Partial Differential Equations and Fourier Analysis — A Short Introduction

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Preface

This short book is intended for a one-semester course for students in the sciences and engineering after they have taken one year of calculus and one term of ordinary differential equations. For universities on quarter systems, sections labelled "optional" can be omitted without loss of continuity. A course based on this book can be offered to sophomores and juniors.

Examples used in this book are drawn from traditional application areas such as physics and engineering, as well as from biology, music, finance and geophysics. I have tried, whenever appropriate, to emphasize physical motivation and have generally avoided theorems and proofs. I also have tried to teach solution techniques, which will be useful in a student's other courses, instead of the theory of partial differential equations.

I believe that the subjects of partial differential equations and Fourier analysis should be taught as early as feasible in an undergraduate's curriculum. Towards this end the book is written to present the subject matter as simply as possible. Ample worked examples are given at the end of the chapters as a further learning aid. Exercises are provided for the purpose of reinforcing standard techniques learned in class. Tricky problems, whose purpose is mainly to test the student's mental dexterity, are generally avoided.

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Chapter 1

Introduction

1.1 Review of Ordinary Differential Equations

This course is mainly about partial differential equations (PDEs). Previously you have studied ordinary differential equations (ODEs). We will review two common types of ordinary differential equations here. If you have no difficulty with these, you have no problem with the prerequisites for this course.

1.1.1 First and Second Order Equations

Example. *Population growth:*

$$\boxed{\frac{dN}{dt} = rN}\,, \tag{1.1}$$

where $N(t)$ is the population density of a species at time t. The above equation is simply a statement that the rate of population growth, $\frac{dN}{dt}$, is proportional to the population itself, with the proportionality constant r. To solve it, we move all the N's to one side and all the t's to the other side of the equation. (This process is called "separation of variables" in the ODE literature. We will not use this term here as it may get confused with a PDE solution method with the same name which we will discuss later.) Thus:

$$\frac{dN}{N} = r dt. \tag{1.2}$$

Integrating both sides yields:

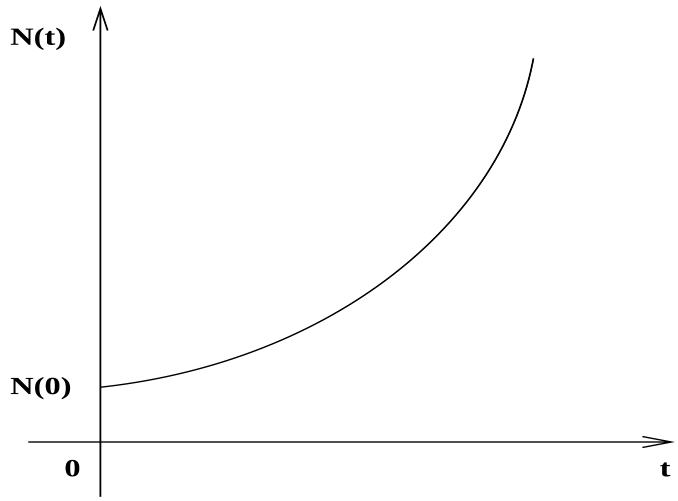


Figure 1.1: Solution to Equation 1.1

$$\ell n N = rt + \text{ constant},$$

which can be rewritten as

$$N(t) = \text{ constant } \cdot e^{rt}.$$

In order for the left-hand side to equal to the right-hand side at $t = 0$, the "constant" in the second equation must be $N(0)$. Thus,

$$\boxed{N(t) = N(0)e^{rt}}\,. \tag{1.3}$$

Population grows exponentially from an initial value $N(0)$, with an e-folding time of r^{-1}. That is, $N(t)$ increases by a factor of e with every increment of r^{-1} in t. The solution is plotted in Figure 1.1.

Equation (1.1) is perhaps an unrealistic model for most population growths. Among other things, its solution implies that the population will grow indefinitely. A better model is given by the following equation:

$$\frac{dN}{dt} = rN \cdot (1 - N/k). \tag{1.4}$$

Try solving it using the same method. The solution is plotted in Figure 1.2 for $0 < N(0) < k$.

Example. *Harmonic Oscillator Equation:*

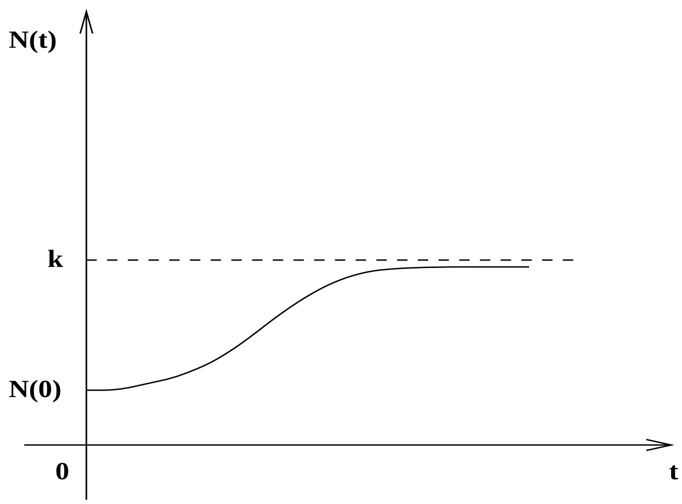


Figure 1.2: Solution to Equation 1.4

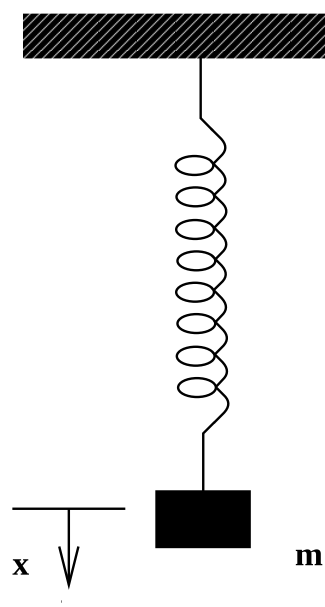


Figure 1.3: A spring of mass m suspended under gravity and in equilibrium. x is the displacement from the equilibrium position.

$$\boxed{m\frac{d^2x}{dt^2} + kx = 0}\,. \tag{1.5}$$

Here x is the vertical displacement from the equilibrium position of the spring, which has a mass m and a spring constant k. Equation (1.5) is a statement of Newton's Law of Motion: $m\frac{d^2x}{dt^2}$ is mass times acceleration. This is required to be equal to the spring's restoring force $-kx$. This force is assumed to be proportional to the displacement from equilibrium.

It is harder to solve a second order ODE, although this particular equation is so common that we were taught to try exponential solutions wherever we see linear equations with constant coefficients.

Solution by trial method: Try $e^{\alpha t}$.

Plugging the guess in Equation (1.5) for x then suggests that α must satisfy

$$m\alpha^2 + k = 0,$$

which means

$$\alpha = i\sqrt{k/m}, \quad \text{or } \alpha = -i\sqrt{k/m},$$

where $i \equiv \sqrt{-1}$ is the imaginary number. There are two different values of α which will make our trial solution satisfy equation (1.5). So the general solution should be a linear combination of the two:

$$\boxed{x(t) = c_1 e^{i\sqrt{k/m}t} + c_2 e^{-i\sqrt{k/m}t}}\,, \tag{1.6}$$

where c_1 and c_2 are two arbitrary (complex) constants.

If you do not like using complex notations (numbers that involve i), you can rewrite (1.6) in real notation, making use of the Euler's Identity, which we will derive a little later:

$$e^{i\theta} = \cos\theta + i\sin\theta. \tag{1.7}$$

Thus the rest solution (1.6) can be rewritten as

$$\boxed{x(t) = A\sin(\sqrt{k/m}t) + B\cos(\sqrt{k/m}t)}\,, \tag{1.8}$$

where A and B are some arbitrary real constants (since c_1 and c_2 were undetermined).

We can verify that (1.8) is indeed the solution to the harmonic oscillator equation (1.5) by noting, from calculus:

$$\frac{d}{dt}\sin\omega t = \omega\cos\omega t, \quad \frac{d}{dt}\cos\omega t = -\omega\sin\omega t$$

so

$$\frac{d^2}{dt^2}\sin\omega t = \frac{d}{dt}(\omega\cos\omega t) = -\omega^2\sin\omega t$$

and

$$\frac{d^2}{dt^2}\cos\omega t = \frac{d}{dt}(-\omega\sin\omega t) = -\omega^2\cos\omega t.$$

Therefore, the sum (1.8) satisfies

$$\frac{d^2}{dt^2}x = -\omega^2 x, \tag{1.9}$$

which is the same as (1.5), provided that $\omega^2 = k/m$.

Euler's Identity:

Euler's Identity, as used in (1.7), deserves some comment. We will also need this identity later when we deal with Fourier series and transforms.

In calculus, we learned how to differentiate an exponential

$$\frac{d}{d\theta}e^{a\theta} = ae^{a\theta}.$$

Although you have always assumed a to be a real number, it does not make any difference if a is complex. So letting $a = i$, we find

$$\frac{d}{d\theta}e^{i\theta} = ie^{i\theta}$$

$$\frac{d^2}{d\theta^2}e^{i\theta} = \frac{d}{d\theta}(ie^{i\theta}) = i^2e^{i\theta} = -e^{i\theta}.$$

We have thus shown that the function

$$y(\theta) = e^{i\theta} \tag{1.10}$$

satisfies the second-order ODE:

$$\frac{d^2}{d\theta^2}y + y = 0. \tag{1.11}$$

$e^{i\theta}$ also happens to satisfy the *initial conditions*:

$$y(0) = 1, \quad \frac{d}{d\theta}y(0) = i. \tag{1.12}$$

On the other hand, we have just verified in (1.9) that

$$y = A\sin\theta + B\cos\theta \tag{1.13}$$

also satisfies (1.11), which is the same as (1.9) if we replace t by θ and ω by 1. If we furthermore require the sum (1.13) to also satisfy the initial condition (1.12), we will find that $B = 1$ and $A = i$. Since,

$$y(\theta) = \cos\theta + i\sin\theta \tag{1.14}$$

satisfies the same ODE (1.11) and the same initial conditions (1.12) as (1.10), (1.14) and (1.10) must be the same by the Uniqueness Theorem for ODEs. What we have outlined is one way for proving the Euler Identity (1.7):

$$\boxed{e^{i\theta} = \cos\theta + i\sin\theta}\,.$$

Solution from First Principles:

If you prefer to find the solution from first principles, i.e. not by guessing that it should be in the form of an exponential, it can be done by "reduction of order", although we normally do not bother to do it this way:

We recognize that Equation (1.5) is a type of ODE with its "independent variable missing". The method of reduction of order suggests that we let

$$p \equiv \frac{dx}{dt},$$

and write

$$\frac{d^2x}{dt^2} = \frac{dp}{dt} = \frac{dx}{dt}\frac{dp}{dx} = p\frac{dp}{dx}.$$

Treating p now as a function of x, Equation (1.5) becomes

$$p\frac{dp}{dx} + \omega^2 x = 0, \tag{1.15}$$

where we have used ω^2 for k/m.

Equation (1.15), a first order ODE, can be solved by the same method we used in Example 1:

Integrating $pdp + \omega^2 x dx = 0$ yields,

$$p^2 + \omega^2 x^2 = \omega^2 a^2.$$

with $\omega^2 a^2$ being an arbitrary constant of integration. From $p = \pm\omega\sqrt{a^2 - x^2}$, we have, since $p = \frac{d}{dt}x$,

$$\frac{dx}{dt} = \pm\alpha\sqrt{a^2 - x^2}.$$

This is again a first order ODE, which we solve as before.

Integrating both sides of

$$\frac{dx}{\sqrt{a^2 - x^2}} = \pm\omega dt$$

and using the integral formula:

$$\int \frac{dx}{\sqrt{a^2 - x^2}} = \sin^{-1}\frac{x}{a} + b, \quad b \text{ being a constant,}$$

we find

$$\sin^{-1}\frac{x}{a} = \pm\omega t + b.$$

Inverting, we find:

$$\frac{x}{a} = \sin(\pm\omega t + b),$$

which can (finally!) be rewritten as

$$x(t) = A\sin\omega t + B\cos\omega t\ . \tag{1.16}$$

1.2 Nonhomogeneous Ordinary Differential Equations

1.2.1 First-Order Equations:

A nonhomogeneous version of the example in (1.1) is

$$\boxed{\frac{dN}{dt} - rN = f(t),} \tag{1.17}$$

where $f(t)$ is a (known) specified function of t, independent of the "unknown" N. It is called the "inhomogeneous term" or the "forcing term". In the population growth example we discussed earlier, $f(t)$ can represent the rate of population growth of the species due to migration.

We are here concerned with the method of solution of (1.17) for any given $f(t)$. We proceed to multiply both sides of (1.17) by a yet-to-be-determined function $\mu(t)$, called the *integrating factor*:

$$\mu \frac{dN}{dt} - r\mu N = \mu f. \tag{1.18}$$

We choose $\mu(t)$ such that the product on the left-hand side of (1.18) is a perfect derivative, i.e.

$$\mu \frac{dN}{dt} - r\mu N = \frac{d}{dt}(\mu N). \tag{1.19}$$

If this can be done, then (1.10) would become:

$$\frac{d}{dt}(\mu N) = \mu f,$$

which can be integrated from $t = 0$ to t to yield:

$$\mu(t)N(t) - \mu(0)N(0) = \int_0^t \mu(t)f(t)dt. \tag{1.20}$$

The notation on the right-hand side of (1.20) is rather confusing. A better way is to use a different symbol, say, τ, in place of t as the dummy variable of integration. Then, (1.20) can be rewritten as

$$N(t) = N(0)\mu(0)\mu^{-1}(t) + \mu^{-1}(t) \int_0^t \mu(\tau)f(\tau)d\tau. \tag{1.21}$$

The remaining task is to find the integrating factor $\mu(t)$. In order for (1.19) to hold, we must have the right-hand side

$$\mu \frac{dN}{dt} + N\frac{d\mu}{dt}$$

equal the left-hand side, implying

$$\frac{d\mu}{dt} = -r\mu. \tag{1.22}$$

The solution to (1.22) is simply

$$\mu(t) = \mu(0)e^{-rt}. \tag{1.23}$$

Substituting (1.23) back into (1.21) then yields

$$\boxed{N(t) = N(0)e^{rt} + e^{rt}\int_0^t e^{-r\tau} f(\tau) d\tau} . \tag{1.24}$$

This then completes the solution of (1.17). If r is not a constant, but is a function t, the procedure remains the same up to, and including (1.22). The solution to (1.22) should now be

$$\mu(t) = \mu(0)e^{-\int_0^t r(t')dt'} . \tag{1.25}$$

The final solution is obtained by substituting (1.25) into (1.21).

Notice that the solution to the (linear) nonhomogeneous equation consists of two parts: a part satisfying the general homogeneous equation and a part that is a particular solution of the nonhomogeneous equation (the first and second terms on the right-hand side of (1.24) respectively). For some simple forcing functions $f(t)$, there is no need to use the general procedure of integrating factors if we can somehow guess a particular solution. For example, suppose we want to solve

$$\boxed{\frac{dN}{dt} - rN = 1} . \tag{1.26}$$

We write

$$N(t) = N_h(t) + N_p(t),$$

where $N_h(t)$ satisfies the homogeneous equation

$$\frac{dN_h}{dt} - rN_h = 0$$

and so is

$$N_h(t) = ke^{rt},$$

for some constant k. $N_p(t)$ is any solution of the Eq. (1.26). By the "method of judicious guessing", we try selecting a constant for $N_p(t)$. Upon substituting $N_p(t) = a$ into (1.26), we find the only possibility: $a = -\frac{1}{r}$. Thus the full solution is

$$N(t) = ke^{rt} - \frac{1}{r} = N(0)e^{rt} + \frac{1}{r}(e^{rt} - 1).$$

1.2.2 Second-Order Equations:

For our purpose here we will be using only the "method of judicious guessing" for linear second-order equations. The more general method of "variation of parameters" is too cumbersome for our limited purposes.

Example: Solve

$$\frac{d^2}{dt^2}x + \omega^2 x = 1. \tag{1.27}$$

We write the solution as a sum of a homogeneous solution x_h and a particular solution x_p, i.e.

$$x(t) = x_h(t) + x_p(t).$$

We already know that the homogeneous solution (to (1.5)) is of the form

$$x_h(t) = A\sin\omega t + B\cos\omega t. \tag{1.28}$$

We guess that a particular solution to (1.27) is a constant

$$x_p(t) = a. \tag{1.29}$$

Subsituting (1.29) into (1.27) then shows that constant is $1/\omega^2$. Thus the general solution to (1.27) is

$$\boxed{x(t) = A\sin\omega t + B\cos\omega t + 1/\omega^2}\,. \tag{1.30}$$

The arbitrary constants A and B are to be determined by initial conditions.

Example: Solve

$$\boxed{\frac{d^2}{dt^2}x + \omega^2 x = \sin\omega_0 t}\,. \tag{1.31}$$

Again we write the solution as a sum of the homogeneous solution and a particular solution. For the particular solution, we try:

$$x_p(t) = a\sin\omega_0 t. \tag{1.32}$$

Upon substitution of (1.32) into (1.31), we find

$$a = (\omega^2 - \omega_0^2)^{-1},$$

and so the general solution is

$$\boxed{x(t) = A\sin\omega t + B\cos\omega t + \frac{\sin\omega_0 t}{(\omega^2 - \omega_0^2)}.} \tag{1.33}$$

The solution in (1.33) is valid as is for $\omega_0 \neq \omega$. Some special treatment is helpful when the forcing frequency ω_0 approaches the natural frequency ω. Let us write

$$\omega_0 = \omega + \epsilon$$

and let $\epsilon \to 0$. The particular solution can be written as

$$\begin{aligned} x_p(t) &= \frac{\sin\omega_0 t}{(\omega^2 - \omega_0^2)} = \frac{\sin(\omega t + \epsilon t)}{\omega^2 - (\omega+\epsilon)^2} \\ &= \frac{\sin\omega t\cos\epsilon t + \cos\omega t\sin\epsilon t}{-2\omega\epsilon - \epsilon^2} \to -\frac{\cos\omega t}{2\omega}\cdot t - \frac{\sin\omega t}{2\omega\epsilon} \text{ as } \epsilon \to 0 \end{aligned}$$

Thus for the case of *resonance*, $\omega_0 = \omega$, the solution (1.33) becomes

$$x(t) = A'\sin\omega t + B\cos\omega t - \frac{1}{2\omega}t\cos\omega t,$$

where we have written $A = A' + \frac{1}{2\omega\epsilon}$, with A' being a (finite) arbitrary constant. The solution grows secularly in t.

