(t)}{dt^2} + \omega^2 x(t) = 0$$

where ω is a constant. Solve this equation for $x(t)$ given the following initial conditions.

(a) $x(0) = 0$ and $\left.\dfrac{dx}{dt}\right|_{t=0} = u_0$ (b) $x(0) = x_0$ and $\left.\dfrac{dx}{dt}\right|_{t=0} = u_0$

In each case, prove that $x(t)$ oscillates with frequency $\nu = \dfrac{\omega}{2\pi}$ and period $T = \dfrac{2\pi}{\omega} = \dfrac{1}{\nu}$.

11.9 The second order differential equation

$$\frac{d^2 f(x)}{dx^2} + \frac{25\pi^2}{L^2} f(x) = 0$$

models the displacement, $f(x)$, of a plucked string that is fixed at each end leading to the boundary conditions $f(0) = f(L) = 0$ and $\frac{df}{dx}|_{x=0} = 5$.

(a) Determine the general solution of the form

$$f(x) = c_1 \, e^{\alpha_+ x} + c_2 \, e^{\alpha_- x}$$

(b) Simplify your result by expressing your solution in terms of a sinusoidal function.

11.10 Consider the second order inhomogeneous ordinary differential equation describing the height, $z(t)$, of a mass, m, falling under the force of gravity with constant rate of acceleration, g, and experiencing a frictional drag force proportional to the speed, $u(t) = \dfrac{dz(t)}{dt}$, written

$$m \frac{d^2 z(t)}{dt^2} = -\gamma \frac{dz(t)}{dt} + mg$$

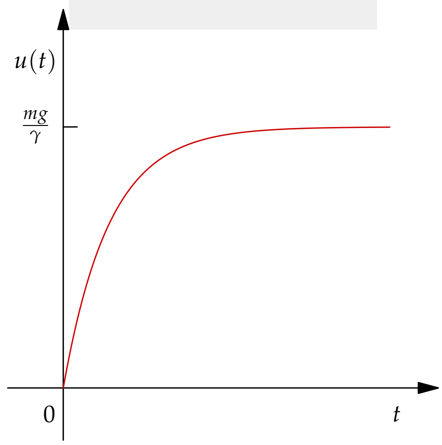
where γ is the friction constant.

(a) Show that this equation is equivalent to the first order ordinary differential equation for the speed of the particle

$$\frac{du(t)}{dt} + \frac{\gamma}{m} u(t) = g$$

(b) Solve the differential equation for $u(t)$ given that $u(0) = 0$.

(c) Show that as $t \to \infty$, the speed of the falling mass approaches a constant terminal speed $u_T = \dfrac{mg}{\gamma}$ as shown in the figure below.



11.11 Determine the coefficients a_n for which the equation

$$\sum_{n=1}^{\infty} n a_n x^{n-1} + 2 \sum_{n=0}^{\infty} a_n x^n = 0$$

is satisfied. Substitue the resulting coefficients a_n in the power series

$$\sum_{n=0}^{\infty} a_n x^n$$

and identify the corresponding function.

11.12* Consider the differential equation

$$(x^2+1)\frac{d^2}{dx^2}y(x) - 4x\frac{d}{dx}y(x) + 6y(x) = 0$$

with the boundary conditions $y(0) = 1$ and $y'(0) = 2$.

(a) Propose a solution in the form of the power series

$$y(x) = \sum_{n=0}^{\infty} a_n x^n$$

Derive the recursion relation

$$a_{n+2} = -\frac{(n-2)(n-3)}{(n+2)(n+1)}\, a_n$$

(b) Using the recursion relation above, determine the four coefficients a_n that are non-zero in terms of a_0 and a_1.

(c) Apply the boundary conditions to determine the solution for $y(x)$.

11.13* Show that

$$c_1\cos(\omega t) + c_2\sin(\omega t) = A\sin(\omega t + \varphi)$$

where

$$A = \sqrt{c_1{}^2 + c_2{}^2} \qquad \varphi = \tan^{-1}\left(\frac{c_1}{c_2}\right)$$

or equivalently

$$c_1\cos(\omega t) + c_2\sin(\omega t) = A\cos(\omega t + \varphi)$$

where

$$A = \sqrt{c_1{}^2 + c_2{}^2} \qquad \varphi = \tan^{-1}\left(-\frac{c_2}{c_1}\right)$$

HINT: Make use of the trigonometric identities provided in Supplement S3. Consider working backward from the identity $\cos(\alpha+\beta) = \cos(\alpha)\cos(\beta) - \sin(\alpha)\sin(\beta)$. Also note that $\sin\left(\tan^{-1}(x)\right) = \frac{x}{\sqrt{x^2+1}}$ and $\cos\left(\tan^{-1}(x)\right) = \frac{1}{\sqrt{x^2+1}}$.

11.14* Consider the differential equation

$$\frac{d^2}{dx^2}y(x) - \frac{d}{dx}y(x) = y(x)$$

with the boundary conditions $y(0) = 0$ and $y'(0) = 1$.

(a) Derive the corresponding auxiliary equation and show that the two roots are $\alpha_+ = \varphi$ and $\alpha_- = 1 - \varphi$ where

$$\varphi = \frac{1}{2}\left(1+\sqrt{5}\right)$$

is the *golden ratio*.

(b) Using the result from (a) and the boundary conditions, determine the solution for $y(x)$.

(c) Propose a solution to the original differential equation in the form of the power series

$$y(x) = \sum_{n=0}^{\infty} a_n x^n$$

and show that the coefficients

$$a_n = \frac{1}{n!} f_n$$

where f_n are the *Fibonacci numbers* and $f_0 = 0$, $f_1 = 1$, $f_2 = 1$, $f_3 = 2$, $f_4 = 3$, $f_5 = 5$, $f_6 = 8$, and so on.

(d) Expand your result from (b) in a Maclaurin series. Compare that series term-by-term with the result from (c). Show that

$$f_n = \frac{1}{\sqrt{5}}\left[\left(\frac{1+\sqrt{5}}{2}\right)^n - \left(\frac{1-\sqrt{5}}{2}\right)^n\right] = \frac{1}{\sqrt{5}}\left[\varphi^n - (1-\varphi)^n\right]$$

This equation relating the Fibonacci numbers to the golden mean is known as *Binet's formula*.

11.15* Consider the second order differential equation known as *Bessel's equation*

$$x^2\frac{d^2y(x)}{dx^2} + x\frac{dy(x)}{dx} + (x^2 - c^2)y(x) = 0$$

where c is a constant. The method we have developed in this chapter cannot be used to solve this problem as the term $x^2y(x)$ leads to terms of order x^{n+2} in addition to the usual terms of order x^n.

(a) Propose a solution of the form $y(x) = x^r \sum_{n=0}^{\infty} a_n x^n$. Inserting into Bessel's equation will lead to a sum of two power series. Assuming that $a_0 \neq 0$, show that a consistent solution can be found if $(n+r)(n+r-1)+(n+r)-c^2 = 0$ for $n = 0$. Solve that equation to identify the two allowed values of $r = c$ and $r = -c$.

(b) For $r = c$, show that $a_1 = 0$ and therefore $a_{2n+1} = 0$ for $n \geq 1$.

(c) For $r = c$, determine the recursion relation for the coefficients a_{2n} in terms of a_0. Use your coefficients to determine the solution $y_+(x)$ to Bessel's equation.

(d) Repeat steps (b) and (c) for $r = -c$ to arrive at a second solution $y_-(x)$ to Bessel's equation.