1.3 Summary of ODE solutions

In this course we will be mostly dealing with linear differential equations with constant coefficients. For these, simply try an exponential solution. This is the easiest way. You are not expected to have to repeat each time the derivation given in the previous sections on why the exponentials are the right solutions to try. Just do the following:

(a) $\boxed{\frac{d}{dt}N = rN}$

Try $N(t) = ae^{\alpha t}$ and find $\alpha = r$ so the solution is

$$\boxed{N(t) = ae^{rt}}.$$

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

Try $x(t) = ae^{\alpha t}$ and find $\alpha = \pm i\omega$ so the complex solution is

$$\boxed{x(t) = a_1 e^{i\omega t} + a_2 e^{-i\omega t}},$$

and the real solution

$$x = A\cos\omega t + B\sin\omega t$$

1.4 Partial Derivatives

The ordinary differential equations we discussed in the last section describe functions of only one independent variable. For example, the unknown N in (1.1) is a function of t only, and Eq. (1.1) describes the rate of change of $N(t)$ with respect to t. It is not hard to imagine a physical situation where the population N depends not only on time t, but also on space x (more realistically on all three spatial dimensions, x, y, z). For a function of more than one independent variables, for example,

$$N = N(x, t),$$

we need to distinguish the derivative with respect to t from the derivative with respect to x. For this purpose, we define the *partial derivatives* in the following way.

The partial derivative of $N(x, t)$ with respect to t, denoted by $\frac{\partial}{\partial t}N(x, t)$, or $N_t(x, t)$ for short, is defined as the derivative of N with respect to t *holding all other independent variables—in this case x—constant*:

$$\boxed{\frac{\partial}{\partial t}N(x,t) = \lim_{\substack{\Delta t\to 0\\ x \text{ held constant}}} \frac{N(x, t+\Delta t) - N(x,t)}{\Delta t}}. \tag{1.34}$$

Similarly, the partial derivative of $N(x, t)$ with respect to x, denoted by $\frac{\partial}{\partial x}N(x, t)$, or $N_x(x, t)$ for short, is defined as:

$$\boxed{\frac{\partial}{\partial x}N(x,t) = \lim_{\substack{\Delta x\to 0\\ t \text{ held constant}}} \frac{N(x+\Delta x, t) - N(x,t)}{\Delta x}.} \tag{1.35}$$

Compare the partial derivatives with the ordinary derivatives:

$$\frac{d}{dt}N(t) = \lim_{\Delta t\to 0} \frac{N(t+\Delta t) - N(t)}{\Delta t},$$

and you will see that the partial derivative is the same as the ordinary derivative if you can just pretend that the other independent variables were constants.

Example: The (first) partial derivatives of

$$N(x,t) = x^3 + t^2 \tag{1.36}$$

are

$$N_t = 2t, \qquad \text{and} \qquad N_x = 3x^2. \tag{1.37}$$

When N is a function of x and t, its integral with respect to t is done by pretending that x is a constant, as in the following example.

Example: For $N(x,t)$ given by (1.36)

$$\int^t N(x,t)dt = x^3 t + \frac{1}{3}t^3 + f(x), \tag{1.38}$$

where $f(x)$ plays the role of a "constant of integration" with respect to t and is actually an arbitrary function of x. To verify this, we can take the (partial) derivative of (1.38) with respect to t and recover $N(x,t)$ in (1.36).

Example: The solution $N(x,t)$ of the PDE:

$$\frac{\partial}{\partial t}N = rN \tag{1.39}$$

for $t > 0$ is

$$N(x,t) = a(x)e^{rt}. \tag{1.40}$$

Here $a(x)$ plays the role of the "constant" in the solution to the ODE (1.1). Setting $t = 0$, we find

$$a(x) = N(x,0),$$

which is to be given by the initial distribution of the population.

1.5 Exercise I

Review of ordinary differential equations:

1. Find the most general solution to:

   (a) $\frac{d}{dt}N = rN + b$; r, b are constants,

   (b) $\frac{d^2}{dt^2}x + \beta\frac{d}{dt}x + \omega^2 x = 0$; β, ω^2 are constants,

   (c) $\frac{d^2}{dt^2}x + \omega^2 x = \cos\omega_0 t$, $\omega \neq \omega_0$,

   (d) $\frac{d^2}{dt^2}x + \omega_0^2 x = \cos\omega_0 t$.

2. Find the solution satisfying the specified initial conditions:

   (a) $\frac{d}{dt}N = rN + b$
   $N(0) = 0$.

   (b) $\frac{d^2}{dt^2}x + \beta\frac{d}{dt}x + \omega^2 x = 0$
   $x(0) = 1$, $\frac{d}{dt}x(0) = 0$.

   (c) $\frac{d^2}{dt^2}x + \omega^2 x = \cos\omega_0 t$, $\omega \neq \omega_0$
   $x(0) = 0$, $\frac{d}{dt}x(0) = 0$.

   (d) $\frac{d^2}{dt^2}x + \omega_0^2 x = \cos\omega_0 t$
   $x(0) = 0$, $\frac{d}{dt}x(0) = 0$.

1.6 Solutions to Exercise I

1. (a) $N(t) = N_h(t) + N_p(t)$, where $N_h(t)$ is the solution to the homogeneous equation and $N_p(t)$ is a particular solution to the non-homogeneous equation. For $N_p(t)$, we try a constant, i.e. $N_p(t) = c$. Substituting it into $\frac{d}{dt}N = rN + b$ yields $0 = rc + b$, implying $c = -b/r$.

The solution to the homogeneous equation $\frac{d}{dt}N = rN$ is: $N_h(t) = ae^{rt}$, where a is an arbitrary constant.

Combining:

$$N(t) = ae^{rt} - b/r.$$

(b) Try

$$x(t) = ae^{\alpha t}.$$

Substituting into the ODE yields:

$$\alpha^2 + \alpha\beta + \omega^2 = 0.$$

So $\alpha = \alpha_1$ or $\alpha = \alpha_2$, where

$$\alpha_1 \equiv -\frac{\beta}{2} + \sqrt{\frac{\beta^2}{4} - \omega^2} \quad \text{and} \quad \alpha_2 \equiv -\frac{\beta}{2} - \sqrt{\frac{\beta^2}{4} - \omega^2}$$

The general solution is

$$x(t) = a_1 e^{\alpha_1 t} + a_2 e^{\alpha_2 t}$$

(c) $x(t) = x_h(t) + x_p(t)$.

For $x_p(t)$, try $x_p(t) = a\cos\omega_0 t$. Substituting into the ODE yields

$$-\omega_0^2 a + \omega^2 a = 1.$$

So $a = 1/(\omega^2 - \omega_0^2)$. For $x_h(t)$, we know the general solution to the homogeneous ODE is

$$x_h(t) = A\sin\omega t + B\cos\omega t; A, B \text{ are arbitrary constants.}$$

The full solution is

$$x(t) = A\sin\omega t + B\cos\omega t + \cos\omega_0 t/(\omega^2 - \omega_0^2).$$

(d) This is the resonance case. Still try $x(t) = x_h(t) + x_p(t)$.

For $x_p(t)$, try $x_p(t) = at\sin\omega_0 t$. Substituting into the nonhomogeneous ODE yields

$$2a\omega_0\cos\omega_0 t - a\omega_0^2 t\sin\omega_0 t + \omega_0^2 at\sin\omega_0 t = \cos\omega_0 t.$$

Thus

$$2a\omega_0 = 1.$$

So $x_p(t) = t \sin \omega_0 t / 2\omega_0$. The general solution to the homogeneous ODE is:

$$x_h(t) = A \sin \omega_0 t + B \cos \omega_0 t.$$

The full solution is

$$x = A \sin \omega_0 t + B \cos \omega_0 t + t \sin \omega_0 t / 2\omega_0.$$

2. (a) $N(t) = ae^{rt} - b/r$

$$N(0) = a - b/r = 0 \text{ implies } a = b/r.$$

So,

$$N(t) = \frac{b}{r}(e^{rt} - 1)$$

(b) $x(t) = a_1 e^{\alpha_1 t} + a_2 e^{\alpha_2 t}$

$$x(0) = a_1 + a_2 = 1$$

$$\frac{d}{dt}x(0) = \alpha_1 a_1 + \alpha_2 a_2 = 0$$

Thus $a_1 = -\alpha_2/(\alpha_1 - \alpha_2)$, $a_2 = \alpha_1/(\alpha_1 - \alpha_2)$.
Finally

$$x(t) = \frac{1}{(\alpha_1 - \alpha_2)}[-\alpha_2 e^{\alpha_1 t} + \alpha_1 e^{\alpha_2 t}]$$

(c) $x(t) = A \sin \omega t + B \cos \omega t + \cos \omega_0 t/(\omega^2 - \omega_0^2)$

$$x(0) = B + 1/(\omega^2 - \omega_0^2)$$

$$\frac{d}{dt}x(0) = A\omega = 0$$

Thus $A = 0$, $B = -1/(\omega^2 - \omega_0^2)$ and

$$x(t) = \frac{1}{(\omega^2 - \omega_0^2)}[\cos \omega_0 t - \cos \omega t]$$

(d) $x(t) = A \sin \omega_0 t + B \cos \omega_0 t + t \sin \omega_0 t/\omega_0$

$$x(0) = B = 0$$

$$\frac{d}{dt}x(0) = A\omega_0 = 0.$$

Thus $A = 0$, $B = 0$, and

$$x(t) = t \sin \omega_0 t/\omega_0.$$

1.7 Exercise II

Partial derivatives:

1. Evaluate $\frac{\partial}{\partial x}u(x, y)$ for

   (a) $u(x, y) = e^{xy}$

   (b) $u(x, y) = (x + y)^2$

   (c) $u(x, y) = x^2 + y^2$

2. Evaluate $\int^y u(x, \eta)d\eta$ (as an indefinite integral) for $u(x, y)$ given by (a), (b) and (c) from Problem 1 above.

3. (a) Find the general solution $u(t)$ to the ODE

$$m\frac{d^2}{dt^2}u + ku = 0,$$

   where m and k are constants.

   (b) Find the general solution $u(x, y)$ to the PDE

$$\frac{\partial^2}{\partial x^2}u + (1 + y^2)u = 0$$

1.8 Solutions to Exercise II

1. Evaluate $\frac{\partial}{\partial x}u(x,y)$ for

   $u(x,y) = e^{xy}, \qquad \frac{\partial}{\partial x}u = ye^{xy}$

   $u(x,y) = (x+y)^2, \quad \frac{\partial}{\partial x}u = 2(x+y)$

   $u(x,y) = x^2 + y^2, \quad \frac{\partial}{\partial x}u = 2x.$

2. Evaluate $\int^y u(x,\eta)d\eta$ from problem 1

   $\int^y e^{x\eta}d\eta = \frac{1}{x}e^{xy} + f(x)$

   $\int^y (x+\eta)^2 d\eta = \frac{(x+y)^3}{3} + g(x)$

   $\int^y (x^2+\eta^2)d\eta = x^2y + \frac{y^3}{3} + h(x),$

   where f,g, and h are arbitrary functions of x.

3a. Find the general solution u(t) to $m\frac{d^2}{dt^2}u + ku = 0$, where m and k are constants.

   Try $u(t) = A\cos\alpha t + B\sin\alpha t$.

   Substitute into $m\frac{d^2}{dt^2}u + ku = 0$ to find $\alpha = \sqrt{k/m}$.

   So the general solution is $u(t) = A\cos\sqrt{k/m}t + B\sin\sqrt{k/m}t$ with A and B arbitrary constants.

3b. Find the general solution $u(x,y)$ to $\frac{\partial^2}{\partial x^2}u + (1+y^2)u = 0$.

   Treat y as a constant with respect to x-partial derivative.

   Try $u(x,y) = A(y)\cos(\alpha(y)x) + B(y)\sin(\alpha(y)x)$.

   Find $\alpha(y) = \sqrt{(1+y^2)}$.

   Thus we have $u(x,y) = A(y)\cos(\sqrt{(1+y^2)}x) + B(y)\sin(\sqrt{(1+y^2)}x)$, with A and B arbitrary functions of y.

Chapter 2

Physical Origins of Some PDEs

2.1 Introduction

In physical applications, PDEs are more ubiquitous than ODEs. This situation can be understood because physical quantities more often depend on space and time than on, say, time alone. A partial differential equation relates the variations of this physical quantity in time and in space. Of course, in mathematical abstraction, one does not need to assign the physical meaning of time to the symbol t, or space to the symbol x; one is simply concerned with the variations of the unknown with respect to more than one independent variable as governed by a PDE.

We will be dealing with first and second order PDEs in this course. In this chapter we will discuss the physical origin of these equations. This chapter is suitable for assigned casual reading.

2.2 Conservation Laws:

Many physical laws can be expressed as a *conservation law* of the form

$$u_t + q_x = 0. \tag{2.1}$$

Here $u(x,t)$ is the "concentration" of something under consideration and q is its "flux" in the x-direction. If the quantity under consideration is nonconservative, we need to add a "source or sink" term to the right-hand side of (2.1). We will provide physical examples of such terms in a moment.

In more than one space dimensions, q would be a vector $\mathbf{q}$, and (2.1) would be replaced by

$$u_t + \nabla \cdot \mathbf{q} = 0$$

for the gradient vector ∇. We will however not be concerned with more than one space dimension here; so you will not need to know vectors or divergence of a vector $(\nabla \cdot \mathbf{q})$.

If q in (2.1) is a function of u only and does not depend on its derivatives, then it can be written as

$$u_t + a(u)u_x = 0, \quad \text{where } a(u) \equiv \frac{dq}{du}. \tag{2.2}$$

(2.2) is a first order PDE. On the other hand, if the flux q depends on u_x, as is often the case for "down-gradient" fluxes, e.g.

$$q = -ku_x, \quad \text{for a constant } k,$$

(2.1) will become

$$u_t - ku_{xx} = 0, \tag{2.3}$$

which is a second-order PDE.

2.2.1 Diffusion of a tracer:

Let c be the concentration of a substance under consideration (in gm/volume). Let ρ be the density of the medium into which it is diffusing. For example, for the problem of diffusion of salt in water, c is the weight of salt per unit volume, and ρ is the weight of water per unit volume. Let $u = c/\rho$ be called the mass ratio of salt to water.

We now consider diffusion in one dimension, x. This can approximate the situation of diffusion in a thin tube of constant cross-sectional area A, with its axis oriented in the x-direction. The tube is filled with water and some salt is put into this tube initially. Since the tube is thin, we can ignore the diffusion of salt radially, assuming the salt quickly manages to diffuse radially to attain the same concentration throughout the cross-section. Its concentration varies mainly with x.

Consider the amount of salt between the sections x and $x + \Delta x$, a small distance apart. If Δx is so small that the variation of c with x can be ignored, that amount of salt contained is $cA\Delta x = \rho A\Delta x \cdot u$, since $A\Delta x$ is the volume of the section under consideration. Since the mass of salt is conserved, we can state that the time rate of change of salt in this volume,

$$\frac{\partial}{\partial t}\rho A\Delta x u,$$

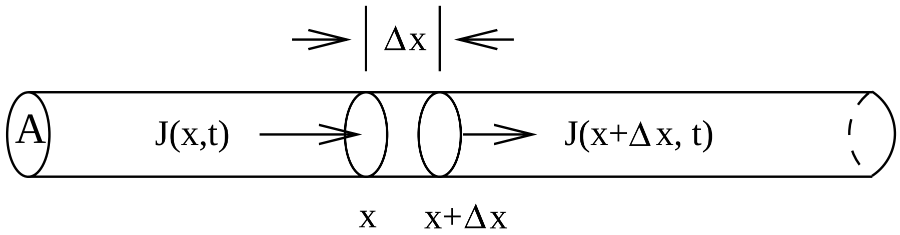


Figure 2.1: Diffusion in a tube of cross-sectional area A.

is equal to the flux of salt into the volume at x, minus the flux of salt out of the volume at $x + \Delta x$, i.e.

$$[J(x,t)A - J(x+\Delta x, t)A],$$

where $J(x,t)$ is the flux at x. It is defined as the time rate of salt flowing across x per unit area.

Thus the equation for the conservation of salt is:

$$\rho A \Delta x \frac{\partial}{\partial t} u = A[J(x,t) - J(x+\Delta t, t)]. \tag{2.4}$$

Dividing both sides by $A\Delta x$, we get

$$\rho \frac{\partial}{\partial t} u = -\frac{J(x+\Delta x, t) - J(x,t)}{\Delta x}. \tag{2.5}$$

We now take the limit as $\Delta x \to 0$, since the smaller Δx is, the better our previous approximation of assuming c to be constant between x and Δx is. The right-hand side of Equation (2.5) becomes,

$$-\lim_{\Delta x \to 0} \frac{J(x+\Delta x, t) - J(x,t)}{\Delta x} = -\frac{\partial J}{\partial x}(x,t).$$

Equation (2.5) is now in the form of a "conservation law", Equation (2.1), if we write $q \equiv J/\rho$:

$$\frac{\partial}{\partial t} u = -\frac{\partial}{\partial x} q. \tag{2.6}$$

To relate the flux q to u, we use *Fick's law of diffusion*, which is obtained from experimental descriptions. It says:

The flux (of salt) is proportional to the negative gradient (of salt) (since salt always diffuses from a high concentration region to a low concentration region). Mathematically, we write this law as

$$J(x,t) = -k \frac{\partial}{\partial x} c = -k\rho \frac{\partial}{\partial x} u, \tag{2.7}$$

where the proportionality constant, k, is the coefficient of diffusivity for salt. Equation (2.6) finally becomes:

$$\boxed{\frac{\partial u}{\partial t} = k\frac{\partial^2 u}{\partial x^2}}\,. \tag{2.8}$$

It is a second-order PDE, because its highest derivative, $\frac{\partial^2 u}{\partial x^2}$, is second order. Equation (2.8) is called the *diffusion equation.* With a different value for k it can be applied to the problem of diffusion of pollutants in air (with ρ being the density of air and c the concentration of the pollutant). In biology and ecology, c could be the population of a species.

2.2.2 Advection of a tracer:

The diffusion of a tracer, say salt in water discussed in 2.2.1, is a macroscopic result of small-scale random molecular motion of salt and water molecules. This is a slow process. Advection, on the other hand, is a faster process if it occurs. If a pollutant of concentration c is put into a river whose water is flowing with speed V, the flux of that pollutant, defined as the time rate of the pollutant flowing across x per unit area, is

$$J(x,t) = V \cdot c, \tag{2.9}$$

because the pollutant is carried by the water with speed V across x. Letting $u = c/\rho$, and $q = J/\rho$, we have, from (2.6)

$$\frac{\partial}{\partial t}u = -\frac{\partial}{\partial x}q$$

or

$$\boxed{\frac{\partial}{\partial t}u + V\frac{\partial}{\partial x}u = 0}\,. \tag{2.10}$$

Equation (2.10) is a first-order PDE. It describes the advection of a tracer by a medium with velocity V.

If the time scales of advection and diffusion are comparable, we should include them both. In that case, the flux becomes

$$J(x,t) = V \cdot c - k\frac{\partial}{\partial x}c, \tag{2.11}$$

and the governing PDE becomes:

$$\boxed{\frac{\partial}{\partial t}u + V\frac{\partial}{\partial x}u = k\frac{\partial^2}{\partial x^2}u.} \tag{2.12}$$

Equation (2.9) is called the *advection-diffusion equation.*

2.2.3 Nonlinear advection:

The advection equation, (2.10), is *linear* if V does not depend on the unknown u. Otherwise it is *nonlinear*. A linear PDE is one where the unknown and its derivatives appear linearly, i.e. not multiplied by itself or its partial derivatives.

Nonlinear advection arises if the quantity u, whose conservation is being considered, is also related to the advecting velocity V. This is the case, for example, when we are considering the conservation of momentum ρu of the fluid, where ρ is the density of the fluid and u is the fluid's velocity in the x-direction. Since the momentum is advected by the fluid velocity u, the conservation law will look something like:

$$\rho\left[\frac{\partial}{\partial t}u + u\frac{\partial}{\partial x}u\right] = \text{ the forces acting.}$$

The simplest such equation is the nonlinear advection equation:

$$\boxed{\frac{\partial}{\partial t}u + u\frac{\partial}{\partial x}u = 0}\,. \tag{2.13}$$

If nonconservative forces, such as molecular diffusion (so-called viscosity) is included, one obtains the nonlinear counterpart to (2.12):

$$\boxed{\frac{\partial}{\partial t}u + u\frac{\partial}{\partial x}u = \nu\frac{\partial^2}{\partial x^2}u}\,. \tag{2.14}$$

Equation (2.14) is the famous *Burgers' equation.* Burgers' equation has been studied by mathematicians as a prototype model of the balance between nonlinear advection and viscosity in fluid flows (where ν is the coefficient of viscosity), although the equations governing real fluid flows are more complicated. [Burgers' equation does not include, among other things, the pressure forces.]

2.2.4 Heat conduction in a rod:

Consider a long cylindrical rod, insulated at the curved sides so that heat can flow in or out only through the ends. The rod is thin, so that the radial variation of temperature u can be ignored. We consider the variation of u with respect to x, measured along the axis of the cylinder, and time t, i.e.

$$u = u(x,t)$$

The time rate of change of heat energy in a small volume $A\Delta x$, situated between sections x and $x+\Delta x$, is

$$c\rho A\Delta x \frac{\partial u}{\partial t},$$

where c is the specific heat and ρ the density of the material of the rod (e.g. copper). This should be equal to the net flux of heat into the volume, i.e.

$$c\rho A\Delta x \frac{\partial u}{\partial t} = J(x,t)A - J(x+\Delta x, t)A. \tag{2.15}$$

where $J(x,t)$ is the flux of heat into the positive x direction across the section at x. Taking the limit as $\Delta x \to 0$, Equation (2.15) becomes

$$\frac{\partial u}{\partial t} = -\frac{\partial q}{\partial x}, \qquad \text{where } q \equiv J/c\rho, \tag{2.16}$$

Equation (2.16) is in the form of a conservation law, (2.1).

To express the flux J in terms of the temperature u, we use Fourier's law of heat conduction: If there are differences in temperature in a conducting medium, the heat energy would flow from the hotter to the colder region. Therefore there is "down gradient" heat flux, proportional to the negative of the temperature gradient, i.e.

$$q(x,t) = -\alpha^2 \frac{\partial}{\partial x} u. \tag{2.17}$$

Here α^2 is the coefficient of thermal diffusivity. For a uniform α^2, Equation (2.7) becomes

$$\boxed{\frac{\partial}{\partial t} u = \alpha^2 \frac{\partial^2}{\partial x^2} u}\ . \tag{2.18}$$

Equation (2.9) is called the *heat equation.* It has the same form as the diffusion equation derived earlier.

2.2.5 Ubiquity of the Diffusion Equation

We have seen that the same diffusion equation arises from seemingly unrelated phenomena, from diffusion of salt and pollutants to conduction of heat. The ubiquity of the diffusion equation arises from (a) the ubiquity of the conservation law (2.1) and (b) the *Fickian flux-gradient relationship* (2.7):

$$J \propto -\frac{\partial c}{\partial x},$$

which is simply a statement that diffusion tends to transport matter or heat from high to low levels. This experimental law is a reflection of the underlying random molecular motion. Consider an imaginary interface at x separating water with no salt to the left and water with salt to the right. Suppose on average it is as likely, through their random motion, for molecules from the right to cross x to the left as it is for molecules from the left to go to the right. Since some of the molecules at the right are salt molecules, after a while some salt molecules have moved to the left while the water molecules from the left have taken their place at the right. The macroscopic result is that there is a *flux* of salt from the high salt concentration region to the low concentration region.

Similarly, let us consider the region of high temperature as consisting of molecules of higher vibrational energy. The energy can be transfered to other molecules upon collison. Thus, although it is equally likely for an energetic molecule to move to the left as it is for it to move to the right, when it moves to the left it has a higher probability of hitting a less energetic molecule, and transfering "heat" in the process. Therefore, macroscopically, heat flows from hot to cold regions.

Diverse phenomena in biology, ranging from animal and insect dispersal to the spread of diseases, can be modeled approximately by a Fickian flux-gradient relationship, and hence can be described by some sort of diffusion equation. (see Okubo (1980): *Diffusion and Ecological Problems: Mathematical Models*, Springer).

2.3 Random Walk

2.3.1 A drunken sailor

Consider the problem of predicting where a (microscopic) "drunken sailor" will be at time t if he walks randomly from an initial position at $x = 0$. For simiplicity let us consider here the one dimensional problem where he is constrained to walk straight along a narrow alley (assuming that the sailor can indeed walk straight!). He takes a step of size Δx in a time interval Δt, and it is equally likely for him to take that step in either direction.

Let $p(x,t)$ be the probability that we will find him at x in time t. In a previous time step $t - \Delta t$, he could be either at the neighboring locations $x - \Delta x$ or at $x + \Delta x$, with equal probability. Therefore we have

$$p(x,t) = \frac{1}{2}p(x - \Delta x, t - \Delta t) + \frac{1}{2}p(x + \Delta x, t - \Delta t). \qquad (2.19)$$

(2.19) is simply a statement that the sailor could have arrived at x from either $x - \Delta x$ by taking a forward step (or lurch), or from $x + \Delta x$ by stepping backward, with equal likelihood. If we take Δx and Δt to be small in some sense, we can expand the right-hand side of (2.17) in a Taylor series about its two variables:

$$\begin{aligned} p(x-\Delta x, t-\Delta t) &\simeq p(x, t-\Delta t) + \frac{\partial p(x,t-\Delta t)}{\partial x}(-\Delta x) \\ &\quad + \frac{1}{2}\frac{\partial^2 p(x,t-\Delta t)}{\partial x^2}(\Delta x)^2 + \ldots \\ &\simeq p(x,t) + \frac{\partial p(x,t)}{\partial t}(-\Delta t) + \frac{1}{2}\frac{\partial^2 p(x,t)}{\partial t^2}(-\Delta t)^2 \\ &\quad + \frac{\partial p(x,t)}{\partial x}(-\Delta x) + \frac{\partial^2 p(x,t)}{\partial x \partial t}(-\Delta t)(-\Delta x) + \ldots \\ &\quad + \frac{1}{2}\frac{\partial^2 p(x,t)}{\partial x^2}(-\Delta x)^2 + \ldots . \end{aligned}$$

Similarly the Taylor series expansion for $p(x+\Delta x, t-\Delta t)$ is the same as for $p(x-\Delta x, t-\Delta t)$ except with $-\Delta x$ replaced by Δx. Therefore (2.19) becomes:

$$p(x,t) = p(x,t) - \frac{\partial}{\partial t}p(x,t)\Delta t + \frac{1}{2}\frac{\partial^2}{\partial t^2}p(x,t)(\Delta t)^2 + \frac{1}{2}\frac{\partial^2}{\partial x^2}p(x,t)(\Delta x)^2 + \ldots .$$

Upon taking the limit $\Delta t \to 0$, $\Delta x \to 0$, we find

$$\boxed{\frac{\partial}{\partial t}u(x,t) = D\frac{\partial^2}{\partial x^2}u(x,t)}\,, \tag{2.20}$$

where $u(x,t) \equiv p(x,t)/\Delta x$ is the *probability density*, which is finite no matter how small Δx is, and $D \equiv \lim_{\substack{\Delta x \to 0 \\ \Delta t \to 0}} \frac{(\Delta x)^2}{2\Delta t}$ is assumed to exist.

Equation (2.20) has the same form as the diffusion equation. Although we used the drunken sailor as an example, the derivation we have just outlined applies better to an ensemble of microscopic particles in random motion, where it makes more sense to take $\Delta x \to 0$, $\Delta t \to 0$, and to treat x and t as continuous variables.

2.3.2 Price of stocks as a random walk

In an efficient market, the price for a share of a company stock is an amount for which as many people wish to buy as to sell. Those wishing to buy are probably expecting the stock price to rise in the near future, while those willing to sell at that price are probably anticipating the stock to drop in price. In such a market, insider trading is curbed. Any information known at time t about the company which might impact its stock price is already reflected in the price at that time. It is equally likely for the price of that stock to rise a given amount Δx at a future time $t+\Delta t$ as it is to fall by the same amount. Consequently, the expectation of a change in price of a stock in a future time should behave like a random walk, and therefore should be governed by the same diffusion equation (2.20), with however a different value for the "diffusion coefficient" D depending on the "volatility" of each stock.

2.4 The Wave Equation

Let us consider as an example the problem of a vibrating (guitar) string. The string is stretched lengthwise with uniform tension T. To fix ideas, let us say that in its equilibrium position the string lies horizontally (in the x-direction), and we consider a vertical displacement $u(x,t)$ from this equilibrium position. We assume that these displacements are small, as compared to the equilibrium length of the string.

We consider a small section of the string between x and $x+\Delta x$. See Figure 2.2.

We apply Newton's law of motion:

$$ma = F$$

(mass times acceleration balancing force), to the vertical motion of this small section of the string. Its mass m is $\rho A \Delta x$, where ρ is the density of the material of the string and A its cross-sectional area. The acceleration in the vertical direction is

$$a = \frac{\partial^2}{\partial t^2} u.$$

The force should be the vertical component of the tension, plus other forces such as gravity and air friction.

The net vertical component of tension is

$$\begin{aligned} & T\sin\theta_2 - T\sin\theta_1 \\ \cong\ & T[\theta_2 - \theta_1] \\ \cong\ & T[u_x(x+\Delta x,t) - u_x(x,t)], \end{aligned}$$

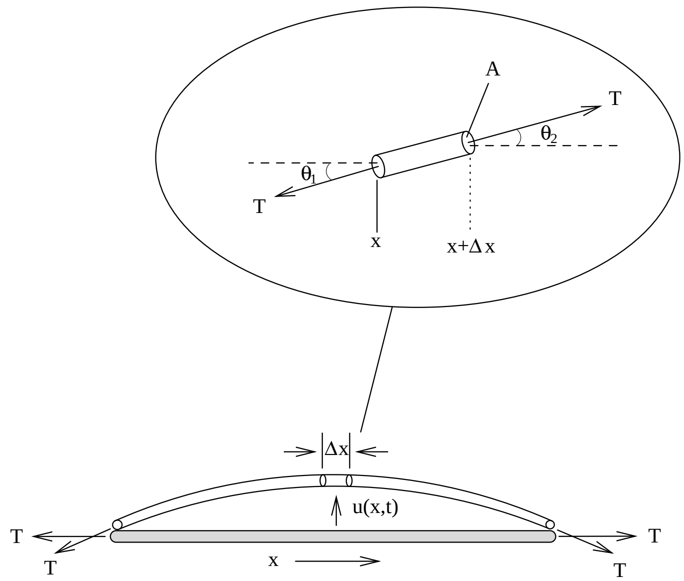


Figure 2.2: A stretched elastic string

assuming that the angles θ_1 and θ_2 are small. Putting these all together, we have

$$\rho A \Delta x \frac{\partial^2}{\partial t^2} u = TA[u_x(x+\Delta x, t) - u_x(x,t)] + \rho A \Delta x \cdot f \tag{2.21}$$

where f represents all additional force per unit mass. Equation (2.21) is

$$\frac{\partial^2}{\partial t^2} u = \frac{T}{\rho} \frac{1}{\Delta x} [u_x(x+\Delta x, t) - u_x(x,t)] + f,$$

which becomes, as $\Delta x \to 0$:

$$\frac{\partial^2}{\partial t^2} u = c^2 \frac{\partial^2}{\partial x^2} u + f, \tag{2.22}$$

where $c^2 \equiv T/\rho$.

The additional force f could represent gravity, in which case $f = -g$ ($g = 980$ cm/s^2), or a frictional force of the form: $f = -\gamma u_t$, where γ is a damping coefficient. In most of the examples to be considered, f will be ignored, and we will be dealing with the simple homogeneous wave equation

$$\boxed{\frac{\partial^2}{\partial t^2} u = c^2 \frac{\partial^2}{\partial x^2} u}\,. \tag{2.23}$$

The wave equation is also quite ubiquitous. Equation (2.23) also governs the propagation of sound waves in the atmosphere, with c changed to the speed of sound. It also governs water waves travelling on the surface of shallow water, with c replaced by $\sqrt{gh}$ and h being the depth of the water.

2.5 Multiple Dimensions

Although our discussions have so far used one dimensional examples, extensions to two or three spatial dimensions are straightforward. These are indicated below:

1-D diffusion equation:

$$\frac{\partial}{\partial t}u = k\frac{\partial^2}{\partial x^2}u.$$

3-D diffusion equation:

$$\boxed{\frac{\partial}{\partial t}u = k\nabla^2 u}\,, \tag{2.24}$$

where $\nabla^2 \equiv \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$ is the Laplacian operator.

1-D wave equation:

$$\frac{\partial^2}{\partial t^2}u = c^2\frac{\partial^2}{\partial x^2}u.$$

3-D wave equation:

$$\boxed{\frac{\partial^2}{\partial t^2}u = c^2\nabla^2 u}\,. \tag{2.25}$$

Essentially, in multi-dimensions, the Laplacian operator replaces the $\frac{\partial^2}{\partial x^2}$ term of the one-dimensional problem.

At steady state the heat equation in multi-dimensions is

$$\boxed{\nabla^2 u = 0}\,. \tag{2.26}$$

Equation (2.24) is called Laplace's equation. Its solution gives the steady state temperature distribution in multi-dimensions, for example, Laplace's equation also governs the distribution of electrostatic potential and the velocity potential in ideal fluid flows.

2.6 Types of second-order PDEs

There are three types of second-order PDEs, whose solutions have distinctly different behaviors. These are *parabolic*, *hyperbolic*, and *elliptic* PDEs. Parabolic equations are diffusion like, while hyperbolic equations are typified by the wave equation. Laplace's equation belongs to the category of elliptic PDEs. Namely:

$\frac{\partial}{\partial t}u = k\frac{\partial^2}{\partial x^2}u$:	Parabolic type
$\frac{\partial^2}{\partial t^2}u = c^2\frac{\partial^2}{\partial x^2}u$:	Hyperbolic type
$\frac{\partial^2}{\partial x^2}u + \frac{\partial^2}{\partial y^2}u = 0$:	Elliptic type

In general a second-order linear PDE in two independent variables (denoted by x and y) can be written in the form (with u_{xx} denoting $\frac{\partial^2}{\partial x^2}u$ etc.):

$$Au_{xx} + Bu_{xy} + Cu_{yy} + Du_x + Eu_y + Fu = G,$$

where A, B, C, D, E, F and G are given functions of x and y. This equation is said to be *parabolic* if $B^2 - 4AC = 0$, *hyperbolic* if $B^2 - 4AC > 0$, and *elliptic* if $B^2 - 4AC < 0$.

The equation is homogeneous if $G \equiv 0$.

2.7 Boundary Conditions

The mathematical specification of a problem involving a partial differential equation in space x and time t is incomplete without the imposition of *boundary conditions* and *initial conditions.*

Three different types of boundary conditions for second order PDEs:

A. *Dirichlet conditions*, where the value of the unknown u is specified at the spatial boundaries.

For example, suppose we want to solve for $u(x,t)$ for $0 < x < L$, the boundaries of the domain are at $x = 0$ and $x = L$. We specify $u = T_1$ at $x = 0$ and $u = T_2$ at $x = L$, this is a Dirichlet boundary condition, because here the values of the unknown u is specified at the boundaries $x = 0$ and

$x = L$. If the values specified at the boundaries are zero, then we call this the *homogeneous* Dirichlet boundary condition. So

$$\boxed{u(0,t) = 0,\ u(L,t) = 0}$$

is a homogeneous Dirichlet boundary condition for a problem in $0 < x < L$.

For the heat conduction problem discussed in 2.2.3, this boundary condition is equivalent to specifying the value of the temperatures at the two ends of the rod.

B. *Neumann Condition*, where the value of the normal derivative of the unknown is specified at the boundaries. [The normal derivative is the derivative normal to the boundary. In a one-dimensional space x, u_x is the normal derivative of u.] For the above mentioned domain,

$$\boxed{u_x(0,t) = b_1, \quad u_x(L,t) = b_2}$$

is a Neumann boundary condition if b_1 and b_2 are specified. If $b_1 = 0$ and $b_2 = 0$, we then have a homogeneous Neumann boundary condition.

For the heat conduction problem, the Neumann condition is equivalent to specifying the heat fluxes at the two ends of the rod. A zero flux represents the fact that the ends of the rod are insulated.

C. *Robin condition*, which involves the specification of a linear combination of u and its normal derivative. An example is

$$\boxed{\begin{aligned} ku_x(0,t) &= h[u(0,t) - b_1] \\ ku_x(L,t) &= h[u(L,t) - b_2] \end{aligned}}\,.$$

For the heat conduction problem, the above condition describes the heat fluxes at the ends of the rod as a difference of the rod temperature and the temperature b_1 and b_2 of the ambient medium with which the rod is in contact.

2.8 Initial Conditions

For the diffusion or heat equation, the PDE governs the diffusion of a tracer or the conduction of heat, whereas the boundary conditions tells us what is happening at the boundaries to affect the solution inside the domain of interest. The initial condition tells us the state from which the solution evolves. Without it, the mathematical specification of the problem is incomplete.

Physically, we understand that two identical conducting rods with the same boundary conditions can evolve differently if they start with different initial temperatures. A completely specified problem can be, for example:

$$\begin{array}{ll} \text{PDE:} & u_t = ku_{xx}, \quad 0 < x < L, \quad t > 0 \\ \text{BC:} & u(0,t) = 0, \quad u(L,t) = 0, \quad t > 0 \\ \text{IC:} & u(x,0) = f(x), \quad 0 < x < L, \quad \text{where} f(x) \text{ is given.} \end{array}$$

For the wave equation, which has a second-order derivative in time, we need two initial conditions. An example of a completely specified problem is:

$$\begin{array}{ll} \text{PDE:} & u_{tt} = c^2 u_{xx}, \quad 0 < x < L, \quad t > 0 \\ \text{BC:} & u(0,t) = 0, \quad u(L,t) = 0, \quad t > 0 \\ \text{IC:} & u(x,0) = f(x), \quad u_t(x,0) = g(x), \quad 0 < x < L, \end{array}$$

where $f(x)$ and $g(x)$ prescribed.

For the vibrating string problem, $f(x)$ represents the initial position of the string, while $g(x)$ represents the initial velocity with which the string is plucked. Both are needed to completely specify the problem. Physically, we understand that the note emitted by a vibrating guitar string is different if we gently displace it and then let go (with $g = 0$) than if we displace the string with a sudden pull.

For the Laplace equation, there is no need for initial conditions. Only boundary conditions are needed. Physically, Laplace's equation determines the temperature distribution at steady state and so this temperature should depend on the conditions at the boundaries only.

If we nevertheless insist on treating one of the independent variables (say y) in the Laplace equation as time-like, and specify "initial conditions" of the form

$$\begin{aligned} u(x,0) &= f(x), \\ u_y(x,0) &= g(x), \end{aligned}$$

the problem in many cases becomes unphysical ("ill-posed"). An example of an ill-posed problem is:

$$\begin{array}{ll} \text{PDE:} & \dfrac{\partial^2}{\partial x^2}u + \dfrac{\partial^2}{\partial y^2}u = 0, \quad 0 < x < L, \quad y > 0 \\ \text{BC:} & u(0,y) = 0, \quad u(L,y) = 0 \\ \text{IC:} & u(x,0) = f(x), \quad u_y(x,0) = g(x), \quad 0 < x < L. \end{array}$$

2.9 Exercises

1. Classify the following PDEs and their associated boundary conditions:

   (a) PDE: $u_t - u_{xx} = \sin x$, $0 < x < \pi$, $t > 0$

   BC: $u(0,t) = 0$, $u(\pi,t) = 0$, $t > 0$

   (b) PDE: $u_{tt} - a(x)^2 u_{xx} = 0$, $t > 0$, $0 < x < L$ where $a(x)$ is a real and nonzero given function.

   BC: $u_x(0,t) = u_x(L,t) = 0$.

2. Consider the following heat equation

$$u_t = \alpha^2 u_{xx}, \quad 0 < x < L, \quad t > 0, \ \alpha = \text{constant}.$$

for a rod of length L whose ends are maintained at temperature $u = 0$, i.e.

$$u(x,t) = 0 \text{ at } x = 0 \text{ and at } x = L.$$

Initially, at $t = 0$, the temperature distribution is given by

$$u(x,0) = \sin\left(\frac{\pi x}{L}\right), \quad 0 < x < L.$$

Solve for $u(x,t)$ for $t > 0$. [Hint: Assume that the solution can be written in the "separable" form:

$$u(x,t) = T(t) \sin \frac{\pi x}{L}.$$

Find $T(t)$ by substituting it into the PDE. Make sure that the initial condition and the boundary conditions are also satisfied.]

3. Same as problem # 1, except the initial condition is

$$u(x,0) = \sin \frac{\pi x}{L} + \frac{1}{4} \sin \frac{2\pi x}{L}.$$

[Hint: Assume $u(x,t) = T_1(t) \sin \frac{\pi x}{L} + T_2(t) \sin \frac{2\pi x}{L}$.]

2.10 Solutions

1. (a) PDE: *parabolic*, nonhomogeneous, linear, second order, two independent variables

BC: Homogeneous Dirichlet.

(b) PDE: *Hyperbolic*, homogeneous, linear, second order, two independent variables.

BC: Homogeneous Neumann.

2. Solve the heat equation,

$u_t = \alpha^2 u_{xx}, \quad 0 < x < L, \quad t > 0$

with boundary conditions, $u(0,t) = u(L,t) = 0$ and initial condition $u(x,0) = \sin(\pi x/L)$.

Assume that the solution can be written in the "separable" form: $u(x,t) = T(t)\sin(\pi x/L)$.

Substitute into the PDE to find: $dT/dt + (\alpha\pi/L)^2 T = 0$.

This is a first order ODE with general solution: $T(t) = ce^{-(\alpha\pi/L)^2 t}$.

Now we use the initial condition to find: $c = 1$. Thus we have the solution:

$u(x,t) = e^{-(\alpha\pi/L)^2 t}\sin(\pi x/L)$.

3. This problem is the same as problem 2 except that we now have the initial condition:

$u(x,0) = sin(\pi x/L) + \sin(2\pi x/L)/4$.

Following the hint we assume that the solution has the form $u(x,t) = u_1(x,t) + u_2(x,t)$ where $u_1(x,t) = T_1(t)\sin(\pi x/L)$ and $u_2(x,t) = T_2\sin(2\pi x/L)$.

We can see that $u_1(x,t)$ is the solution we found in problem 2 and that in finding the solution $u_2(x,t)$ we do exactly as in problem 2, where the general solution becomes $T_2(t) = c_2 e^{-(2\alpha\pi/L)^2 t}$ with the constant $c_2 = 1/4$.

Thus we have, after adding u_1 and u_2, the solution to problem 3 as:

$u(x,t) = e^{-(\alpha\pi/L)^2 t}\sin(\pi x/L) + e^{-(2\alpha\pi/L)^2 t}\sin(2\pi x/L)/4$.

Chapter 3

Separation of Variables

3.1 Introduction

The method of separation of variables is a standard technique for solving linear PDEs in finite domains. Fourier series arise naturally from this method of solution.

3.2 An example of heat conduction in a rod:

Consider the problem of a copper rod of thermal diffusivity α^2 and of length L with a known initial temperature $u(x,0) = f(x)$. For $t > 0$, the two ends of the rod are maintained at a constant temperature of 0° C. Find the temperature of the rod as a function of x and t.

The mathematical problem is specified by the partial differential equation (PDE) governing the heat conduction process, the boundary conditions (BCs), and the initial condition (IC):

$$\begin{aligned}
&\text{PDE:} \quad && u_t = \alpha^2 u_{xx}, \quad 0 < x < L, \quad t > 0 && (3.1)\\
&\text{BCs:} \quad && u(0,t) = 0, \quad u(L,t) = 0, \quad t > 0 && (3.2)\\
&\text{IC:} \quad && u(x,0) = f(x), \quad 0 < x < L. && (3.3)
\end{aligned}$$

(It is understood that u is expressed in units of $^\circ$C.)

The boundary conditions we have imposed here are of Dirichlet type. We prefer to first make them homogeneous. If the boundary values were instead

$$u(0,t) = T_1, \quad u(L,t) = T_2,$$

we would first try to make them zero by defining a new unknown $\tilde{u}(x,t)$:

$$\tilde{u}(x,t) = u(x,t) - \left[T_1 + \frac{x}{L}(T_2 - T_1)\right],$$

so that the new problem for $\tilde{u}(x,t)$ has homogeneous boundary conditions:

$$\begin{array}{ll} \text{PDE:} & \tilde{u}_t = \alpha^2 \tilde{u}_{xx}, \quad 0 < x < L, \quad t > 0 \\ \text{BCs:} & \tilde{u}(0,t) = 0, \quad \tilde{u}(L,t) = 0, \quad t > 0 \\ \text{IC:} & \tilde{u}(x,0) = f(x) - \left[T_1 + \frac{x}{L}(T_2 - T_1)\right] \equiv g(x), \quad 0 < x < L. \end{array}$$

In the following section we will consider the system (3.1), (3.2), and (3.3), with the understanding that if the boundary conditions are not homogeneous, we can make them so with a redefinition of u and f.

3.3 Separation of variables:

- **Step 1:** We first assume the solution to the PDE (3.1) is of the "separable" form:

$$u(x,t) = T(t)X(x). \tag{3.4}$$

- **Step 2:** Substituting the assumed form (3.4) into Eq. (3.1) yields

$$\frac{d}{dt}T(t) \cdot X(x) = \alpha^2 T(t) \frac{d^2}{dx^2} X.$$

  We divide both sides of the equation by $\alpha^2 T(t) X(x)$ to get

$$\frac{\frac{d}{dt}T(t)}{\alpha^2 T(t)} = \frac{\frac{d^2}{dx^2}X(x)}{X(x)}. \tag{3.5}$$

  [Division by α^2 is not necessary, and will not make any difference to the procedure if this is not done.]

- **Step 3:** Notice that the left-hand side of Eq. (3.5) is a function of t only, while the right-hand side is a function of x only. The only way a function of t can be equal to a function of x is for each to equal to a constant. Let this *separation constant* be denoted by K.

  So (3.5) becomes

$$\frac{d}{dt}T(t)/\alpha^2 T(t) = \frac{d^2}{dx^2}X(x)/X(x) = K. \tag{3.6}$$

This is actually *two* ordinary differential equations:

$$\frac{d^2}{dx^2}X(x) = KX(x), \tag{3.7}$$

and

$$\frac{d}{dt}T(t) = \alpha^2 KT(t). \tag{3.8}$$

- **Step 4:** We know how to solve Eq. (3.7) from Chapter 1 if K is negative. Let us solve this case first and later do the K positive case.

  Let $K = -\lambda^2 < 0$, where λ^2 is some positive constant. Eq. (3.7) becomes the harmonic oscillator equation:

$$\frac{d^2}{dx^2}X(x) + \lambda^2 X(x) = 0, \tag{3.9}$$

  whose solution is, from Chapter 1:

$$X(x) = A\sin\lambda x + B\cos\lambda x. \tag{3.10}$$

  [We can alternatively use the complex notation and write $X(x) = ae^{i\lambda x} + be^{-i\lambda x}$. In the present case it is more convenient, for the purpose of applying boundary condition, to use the real solution (3.10).]

  The constants A and B are (presumably) to be determined from the boundary conditions, which are, from (3.2) and (3.4):

$$X(0) = 0, \quad X(L) = 0. \tag{3.11}$$

  From (3.10), we have

$$X(0) = B,$$

  so the first boundary conditions demands that $B = 0$. Thus,

$$X(x) = A\sin\lambda x, \tag{3.12}$$

$$X(L) = A\sin\lambda L.$$

  The second boundary condition, $X(L) = 0$, then implies either

$$A = 0 \quad \text{or} \quad \sin\lambda L = 0.$$

  The first possibility, $A = 0$, gives a trivial solution

$$X(x) \equiv 0.$$

For nontrivial solutions, we need $\sin \lambda L = 0$, yielding the *eigenvalue*:

$$\lambda = \frac{n\pi}{L} \equiv \lambda_n, \quad n = 1, 2, 3, 4, 5, \ldots \ . \tag{3.13}$$

[The nagative integer values of n doesnot give different solutions from the positive values because $A\sin(-\lambda_n x) = A' \sin(\lambda_n x)$, where $A' = -A$.]

The corresponding *eigenfunction* (from (3.12) and (3.13)) is:

$$X(x) = \sin \lambda_n x \equiv X_n(x). \tag{3.14}$$

[Note that we have set the arbitrary constant A to 1 in (3.14), without loss of generality, because we can always absorb a different A in $T(t)$. It is the *product*, $u(x,t) = T(t)X(x)$, that matters.]

It is easy to show that for $K > 0$, the solution to (3.7) is

$$X(x) = Ae^{\sqrt{K}x} + Be^{-\sqrt{K}x}.$$

$X(0) = 0$ implies

$$A + B = 0, \quad \text{or} \quad A = -B.$$

$X(L) = 0$ implies

$$Ae^{\sqrt{K}x} + Be^{-\sqrt{K}x} = 0,$$

or

$$B\left(-e^{\sqrt{K}L} + e^{-\sqrt{K}L}\right) = 0.$$

Since $K > 0$, $e^{\sqrt{K}L} > e^{-\sqrt{K}L}$, B should be zero. Thus $A = -B$ is also zero, leading to a trivial solution $X(x)$.

For $K = 0$, the ordinary differential equation for $X(x)$ becomes

$$\frac{d^2}{dx^2}X = 0.$$

Its solution is

$$X(x) = Ax + B.$$

Applying the boundary condition $X(0) = 0$ leads to $B = 0$. Applying $X(L) = 0$ then implies that $A = 0$. This again leads to the trivial solution $X(x)$.

Thus we conclude that for nontrivial solutions, K can only be negative, and furthermore K can only equal the following discrete values

$$K = -\lambda_n^2 = -\left(\frac{n\pi}{L}\right)^2, \quad n = 1, 2, 3, 4, \ldots .$$

- **Step 5:** The $T(t)$ equation (3.8) now becomes

$$\frac{d}{dt}T = -\alpha^2\lambda_n^2 T(t). \tag{3.15}$$

We denote the solution for each value of n:

$$T(t) = T_n(t) = T_n(0)e^{-\alpha^2\lambda_n^2 t}. \tag{3.16}$$

- **Step 6:** We have in fact found an infinite number of solutions to the PDE (3.1), each satisfying the boundary conditions (3.2). They are of the form

$$\begin{aligned} u_n(x,t) &\equiv T_n(t)X_n(x) \\ &= T_n(0)e^{-\alpha^2\left(\frac{n\pi}{L}\right)^2 t}\sin\frac{n\pi x}{L}, \end{aligned} \tag{3.17}$$

each corresponding to a value of n, $n = 1, 2, 3, 4, \ldots$.

In (3.17), the $T_n(0)$'s are arbitrary constants, (presumably) to be determined from the initial condition (3.3). However, this is only feasible if the initial condition (3.3) is such a sine function. For example, if the initial condition is

$$u(x,0) = \sin\frac{\pi x}{L}, \tag{3.18}$$

we should then pick $n = 1$, and $T_1(0) = 1$. This leads to the solution

$$u(x,t) = u_1(x,t) = e^{-\alpha^2\left(\frac{\pi}{L}\right)^2 t}\sin\frac{\pi x}{L}. \tag{3.19}$$

You should now verify that (3.19) satisfies the PDE (3.18), and is therefore *the* solution we are looking for in this particular special case.

- **Step 7:** To satisfy more general initial conditions, we need to construct a more general solution. We do so by adding up all possible component solutions in (3.17). [This is referred to as the *principle of superposition.*]

We write:

$$\begin{aligned} u(x,t) &= u_1(x,t) + u_2(x,t) + u_3(x,t) + \ldots \\ &= \sum_{n=1}^{\infty} u_n(x,t) \qquad (3.20) \\ &= \sum_{n=1}^{\infty} T_n(0)e^{-(\alpha\pi/L)^2 t}\sin\frac{n\pi x}{L}. \qquad (3.21) \end{aligned}$$

You should check that the sum in (3.20) satisfies the PDE (3.1) and the boundary condition (3.2), presuming the infinite series converges.

- **Step 8:** We now use the more general solution (3.21) to satisfy the initial condition (3.3). To satisfy

$$u(x,0) = f(x), \quad 0 < x < L.$$

we require

$$f(x) = \sum_{n=1}^{\infty} T_n(0) \sin \frac{n\pi x}{L}, \quad 0 < x < L, \tag{3.22}$$

The remaining task is to evaluate $T_n(0)$ given $f(x)$.

- **Step 9:** If we can express a function $f(x)$ in terms of what is now known as a *Fourier sine series*:

$$f(x) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L}, \quad 0 < x < L, \tag{3.23}$$

then we can equate each term in (3.22) and (3.23) and find that

$$T_n(0) = a_n, \quad n = 1, 2, 3, \ldots$$

and the problem is then completely solved.

The question is, can we always represent an arbitrary function $f(x)$ in the form of a Fourier sine series (3.23)? We will leave this issue to the next chapter, where Fourier series will be discussed.

The French scientist Joseph Fourier faced these questions when he studied the heat conduction problem, much as we presented it here. Fourier claimed in 1807, when he presented his paper on heat conduction to the Paris Academy, that an arbitrary function $f(x)$ could indeed be expressed as a sum of sines in the form of (3.23). There was not much mathematical rigor in Fourier's arguments; he was probably motivated by his physical understanding of the heat conduction problem for which the general solution should be expressible in the form of (3.21). Setting $t = 0$ in this solution would then seen to "require" the initial arbitrary temperature distribution to be expressible as a sum of sines, as in (3.22). This assertion of Fourier's was ridiculed by the mathematician Lagrange at the time. We now know of course that Fourier was right: Any physically reasonable function $f(x)$ can be written in the form of a sum of sines (or cosines for that matter).

Assuming that (3.23) is true and the series converges, we can obtain the coefficient a_n of the Fourier sine series of $f(x)$ in the following manner.

Multiply both sides of Eq. (3.23) by $\sin \frac{m\pi x}{L}$, where m is any integer, and integrate over the domain:

$$\int_0^L f(x) \sin \frac{m\pi x}{L} dx = \sum_{n=1}^{\infty} a_n \int_0^L \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} dx. \tag{3.24}$$

Note that in (3.24) we have switched the order of integration and summation. This is allowable if the series is uniformly convergent. In the next chapter, we will derive the so-called *orthogonality relationship* of sines which states

$$\frac{2}{L} \int_0^L \sin \frac{n\pi x}{L} \sin \frac{m\pi x}{L} dx = \delta mn \equiv \begin{cases} 1 & if \quad m = n \\ 0 & if \quad m \neq n. \end{cases} \tag{3.25}$$

Substituting (3.25) into (3.24), we find that only one term remains in the infinite sum on the right-hand side:

$$\sum_{n=1}^{\infty} a_n \frac{L}{2} \delta mn = \frac{L}{2} a_m. \tag{3.26}$$

Equating (3.26) to the left-hand side of (3.24), we obtain:

$$a_m = \frac{2}{L} \int_0^L f(x) \sin \frac{m\pi x}{L} dx, \quad \text{where } m = 1, 2, 3, 4, \ldots. \tag{3.27}$$

Since m is an arbitrary index, we can use any other symbol, including n. Thus (3.27) is the same as

$$a_n = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi x}{L} dx, \quad n = 1, 2, 3, \ldots. \tag{3.28}$$

Either (3.27) or (3.28) can be used to generate the coefficients $a_1,\ a_2,\ a_3,\ a_4,\ \ldots$.

- **Step 10:** Finally, we have the solution which satisfies the PDE, the BCs, and the IC:

$$u(x,t) = \sum_{n=1}^{\infty} a_n e^{-(\alpha n\pi/L)^2 t} \sin \frac{n\pi x}{L}, \quad 0 < x < L$$

$$\text{where} \quad a_n = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi x}{L} dx. \tag{3.29}$$

You should try to verify *a posteri* that (3.29) does indeed satisfy (3.1), (3.2), and (3.3).

3.4 Physical interpretation of the solution:

The general solution (3.29) to the heat conduction problem, although complicated, has some simple physical interpretations.

It can be rewritten as

$$u(x,t) = \sum_{n=1}^{\infty} a_n e^{-n^2 t/t_e} \sin \frac{n\pi x}{L},$$

where $t_e \equiv (L/(\pi\alpha))^2$ is about an hour for a copper rod of length 2m (with $\alpha^2 = 1.16 \text{ cm}^2/\text{s}$). The initial temperature distribution

$$u(x,0) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L}$$

can be quite complicated and can consist of many sine modes. As time goes on, however, the small scales (i.e. the higher n sine modes) in the sum for $u(x,t)$ decay much faster than the larger scale modes. If a_1 and a_n are nonzero, we can look at the ratio

$$\frac{a_n e^{-n^2 t/t_e}}{a_1 e^{-t/t_e}}$$

of the coefficients of the nth mode and the first mode.

At $t = t_e$, about one hour later, the ratio gets smaller and smaller for increasing n because

$$\begin{aligned} e^{-n^2}/e^{-1} \quad &= 0.05 \quad \text{for } n=2 \\ &3 \times 10^{-4} \quad \text{for } n=3 \\ &3 \times 10^{-7} \quad \text{for } n=4. \end{aligned}$$

Therefore, for most practical purposes, the full solution is dominated by the first term, the lowest sine mode:

$$u(x,t) \simeq a_1 e^{-t/t_e} \sin \frac{\pi x}{L} \quad \text{for } t \gtrsim t_e.$$

Eventually, even this lowest mode decays to zero, as the rod approaches a uniform zero temperature consistent with the temperature specified at the boundaries.

For small times, smaller scale modes are significant, if these were present in the initial temperature distribution. However, the smaller scales decay faster than the larger scales. We see a gradual *smoothing* of the solution. This is a common property of diffusion and heat conduction, which always tends to smooth out gradients that are present.

3.5 A vibrating string problem:

Consider a vibrating (guitar) string of length L—the length of the vibrating part being determined by where the player presses on the string. Let $c^2 = T/\rho$, where T is the tension on the string, which can be adjusted by the player, and ρ is the density of its material.

$$\text{PDE:} \quad u_{tt} = c^2 u_{xx}, \quad 0 < x < L, \quad t > 0 \tag{3.30}$$

$$\text{BCs:} \quad u(0,t) = 0, \quad u(L,t) = 0 \tag{3.31}$$

$$\text{IC:} \quad u(x,0) = f(x), \quad u_t(x,0) = g(x), \quad 0 < x < L. \tag{3.32}$$

A few words are in order about the initial conditions. Mathematically, since there is a second derivative in t in the governing PDE, there should be two initial conditions to completely specify the problem. We will see this as we proceed further with the solution of the problem and discover that there will be undetermined constants in the solution if we don't prescribe a second initial condition. This is unlike the case of the heat equation, which needs only a first order derivative in t be given.

In (3.32), $f(x)$ is the shape of the initial displacement and $g(x)$ is the shape of the initial velocity. We will see that the intensity of the sound and the spectrum of frequencies of sound generated depend on both initial conditions.

We again use the method of separation of variables to solve this problem. Since we have already discussed the ten steps of this method in detail in the previous section, there is no need to repeat every detail here again. You can follow this template in doing your homework and exam problems.

We first assume that the solution can be written in the separable form:

$$u(x,t) = T(t)X(x)$$

anticipating that we will ultimately superpose such solutions to satisfy initial conditions.

Substituting into the PDE yields

$$\frac{1}{c^2}\frac{d^2T}{dt^2}/T = \frac{d^2X}{dx^2}/X = -\lambda^2,$$

where $-\lambda^2$ is the separation constant. Solving the ordinary differential equation for X:

$$\frac{d^2X}{dx^2} + \lambda^2 X = 0,$$

subject to the boundary conditions:

$$X(0) = 0, \quad X(L) = 0,$$

yields the eigenvalues:

$$\lambda = \lambda_n = \frac{n\pi}{L}, \quad n = 1, 2, 3, \ldots$$

and the corresponding eigenfunction:

$$X(x) = X_n(x) = \sin \lambda_n x$$

(again scaling out any multiplicative factor)

The T-equation:

$$\frac{d^2T}{dt^2} = -c^2\lambda^2 T$$

can be solved for each value of $\lambda = \lambda_n$ to yield:

$$T(t) = T_n(t) = A_n \sin(\omega_n t) + B_n \cos(\omega_n t),$$

where $\omega_n = c\lambda_n = cn\pi/L$ is the *frequency* of oscillation and the constants A_n and B_n remain arbitrary.

We construct the general solution by superimposing all possible solutions of the form $T_n(t)X_n(x)$, to yield:

$$\boxed{\begin{aligned} u(x,t) &= \sum_{n=1}^{\infty} T_n(t)X_n(x) \\ &= \sum_{n=1}^{\infty} [A_n \sin(\omega_n t) + B_n \cos(\omega_n t)] \sin \frac{n\pi x}{L} \end{aligned}} . \tag{3.33}$$

To satisfy the initial conditions (3.32), we require

$$u(x,0) = f(x) = \sum_{n=1}^{\infty} B_n \sin \frac{n\pi x}{L}, \quad 0 < x < L, \tag{3.34}$$

and

$$u_t(x,0) = g(x) = \sum_{n=1}^{\infty} \frac{cn\pi}{L} A_n \sin \frac{n\pi x}{L}, \quad 0 < x < L. \tag{3.35}$$

(3.34) is a Fourier sine series for the initial displacement $f(x)$, and so (see (3.29))

$$\boxed{B_n = \frac{2}{L}\int_0^L f(x) \sin \frac{n\pi x}{L} dx} . \tag{3.36}$$

(3.35) is a Fourier sine series for the initial velocity $g(x)$, and so

$$\boxed{A_n = \frac{2}{\pi n c}\int_0^L g(x)\sin\frac{n\pi x}{L}dx}\,. \tag{3.37}$$

The solution (3.33) is now completely specified. Convergence of the series solution remains to be considered.

Physical Interpretation:

Unlike the solution of the heat/diffusion equation, the solution to the wave equation does not decay in time. Instead there are *standing waves* set up between the two ends of the string. The gravest (fundamental) standing-mode, $\sin\frac{\pi x}{L}$, oscillates with a frequency $\omega_1 = c\lambda_1$, and the nth standing-mode, $\sin\frac{n\pi x}{L}$, oscillates with a frequency

$$\omega_n = c\lambda_n = \frac{n\pi c}{L} = \frac{n\pi}{L}\sqrt{\frac{T}{\rho}}.$$

i.e. n times the fundamental frequency w_1.

This property, that all frequencies generated by a vibrating string are integer multiples of the fundamental frequency, is what makes the sound of a violin or guitar pleasing to the human ear. This property is a consequence of the one space dimensionality of the vibrating string, and is not shared by two dimensional vibrating membranes (such as a drumhead), where the higher-order frequencies are not integer multiples of the fundamental one.

The frequencies produced by a vibrating string

$$\omega_n = \frac{n\pi}{L}\sqrt{\frac{T}{\rho}}$$

depend on a few physical parameters, as revealed by the solution. The higher the tension on the string, the higher the frequency; the denser the string material, the lower the frequency; and the longer the length of the vibrating part of the string, the lower the frequency. The latter part is controlled by the guitarist's placement of his (or her) finger when he clamps down on the string.

3.6 Schrödinger equation

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2\mu}\nabla^2\psi + V\psi$$

where $\hbar$ is Planck's constant ($\hbar = 1.054 \times 10^{-34} J \cdot s$), μ is the mass of the particle under consideration, and V is the potential energy (time independent) of the force field ($F = -\nabla V$). ψ is the wave function; $|\psi|^2$ gives the probability density of finding the particle in a particular location. Consider the following simple example:

1-D Schrödinger equation:

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}\psi + V(x)\psi, \qquad -\infty < x < \infty.$$

Suppose $V(x) = 0$ if $0 < x < L$, but ∞ elsewhere. Therefore the particle cannot be located anywhere other than in $0 < x < L$. The problem simplifies to

$$\begin{aligned} &\text{PDE:} \quad i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2\mu}\frac{\partial^2}{\partial x^2}\psi \qquad 0 < x < L \\ &\text{BC:} \quad \psi(0,t) = 0, \quad \psi(L,t) = 0 \end{aligned}$$

Separation of variables:

$$\begin{aligned} \psi(x,t) &= u(x)T(t) \\ \frac{i\hbar T'(t)}{T(t)} &= -\frac{\hbar^2}{2\mu}\frac{u''(x)}{u(x)} = \text{const} \equiv E \\ T'(t) &= -iET(t)/\hbar \\ u''(x) &= -E2\mu/\hbar^2 u(x). \end{aligned}$$

Since

$$T(t) = T(0)e^{-iEt/\hbar}$$

$E/\hbar$ is interpreted as the frequency of oscillation, ω. In quantum mechanics, ω times $\hbar$ is the energy of the oscillator. This is the reason the symbol E was used ($E = \omega\hbar$) as the separation constant. It is to be determined from the boundary value problem as an eigenvalue.

$$\begin{cases} u''(x) = -2\mu E/\hbar^2 u(x) \\ u(0) = 0, \quad u(L) = 0 \end{cases}$$

Solution:

$$u(x) = A\sin\sqrt{\frac{2\mu E}{\hbar^2}}x + B\cos\sqrt{\frac{2\mu E}{\hbar^2}}x$$

$u(0) = 0$ implies $B = 0$. $u(L) = 0$ implies

$$A\sin\sqrt{\frac{2\mu E}{\hbar^2}}L = 0.$$

Therefore $\sqrt{2\mu E}L/\hbar = n\pi$, $n = 1, 2, 3, \ldots$, which is:

$$E = E_n = \frac{n^2\pi^2\hbar^2}{2\mu L^2}, \qquad n = 1,\ 2,\ \ldots.$$

The energy is quantized! The solution is:

$$\psi(x,t) = \sum_{n=1}^{\infty} a_n \sin\frac{n\pi x}{L} e^{-iE_n t/\hbar}, \quad 0 < x < L, \quad 0 \text{ elsewhere}\,.$$

a_n can be found from the initial condition, but this step is often not done. Conceptually the more important result is the quantization of the eigenvalues and hence the quantization of the energy.

3.7 Exercises

1. Solve the following heat equation:

$$\begin{array}{ll} \text{PDE:} & u_t = a^2 u_{xx}, \quad 0 < x < L, \quad t > 0 \\ \text{BCs:} & u(0,t) = 0, \quad u(L,t) = 0, \quad t > 0 \\ \text{IC:} & u(x,0) = \displaystyle\sum_{n=1}^{\infty} a_n \sin\left(\frac{n\pi x}{L}\right), \quad 0 < x < L, \end{array}$$

   where the a_n's are known constants.

2. (a) Solve the following wave equation for a guitar string of density ρ under tension T:

$$\begin{array}{ll} \text{PDE:} & u_{tt} = \left(\dfrac{T}{\rho}\right) u_{xx}, \quad 0 < x < L, \quad t > 0 \\ \text{BCs:} & u(0,t) = 0, \quad u(L,t) = 0, \quad t > 0 \\ \text{IC:} & u(x,0) = a_1 \sin\dfrac{\pi x}{L}, \quad 0 < x < L \\ & u_t(x,0) = 0, \quad 0 < x < L. \end{array}$$

   (b) What is the frequency of oscillation of the string?

3.8 Solutions

1. Solve the following heat equation:

$u_t \; = \; \alpha^2 u_{xx}, \quad 0 < x < L, \quad t > 0$

with initial condition $u(x, 0) \; = \sum_{n=0}^{\infty} a_n \sin(n\pi x/L)$,

and boundary conditions $u(0, t) = 0$, and $u(L, t) = 0$.

We use separation of variables. Since we have homogeneous Dirichlet BCs we use:

$u(x, t) \; = \sum_{n=0}^{\infty} T_n(t) \sin(n\pi x/L)$.

Plugging into the PDE, we are left with a first order ODE in time which has the solution:

$T_n(t) \; = \; A_n e^{-(n\pi/L)^2 \alpha^2 t}$.

Using the initial condition we find:

$\sum_{n=0}^{\infty} A_n \sin(n\pi x/L) = \; \sum_{n=0}^{\infty} a_n \sin(n\pi x/L)$.

Thus $A_n = a_n$ and

$u(x, t) = \sum_{n=0}^{\infty} a_n e^{-(n\pi/L)^2 \alpha^2 t} \sin(n\pi x/L)$.

2. Solve the following vibrating string problem:

$u_{tt} \; = \; (T/\rho) u_{xx}$, $(T/\rho) =$ constant,

with initial conditions $u(x, 0) \; = a_1 \sin(\pi x/L)$, $u_t(x, 0) \; = 0$,

and boundary conditions $u(0, t) = 0$, and $u(L, t) = 0$.

We use separation of variables. Since we have homogeneous Dirichlet BC we find:

$u(x, t) \; = \sum_{n=0}^{\infty} T_n(t) \sin(n\pi x/L)$.

Plugging into the PDE we obtain a second order ODE in time, which has the solution:

$T_n(t) \; = \; A_n \sin(\omega_n t) + B_n \cos(\omega_n t)$, where $\omega_n = (n\pi/L)(T/\rho)^{1/2}$.

Using the initial conditions we find:

$\sum_{n=0}^{\infty} A_n \sin(n\pi x/L) = 0$ and $\sum_{n=0}^{\infty} B_n \sin(n\pi x/L) = a_1 \sin(\pi x/L)$.

Thus we have that: $A_n = 0$ for all n, $B_1 = a_1$ and $B_n = 0$ for $n \neq 1$, leaving us with:

$u(x,t) = a_1 \cos((\pi/L)(T/\rho)^{1/2} t) \sin(\pi x/L).$

The frequency of vibration is $(\pi/L)(T/\rho)^{1/2}$.

Chapter 4

Fourier Sine Series

4.1 Introduction

An important mathematical question raised by Joseph Fourier in 1807, arising from his practical work on heat conduction, is whether an arbitrary function $f(x)$ can be represented in the form of a "Fourier sine series":

$$\boxed{f(x) = \sum_{n=1}^{\infty} a_n \sin\frac{n\pi x}{L}, \quad 0 < x < L.} \tag{4.1}$$

A second question is: suppose we *can* indeed represent $f(x)$ by a Fourier sine series of the form (4.1), how do we calculate the "Fourier sine coefficients", a_n's?

4.2 Finding the Fourier coefficients

Let us deal with the second question first. Suppose (4.1) holds. We multiply both sides by $\sin\frac{m\pi x}{L}$, where m is any integer, and then integrate both sides from 0 to L. Thus,

$$\int_0^L f(x)\sin\frac{m\pi x}{L}dx = \sum_{n=1}^{\infty} a_n \int_0^L \sin\frac{m\pi x}{L}\sin\frac{n\pi x}{L}dx, \tag{4.2}$$

where we have interchanged the order of integration and summation. Using the trigonometric identity:

$$\sin a \sin b = \frac{1}{2}[\cos(a-b) - \cos(a+b)],$$

the integral on the right-hand side of Eq. (4.2) can be evaluated:

$$
\begin{aligned}
I_{mn} \equiv \int_0^L \sin\frac{m\pi x}{L}\sin\frac{n\pi x}{L}dx &= \frac{1}{2}\int_0^L \cos\frac{(m-n)\pi x}{L}dx - \frac{1}{2}\int_0^L \cos\frac{(n+m)\pi x}{L}dx \\
&= \frac{1}{2}\frac{\sin((m-n)\pi x/L)}{(m-n)\pi/L}\Bigg|_0^L - \frac{1}{2}\frac{\sin((m+n)\pi x/L)}{(m+n)\pi/L}\Bigg|_0^L
\end{aligned}
$$

Thus, we obtain the so-called *orthogonality relationship* for sines,

$$I_{mn} = \frac{L}{2}\delta_{mn}, \tag{4.3}$$

where

$$\delta_{mn} \equiv \begin{cases} 1 & \text{if } m = n \\ 0 & \text{if } m \neq n. \end{cases}$$

[When $m = n$, we have

$$
\begin{aligned}
I_{mm} &= \int_0^L \left(\sin\frac{m\pi x}{L}\right)^2 dx = \frac{1}{2}\int_0^L \left(1 - \cos\frac{2m\pi x}{L}\right) dx \\
&= \frac{L}{2}.]
\end{aligned}
$$

Substituting (4.3) into (4.2), we find

$$\int_0^L f(x)\sin\frac{m\pi x}{L}dx = \sum_{n=1}^{\infty} a_n \frac{L}{2}\delta_{mn} = \frac{L}{2}a_m.$$

So for any specified integer m,

$$a_m = \frac{2}{L}\int_0^L f(x)\sin\frac{m\pi x}{L}dx. \tag{4.4}$$

(4.4) gives:

$$
\begin{aligned}
a_1 &= \frac{2}{L}\int_0^L f(x)\sin\frac{\pi x}{L}dx \\
a_2 &= \frac{2}{L}\int_0^L f(x)\sin\frac{2\pi x}{L}dx \\
a_3 &= \frac{2}{L}\int_0^L f(x)\sin\frac{3\pi x}{L}dx \\
&\vdots
\end{aligned}
$$

In particular, we can write

$$\boxed{a_n = \frac{2}{L}\int_0^L f(x)\sin\frac{n\pi x}{L}dx, \quad n = 1, 2, 3, \ldots} \tag{4.5}$$

and thus have completed our task of finding the Fourier sine series coefficients, a_n, in (4.1).

4.3 An Example:

Represent $f(x) = 100$ in the form of a Fourier sine series over the interval $0 < x < L$:

$$f(x) = \sum_{n=1}^{\infty} a_n \sin\frac{n\pi x}{L}, \quad 0 < x < L.$$

The Fourier coefficients, a_n, are given by

$$\begin{aligned} a_n &= \frac{2}{L}\int_0^L f(x)\sin\frac{n\pi x}{L}dx \\ &= \frac{2}{L}\int_0^L 100\sin\frac{n\pi x}{L}dx \\ &= \begin{cases} 0 & \text{if } n \text{ is even} \\ \frac{400}{n\pi} & \text{if } n \text{ is odd.} \end{cases} \end{aligned}$$

So we say that in $0 < x < L$, we have

$$100 = \frac{400}{\pi}\left[\frac{\sin(\pi x/L)}{1} + \frac{\sin(3\pi x/L)}{3} + \frac{\sin(5\pi x/L)}{5} + \ldots\right]. \tag{4.6}$$

(4.6) is rather strange; it says that a constant, 100, can be represented by a sum of sines. Let us see what we will get if we add up the sines in the right-hand side of (4.6). In Figure 4.1, we plot one term in the sum (i.e. $\frac{400}{\pi}\sin(\pi x/L)$). In Figure 4.2, we plot two terms, i.e. $\frac{400}{\pi}[\sin(\pi x/L) + \frac{1}{3}\sin(3\pi x/L)]$. In Figure 4.3, we plot 3 terms, etc. By the time we have included enough terms, we see that the right-hand side of (4.6) approaches the constant value of 100 in the interior of the interval, $0 < x < L$. (Near the edges $x = 0$ and $x = L$, the oscillations get increasingly confined to the edges, where the sum of sines tries very hard to approach 100 in the interior of the domain, $0 < x < L$, while being identically zero at $x = 0$ and $x = L$. A discontinuity is created at the edges. There is also the so-called Gibbs phenomenon present near the edges, where just within the boundaries, there is an overshoot of the true value of 100, by 18%.]

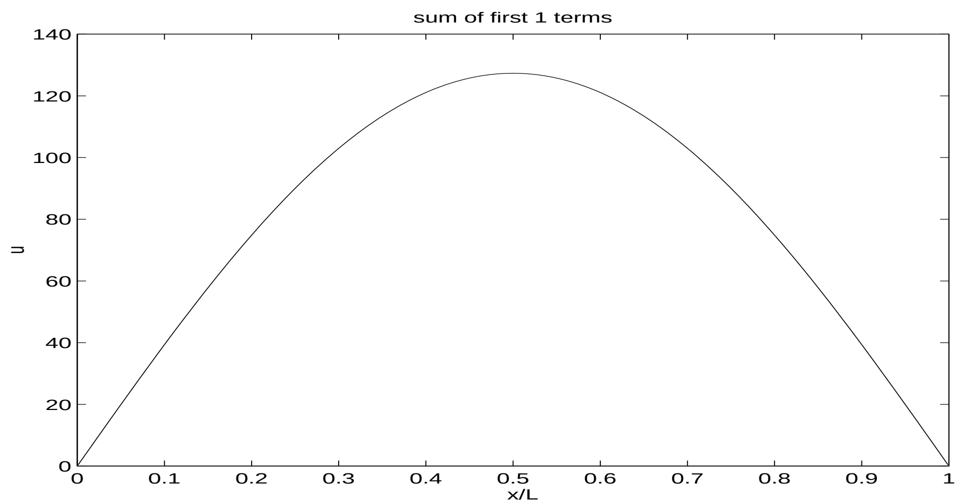


Figure 4.1: Plot of the first term in the Fourier sine expansion of 100.

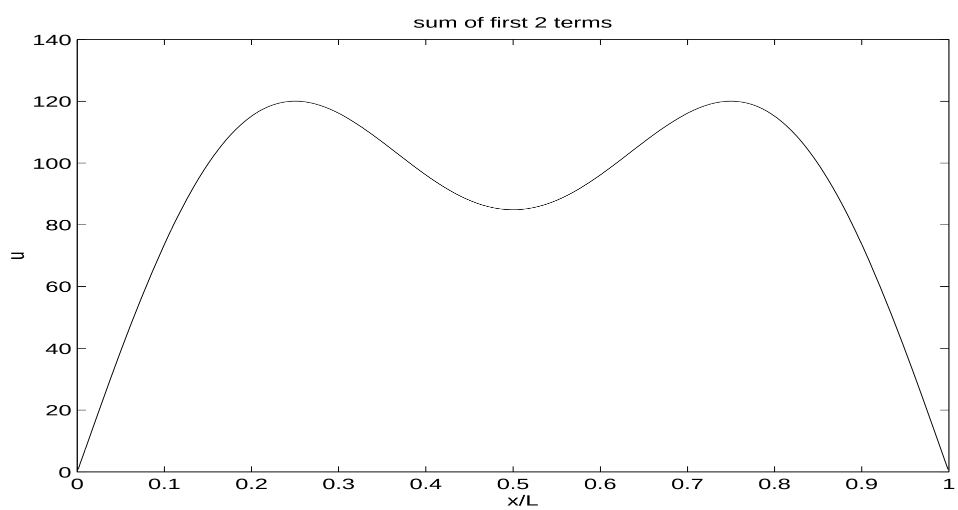


Figure 4.2: Plot of the sum of the first 2 terms in the Fourier sine expansion of 100.

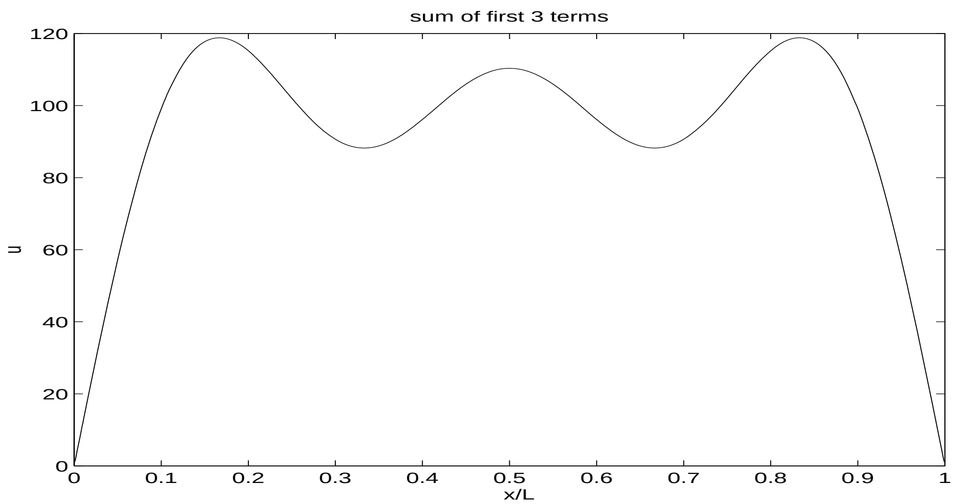


Figure 4.3: Plot of the sum of the first 3 terms in the Fourier sine expansion of 100.

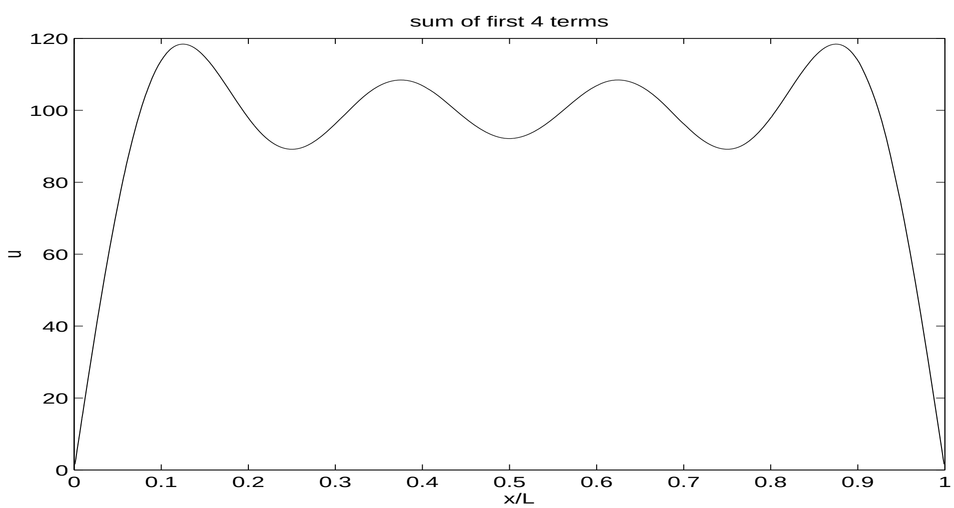


Figure 4.4: Plot of the sum of the first 100 terms in the Fourier sine expansion of 100.

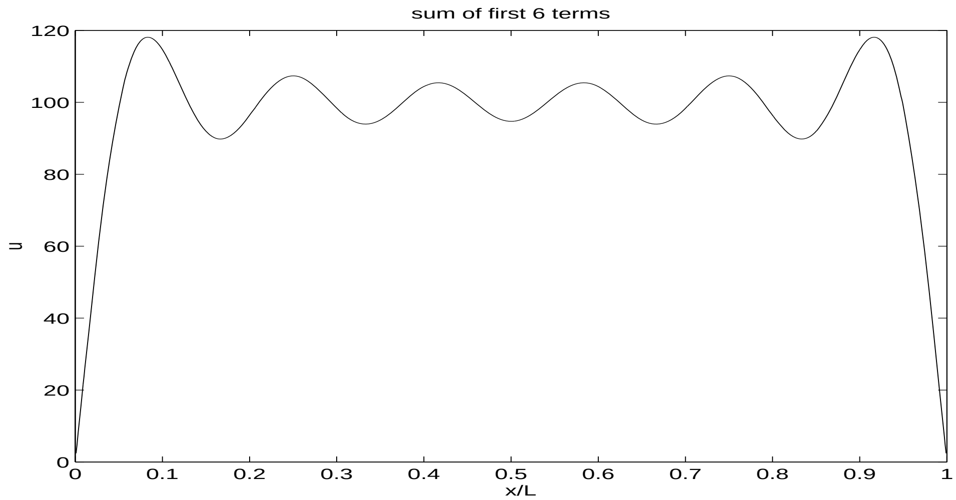


Figure 4.5: Plot of the sum of the first 6 terms in the Fourier sine expansion of 100.

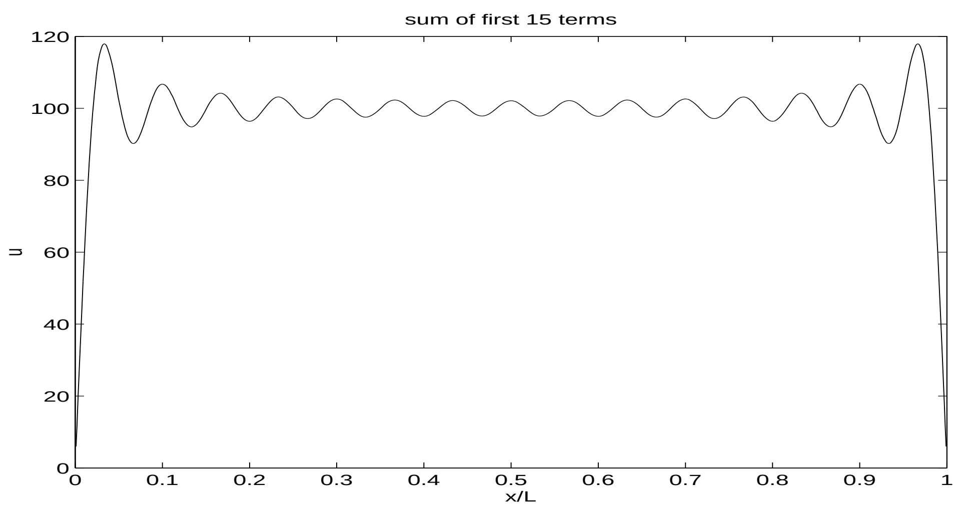


Figure 4.6: Plot of the sum of the first 15 terms in the Fourier sine expansion of 100.

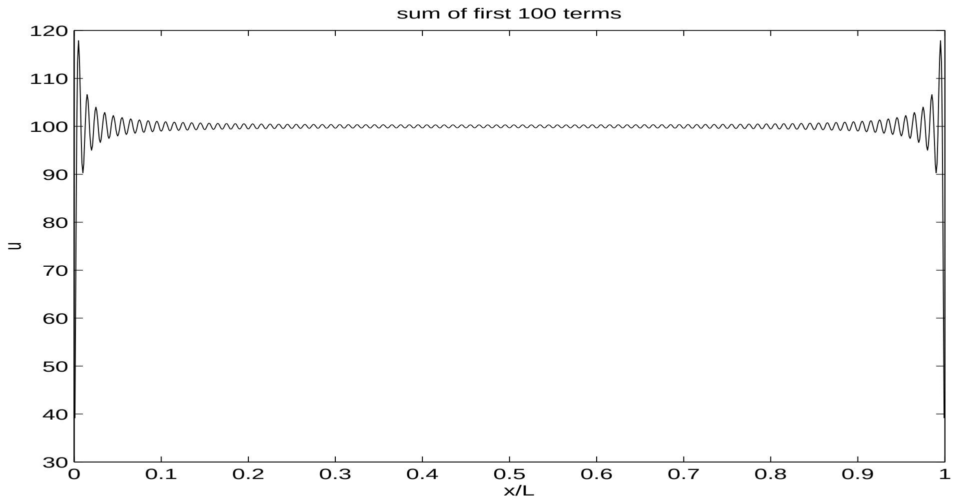


Figure 4.7: Plot of the sum of the first 100 terms in the Fourier sine expansion of 100.

4.4 Some comments:

What the example demonstrates is that the Fourier sine series can indeed represent $f(x)$ in the interval indicated. We can do this for other functions, and you will find that the Fourier sine series does a very good job in representing each of them. Actually, the most difficult function to represent by a Fourier sine series may be the one we have just done, $f(x) =$ constant in $0 < x < L$. This is because the sines all go to zero at $x = 0$ and $x = L$, but they have to add up to a nonzero constant slightly inside the boundaries. Many more terms in the sum are required to create this near discontinuity. For functions which are continuous and actually zero at the boundaries $x = 0$ and $x = L$, you will find that you do not need as many terms in the sum to give a good numerical representation of the original function.

It is not reasonable to expect that the sines can represent a function which blows up (i.e. attains infinite values) in the domain $0 < x < L$. Such unphysical functions are excluded in our consideration. The following mathematical result can be stated in a Theorem (a more general form is called Dirichlet's Theorem):

If $f(x)$ is a bounded function, which is continuous or piecewise continuous in a domain, the Fourier sine series representation of $f(x)$ converges to $f(x)$ for each point x in the domain where $f(x)$ is continuous. At those points where $f(x)$ jumps, the series converges to a value which is the average of the left- and right-hand limits of $f(x)$ at those points, where $f(x)$ is *discontinuous.*

[A piecewise continuous function is one which can take a finite number of finite jumps in the domain and be continuous elsewhere.]

4.5 A mathematical curiosity

If you are convinced that the function $f(x) = 100$ can be represented by a Fourier sine series in the interior of the domain:

$$100 = \frac{400}{\pi}\left(\sin\frac{\pi x}{L} + \frac{\sin\frac{3\pi x}{L}}{3} + \frac{\sin\frac{5\pi x}{L}}{5} + \ldots\right), \quad 0 < x < L,$$

then pick $x/L = \frac{1}{2}$ to get

$$100 = \frac{400}{\pi}(1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \frac{1}{9} - \ldots)$$

or

$$\pi = 4(1 - \frac{1}{3} + \frac{1}{5} - \frac{1}{7} + \frac{1}{9} - \ldots). \tag{4.7}$$

This relationship between π and the odd integers was discovered by Leibniz in 1673 by a different route.

You may try adding up the right-hand side of (4.7) and see how many terms are needed to approximate π to the accuracy you want.

4.6 Representing the cosine by sines

When Fourier presented his work on heat conduction and Fourier series to the Paris Academy in 1807, neither Laplace nor Lagrange would accept his use of Fourier series. In particular, Laplace could not accept the fact that $\cos x$ could be represented using a sum of sines. Let us see if Fourier was right.

Let us try to represent

$$f(x) = \cos x$$

in the interval $0 < x < \pi$ by a sine series

$$f(x) = \sum_{n=1}^{\infty} a_n \sin nx.$$

Fourier's formula for the coefficients gives

$$a_n = \frac{2}{\pi}\int_0^{\pi} \cos x \sin nx \; dx, \quad n = 1, 2, 3, \ldots.$$

Using the trigonometric identity

$$2\cos a \sin b = \sin(a+b) - \sin(a-b),$$

the integral can be evaluated to yield:

$$a_n = \begin{cases} \frac{4n}{\pi(n^2-1)}, & n = \text{even} \\ 0, & n = \text{odd}. \end{cases}$$

Thus, we find

$$\begin{aligned} \cos x &= \sum_{n\ even} \frac{4n}{\pi(n^2-1)} \sin nx, \quad 0 < x < \pi \\ &= \frac{8}{3\pi}\sin 2x + \frac{16}{15\pi}\sin 4x + \ldots, \ 0 < x < \pi. \end{aligned}$$

Try adding up as many terms as you can using a graphing calculator or computer. Does the sum approach $\cos x$ in the interval?

Comment: We can express a cosine in terms of a sine series only for half of its period. It is still true that a cosine cannot be expressed in terms of sines in its full period $-\pi < x < \pi$.

4.7 Application to the Heat Conduction Problem

PDE: $u_t = \alpha^2 u_{xx}, \quad 0 < x < L, \quad t > 0$

BCs: $u(0,t) = 0, \quad u(L,t) = 0, \quad t > 0$

IC: $u(x,0) = f(x), \quad 0 < x < L.$

In particular, we shall consider the case where $f(x) = 100$.

In Chapter 3, we found that the general solution to the PDE which satisfies the BCs is given by

$$u(x,t) = \sum_{n=1}^{\infty} T_n(0) e^{-\alpha^2 (\frac{n\pi}{L})t} \sin \frac{n\pi x}{L}, \quad 0 < x < L. \tag{4.8}$$

where the constants $T_n(0)$ are yet to be determined from the IC.

Setting $t = 0$ in (4.8) and setting $u(x,0) = f(x)$, we arrive at

$$f(x) = \sum_{n=1}^{\infty} T_n(0) \sin \frac{n\pi x}{L}, \quad 0 < x < L, \tag{4.9}$$

Therefore $T_n(0)$ is the Fourier sine coefficient of $f(x)$ and is given by (4.4) as

$$T_n(0) = a_n = \frac{2}{L}\int_0^L f(x)\sin\frac{n\pi x}{L}dx.$$

For $f(x) = 100$, we know that

$$a_n = \begin{cases} 0 & \text{if } n \text{ is even} \\ \frac{400}{n\pi} & \text{if } n \text{ is odd.} \end{cases}$$

Thus finally, the solution to the above PDE problem is

$$\begin{aligned} u(x,t) &= \sum_{n=1}^{\infty} a_n e^{-\alpha^2(\frac{n\pi}{L})^2 t}\sin\frac{n\pi x}{L} \\ &= \sum_{k=1}^{N}\frac{400}{\pi}\frac{1}{(2k-1)}e^{-(2k-1)^2(t/t_e)}\sin\frac{(2k-1)\pi x}{L}, \quad 0 < x < L, \end{aligned} \qquad (4.10)$$

where $t_e \equiv \left(\frac{L}{\alpha\pi}\right)^2$, and $N \to \infty$.

The solution in (4.10) is plotted in Figure 4.8 for different values of t/te. It turns out that unless t/te is very small, only a few terms are needed in the sum in (4.10). In Figure 4.9, we show that the solution can be represented to a high degree of accuracy by the first two terms:

$$u(x,t) \cong \frac{400}{\pi}e^{-t/te}\sin\frac{\pi n}{L} + \frac{400}{3\pi}e^{-9t/te}\sin\frac{3\pi x}{L}, \quad \text{for } t \gtrsim te.$$

Although we obtained this behavior already in Chapter 6, only now do we have the actual coefficients a_1 and a_3 etc calculated explicitly.

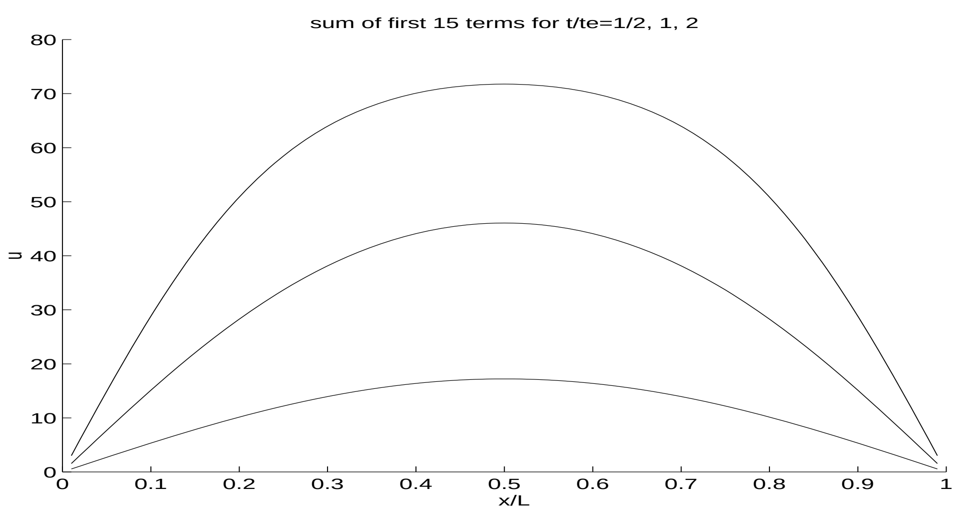


Figure 4.8: Plot of the sum of the first 15 terms in solution for $t/t_e = 1/2$, 1, 2.

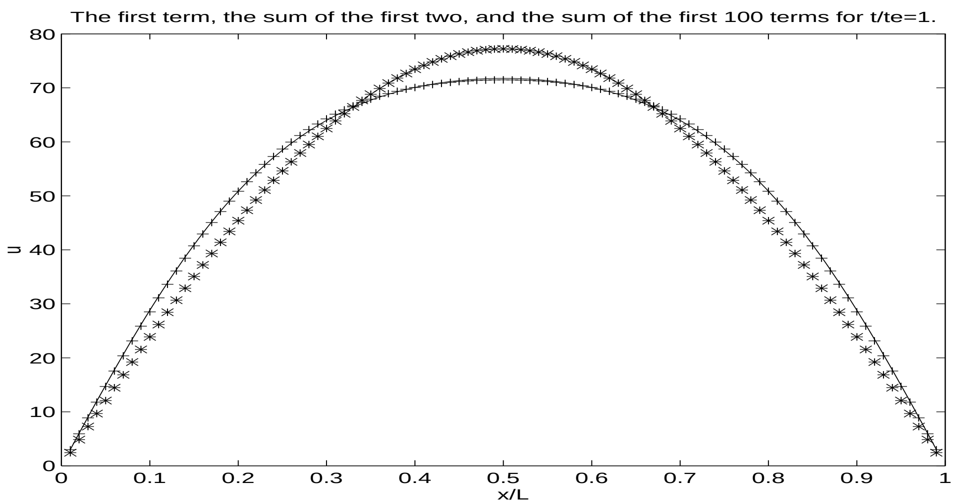


Figure 4.9: The first term, sum of the first two, and sum of the first 100 terms.

4.8 Exercises

1. Let $f(x)$ be given by

$$f(x) = \begin{cases} x, & 0 < x < L/2 \\ (L - x), & L/2 < x < L. \end{cases}$$

   Represent $f(x)$ by a Fourier sine series of the form

$$f(x) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L}, \quad 0 < x < L.$$

   (a) Find a_n, $n = 1, 2, 3, \ldots$.

   (b) Retain the first N terms as an approximation

$$f(x) \cong f_N(x) \equiv \sum_{n=1}^{N} a_n \sin \frac{n\pi x}{L}, \quad 0 < x < L.$$

   Using a graphing calculator or a computer, plot $f_N(x)$ as a function of x/L for $N = 1$, 3, 5, 31, and (optional) 101.

[You will notice that $a_n = 0$ for even n's, so the actual number of nonzero terms in the sum is halved.]

2. The solution to

$$\begin{array}{ll} \text{PDE:} & u_t = \alpha^2 u_{xx}, \quad 0 < x < L \\ \text{BCs:} & u(0,t) = 0, \quad u(L,t) = 0 \\ \text{IC:} & u(x,0) = f(x), \quad \text{where } f(x) \text{ is given in problem 1,} \end{array}$$

is given by

$$u(x,t) = \sum_{n=1}^{\infty} a_n e^{-n^2(t/t_e)} \sin \frac{n\pi x}{L}, \quad 0 < x < L,$$

where $t_e = (L/\pi\alpha)^2$.

Again replace

$$\sum_{n=1}^{\infty} \quad \text{by} \quad \sum_{n=1}^{N} \quad \text{as an approximation.}$$

Plot out the solution as a function of x/L for $t = \frac{1}{2}t_e$, t_e and $2t_e$. Use a large enough N so that your solution does not change noticeably when N is increased. You will find that you need only a few terms in the sum to get an accurate solution.

4.9 Solutions

Problem 1, figures 4.10-4.14

(a) We know that $f(x) = \sum_{n=1}^{\infty} a_n \sin(n\pi x/L)$. Thus $a_n = 2/L \int_0^L f(x) \sin(n\pi x/L) dx$ which upon integration yields;

$a_n = (4L/(n\pi)^2) \sin(n\pi/2)$.

$f(x) = \sum_{n=1}^{\infty} a_n \sin(n\pi x/L)$ where a_n is given above.

(b) see figures 4.10-4.14

Problem 2, figures 4.15-4.17

$u(x,t) = \sum_{n=1}^{\infty} a_n e^{-n^2(t/t_e)} \sin(n\pi x/L)$ where a_n is given above.

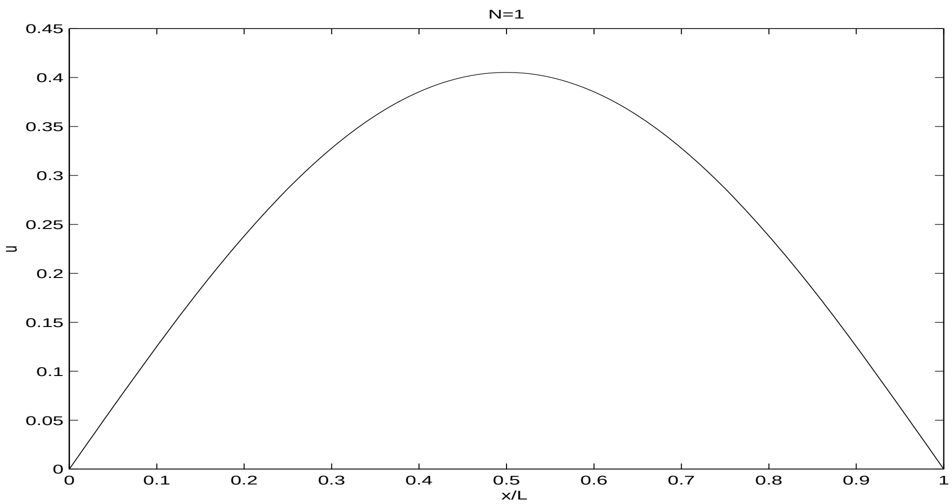


Figure 4.10: Sum of the first 1 terms in the Fourier sine expansion of x(L-x), L=1.

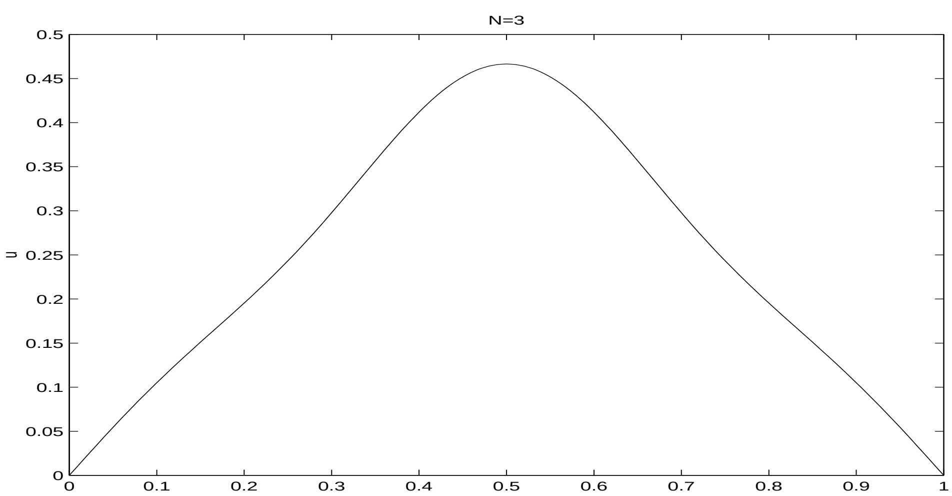


Figure 4.11: Sum of the terms up to N=3 in the Fourier sine expansion of x(L-x), L=1.

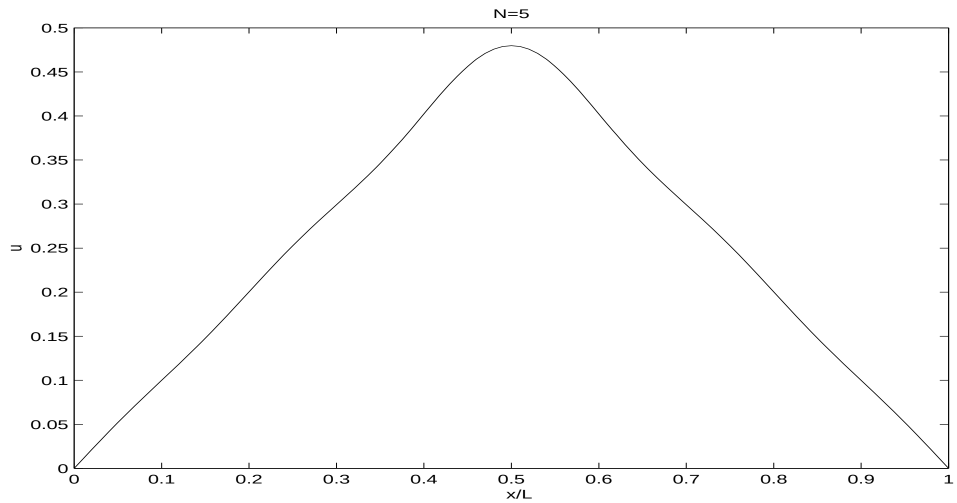


Figure 4.12: Sum of the terms up to N=5 in the Fourier sine expansion of x(L-x), L=1.

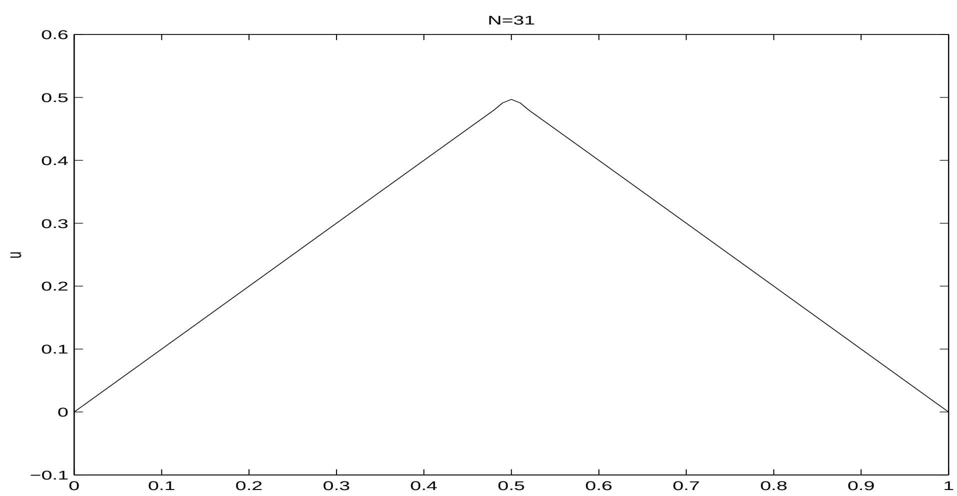


Figure 4.13: Sum of the terms up to N=31 in the Fourier sine expansion of x(L-x), L=1.

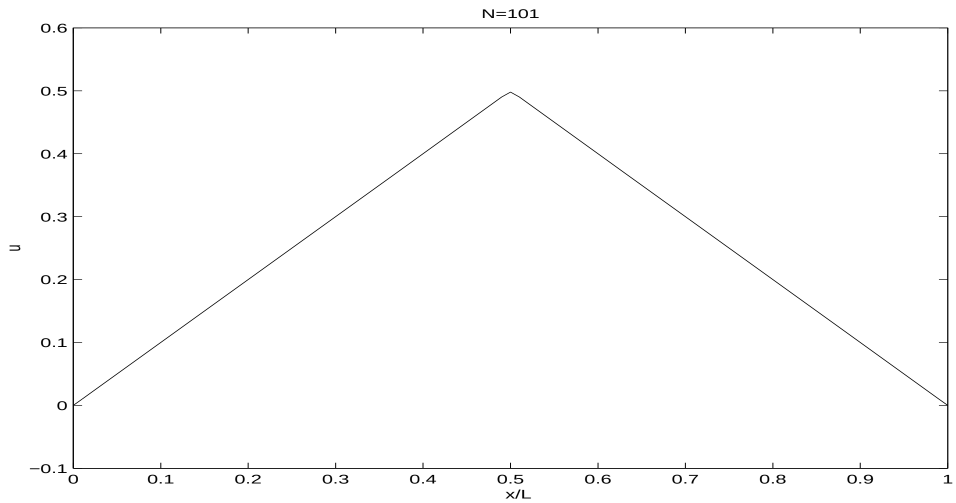


Figure 4.14: Sum of the terms up to N=101 in the Fourier sine expansion of x(L-x), L=1.

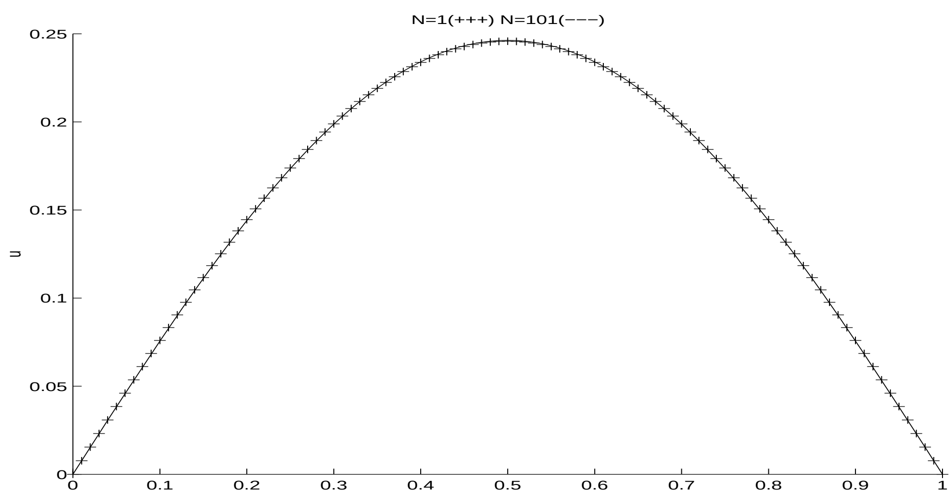


Figure 4.15: Sum of the terms for N=1 and N=101 in u(x,t) for t/te=1/2.

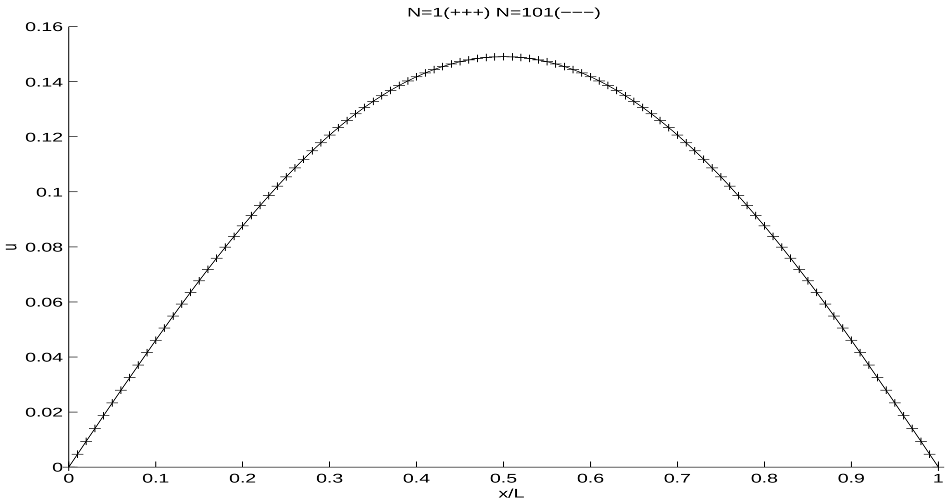


Figure 4.16: Sum of the terms for N=1 and N=101 in u(x,t) for t/te=1.

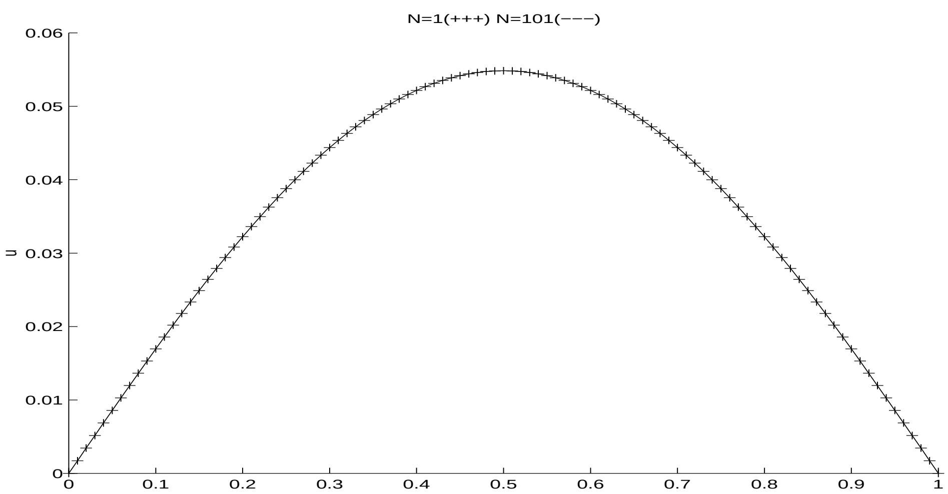


Figure 4.17: Sum of the terms for N=1 and N=101 in u(x,t) for t/te=2.

Chapter 5

Fourier Cosine Series

5.1 Introduction

In the previous chapter, function $f(x)$ were represented by a series of sines. It is also possible to express the same function alternatively in a series of cosines, in the form

$$f(x) = \sum_{n=0}^{\infty} b_n \cos \frac{n\pi x}{L}, \quad 0 < x < L. \tag{5.1}$$

Here the summation starts from $n = 0$, because $\cos 0 = 1$ is not zero. We will delay the motivation for wanting to write $f(x)$ in this form until later. Here we discuss only *how* to find the Fourier cosine series coefficients b_n assuming that $f(x)$ can be represented in the form of (5.1).

5.2 Finding the Fourier coefficients

We multiply both sides of (5.1) by $\cos \frac{m\pi x}{L}$, where m is any integer, $m = 0$, 1, 2, 3, ..., and integrate from 0 to L:

$$\int_0^L f(x) \cos \frac{m\pi x}{L} dx = \sum_{n=0}^{\infty} b_n \int_0^L \cos \frac{m\pi x}{L} \cos \frac{n\pi x}{L} dx. \tag{5.2}$$

There is *an orthogonality* condition for the cosines which can be written as

$$I_{mn} \equiv \int_0^L \cos \frac{m\pi x}{L} \cos \frac{n\pi x}{L} dx = \begin{cases} 0 & \text{if } m \neq n \\ \frac{L}{2} & \text{if } m = n \neq 0 \\ L & \text{if } m = n = 0. \end{cases} \tag{5.3}$$

To show this, we note the trigonometric identity

$$\cos a \cos b = \frac{1}{2}\cos(a-b) + \frac{1}{2}\cos(a+b),$$

so

$$\begin{aligned}
\int_0^L \cos\frac{m\pi x}{L}\cos\frac{n\pi x}{L}dx &= \frac{1}{2}\int_0^L \cos\frac{(m-n)\pi x}{L}dx + \frac{1}{2}\int_0^L \cos\frac{(m+n)\pi x}{L}dx \\
&= \left.\frac{\sin\frac{(m-n)\pi x}{L}}{2(m-n)\pi/L}\right|_0^L + \left.\frac{\sin\frac{(m+n)\pi x}{L}}{2(m+n)\pi/2}\right|_0^L \\
&= 0 \quad \text{if } m \neq n.
\end{aligned}$$

When $n = m \neq 0$

$$\cos\frac{m\pi x}{L}\cos\frac{n\pi x}{L} = \frac{1}{2}\left(1 + \cos\frac{2m\pi x}{L}\right).$$

The integral from 0 to L of the first term, $\frac{1}{2}$, is $L/2$, while the integral of the second term, $-\frac{1}{2}\cos\frac{2m\pi x}{L}$, is zero. When $m = n = 0$,

$$\cos\frac{m\pi x}{L}\cos\frac{n\pi x}{L} = 1,$$

so its integral from 0 to L is L. Thus we have derived the identity in (5.3).

Substituting (5.3) into (5.2) then yields

$$\int_0^L f(x)\cos\frac{m\pi x}{L}dx = b_m I_{mn} = \begin{cases} b_0 L & \text{if } m = 0 \\ b_m \frac{L}{2} & \text{if } m \neq 0. \end{cases}$$

Thus we have the Fourier cosine series representation for $f(x)$ in the form

$$\boxed{f(x) = \sum_{n=0}^{\infty} b_n \cos\frac{n\pi x}{L}, \quad 0 < x < L},$$

where,

$$\begin{aligned}
b_0 &= \frac{1}{L}\int_0^L f(x)dx \\
b_n &= \frac{2}{L}\int_0^L f(x)\cos\frac{n\pi x}{L}dx, \quad n = 1, 2, 3, 4, \ldots.
\end{aligned} \tag{5.4}$$

5.3 Application to PDE with Neumann Boundary Conditions

Consider heat conduction in a rod of length L whose initial temperature is given as

$$\boxed{\text{IC:} \quad u(x,0) = f(x), \quad 0 < x < L}. \tag{5.5}$$

Find the evolution of $u(x,t)$ for $t > 0$ if the ends of the rod are insulated, i.e.

$$\boxed{\text{BCs:} \quad u_x(0,t) = 0, \quad u_x(L,t) = 0, \quad t > 0}. \tag{5.6}$$

Assume heat conduction is governed by the heat equation:

$$\boxed{\text{PDE:} \quad u_t = \alpha^2 u_{xx}, \quad 0 < x < L}. \tag{5.7}$$

The usual method of separation of variables will lead us to the solution in the form:

$$u(x,t) = \sum_n T_n(t) X_n(x), \tag{5.8}$$

where the "eigenfunction", $X_n(x)$, satisfies

$$\frac{d^2}{dx^2} X_n(x) + \lambda_n^2 X_n(x) = 0. \tag{5.9}$$

The only difference between this case and the previous one in Chapter 3, section 2, is the boundary conditions. Here the Neumann condition. (5.6) implies

$$\frac{d}{dx} X_n(0) = 0, \quad \frac{d}{dx} X_n(L) = 0. \tag{5.10}$$

Nontrivial solutions to (5.9) and (5.10) are

$$X_n(x) = \cos \lambda_n x \tag{5.11}$$

provided

$$\lambda_n = \frac{n\pi}{L}, \quad n = 0, 1, 2, 3, \ldots.$$

The $T_n(t)$ satisfies, as in section 3.2:

$$\frac{d}{dt} T_n(t) + \alpha^2 \lambda_n^2 T_n(t) = 0. \tag{5.12}$$

So

$$T_n(t) = T_n(0) e^{-\alpha^2 \lambda_n^2 t}. \tag{5.13}$$

The general solution, satisfying the PDE and the BCs, is

$$\boxed{u(x,t) = \sum_{n=0}^{\infty} T_n(0) e^{-\alpha^2\lambda_n^2 t} \cos\frac{n\pi x}{L}.} \tag{5.14}$$

To satisfy the IC, we require, at $t = 0$,

$$u(x,0) = f(x) = \sum_{n=0}^{\infty} T_n(0) \cos\frac{n\pi x}{L}, \quad 0 < x < L. \tag{5.15}$$

(5.15) implies that the constants, $T_n(0)$'s, are the Fourier cosine coefficients for $f(x)$. Thus

$$\boxed{\begin{aligned} T_n(0) = b_n &= \frac{2}{L}\int_0^L f(x)\cos\frac{n\pi x}{L}dx, \quad n = 1, 2, 3, \ldots \\ T_0(0) = b_0 &= \frac{1}{L}\int_0^L f(x)dx. \end{aligned}}$$

The problem is now completely solved, assuming $f(x)$ is given.

An Example:

Solve

PDE: $u_t = u_{xx}$, $0 < x < 1$, $t > 0$

BCs: $u_x(0,t) = 0$, $u_x(1,t) = 0$, $t > 0$

IC: $u(x,0) = x$, $0 < x < 1$.

Since the boundary conditions are homogeneous Neumann, try a cosine series expansion of the solution

$$u(x,t) = \sum_{n=0}^{\infty} T_n(t) X_n(x), \tag{5.16}$$

where $X_n(x) = \cos n\pi x$. Substituting the assumed form (7.16) into the PDE yields:

$$\frac{d}{dt}T_n(t) = -(n\pi)^2 T_n(t), \quad n = 0, 1, 2, 3, \ldots. \tag{5.17}$$

The solution of (5.17) is

$$T_n(t) = T_n(0)e^{-(n\pi)^2 t}.$$

Therefore,

$$u(x,t) = \sum_{n=0}^{\infty} T_n(0) e^{-(n\pi)^2 t} \cos n\pi x, \quad 0 < x < 1.$$

To satisfy the IC, we require

$$x = \sum_{n=0}^{\infty} T_n(0) \cos n\pi x, \quad 0 < x < 1.$$

So the $T_n(0)$'s are the Fourier cosine coefficients of the function x, and thus

$$T_n(0) = \int_0^1 x dx = \frac{1}{2}$$
$$T_n(0) = 2\int_0^1 x \cos n\pi x dx = \begin{cases} 0 & \text{if } n = \text{even} \\ -\frac{4}{(n\pi)^2} & \text{if } n = \text{odd.} \end{cases}$$

Finally,

$$u(x,t) = \frac{1}{2} - \frac{4}{\pi^2} \sum_{\substack{n=1 \\ n \text{ odd}}}^{\infty} \frac{1}{n^2} e^{-(n\pi)^2 t} \cos n\pi x.$$

Chapter 6

Fourier Series

6.1 Introdution

We discussed the Fourier sine series in Chapter 4 and the Fourier cosine series in Chapter 5. Now, we shall combine the two to form a *periodic* Fourier series (or simply called the Fourier series). Before we do so however, we first try to motivate the need for such a series by looking for the eigenfunctions satisfying periodic boundary conditions.

6.2 Periodic Eigenfunctions

Consider heat conduction in a circular ring. Let us denote the circumference of the ring by $2L$. Denote any point on the ring by $x = 0$. Then the points $x = -L$ and $x = L$ are actually the same point. The problem is to be solved in the domain $-L < x < L$, subject to the boundary condition that the solution should be the same at $x = -L$ and $x = L$.

$$\begin{aligned}
&\text{PDE:} \quad u_t = \alpha^2 u_{xx}, \quad -L < x < L, \quad t > 0 && (6.1)\\
&\text{BCs:} \quad u(-L,t) = u(L,t) && (6.2)\\
&\qquad\quad\; u_x(-L,t) = u_x(L,t) && (6.3)\\
&\text{IC:} \quad\;\; u(x,0) = f(x), \quad -L < x < L. && (6.4)
\end{aligned}$$

As we will show, that these boundary conditions are sufficient to define a periodic function. That is, we can look for a solution for all x, $-\infty < x < \infty$, with the condition that it repeats itself with period $2L$, i.e.

$$\boxed{u(x,t) = u(x + 2L, t)}\,. \qquad (6.5)$$

We will get the same result as (6.2) and (6.3).

We shall again use the method of separation of variables, and we first try

$$u(x,t) = T(t)X(x).$$

Substituting into the PDE yields

$$\frac{T'(t)}{\alpha^2 T(t)} = \frac{X''(x)}{X(x)} = -\lambda^2,$$

where $-\lambda^2$ is the separation constant. The eigenfunction $X(x) = X_n(x)$ is determined from

$$X''(x) + \lambda^2 X(x) = 0 \tag{6.6}$$

$$X(-L) = X(L), \quad X'(-L) = X'(L). \tag{6.7}$$

The boundary conditions for X comes from (6.2) and (6.3). The solution to (6.6) is

$$X(x) = a \sin \lambda x + b \cos \lambda x, \tag{6.8}$$

so the first boundary condition in (6.7) implies

$$-a \sin \lambda L + b \cos \lambda L = a \sin \lambda L + b \cos \lambda L,$$

i.e.

$$2a \sin \lambda L = 0. \tag{6.9}$$

The second boundary condition

$$\lambda a \cos \lambda L + \lambda b \sin \lambda L = \lambda a \cos \lambda L - \lambda b \sin \lambda L,$$

is

$$2b\lambda \sin \lambda L = 0. \tag{6.10}$$

Both (6.9) and (6.10) can be satisfied if $\sin \lambda L = 0$, or by taking

$$\lambda = n\pi/L \equiv \lambda_n, \quad n = 0, 1, 2, 3, \ldots. \tag{6.11}$$

So the eigenfunction corresponding to λ_n is

$$X(x) = a_n \sin \lambda_n x + b_n \cos \lambda_n x \equiv X_n(x), \quad n = 1, 2, 3, \ldots. \tag{6.12}$$

Superposition over all n then yields the general solution of the PDE in the form

$$u(x,t) = \sum_n T_n(t) X_n(x).$$

Thus:

$$\boxed{u(x,t) = \sum_{n=0}^{\infty}[a_n \sin\frac{n\pi x}{L} + b_n \cos\frac{n\pi x}{L}]e^{-(n\pi\alpha/L)^2 t}}\,. \tag{6.13}$$

To satisfy the IC, we need

$$\boxed{f(x) = \sum_{n=0}^{\infty}[a_n \sin\frac{n\pi x}{L} + b_n \cos\frac{n\pi x}{L}], \quad -L < x < L}\,. \tag{6.14}$$

The right-hand side of (6.14) is the Fourier series expansion of $f(x)$ in the domain $-L < x < L$. It is periodic with period $2L$ in $-\infty < x < \infty$.

6.3 Fourier Series

We now return to the mathematical problem of representing an arbitrary, piecewise continuous, function $f(x)$ in a Fourier series of period $2L$,

$$f(x) = \sum_{n=0}^{\infty}[a_n \sin\frac{n\pi x}{L} + b_n \cos\frac{n\pi x}{L}], \quad -L < x < L. \tag{6.15}$$

If $f(x)$ is itself periodic with period $2L$, then the representation is good for all x, $-\infty < x < \infty$. If $f(x)$ is not periodic outside the interval $-L < x < L$, or if $f(x)$ is not defined beyond this interval, the representation is good only in the restricted interval.

There are two ways to find the coefficients a_n and b_n of the Fourier series. The standard way is to use the orthogonality conditions between sines and cosines. They are, for integers m and n:

$$\int_{-L}^{L} \sin\frac{m\pi x}{L}\sin\frac{n\pi x}{L}dx = \begin{cases} 0 & \text{if } m \neq n \\ L & \text{if } m = n \end{cases} \tag{6.16}$$

$$\int_{-L}^{L} \cos\frac{m\pi x}{L}\cos\frac{n\pi x}{L}dx = \begin{cases} 0 & \text{if } m \neq n \\ L & \text{if } m = n \neq 0 \\ 2L & \text{if } m = n = 0 \end{cases} \tag{6.17}$$

$$\int_{-L}^{L} \sin\frac{m\pi x}{L}\cos\frac{n\pi x}{L}dx = 0 \text{ for all } m \text{ and } n \tag{6.18}$$

Of the three orthogonality relations (6.16), (6.17) and (6.18), only the last one is really new. We derived the first two previously when the integration was over half the domain, from 0 to L. Since sines are odd functions of x and cosines are even function of x, the integrands in (6.16) and (6.17) are even in x. Thus,

$$\int_{-L}^{L} \sin\frac{m\pi x}{L}\sin\frac{n\pi x}{L}dx = 2\int_{0}^{L} \sin\frac{m\pi x}{L}\sin\frac{n\pi x}{L}dx$$
$$\int_{-L}^{L} \cos\frac{m\pi x}{L}\cos\frac{n\pi x}{L}dx = 2\int_{0}^{L} \cos\frac{m\pi x}{L}\cos\frac{n\pi x}{L}dx.$$

(6.16) then follows from our previous results, namely (6.7), and (6.17) follows from (5.3). The last identity, (6.18) follows from the fact that the integrand in (6.18) is odd in x and so the integral over positive and negative values of x yields zero.

Using these orthogonality relations, we can now obtain the coefficients a_n and b_n in the following way. Multiply both sides of (6.15) by $\sin\frac{m\pi x}{L}$ and integrate with respect to x from $-L$ to L to get

$$\begin{aligned}\int_{-L}^{L} f(x)\sin\frac{m\pi x}{L}dx &= \sum_{n=0}^{\infty}[a_n\int_{-L}^{L}\sin\frac{m\pi x}{L}\sin\frac{n\pi x}{L}dx \\ &\quad + b_n\int_{-L}^{L}\sin\frac{m\pi x}{L}\cos\frac{n\pi x}{L}dx] \\ &= a_m L.\end{aligned}$$

so

$$a_m = \frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{m\pi x}{L}dx, \quad m = 0,1,2,3,\ldots.$$

Multiplying (6.15) by $\cos\frac{m\pi x}{L}$ and integrating with respect to x from $-L$ to L yields, similarly,

$$b_m = \frac{1}{L}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}dx, \quad m \neq 0$$
$$b_0 = \frac{1}{2L}\int_{-L}^{L} f(x)dx.$$

Summary: The Fourier series representation of a piecewise continuous function $f(x)$ in the interval $-L < x < L$ is given by

$$\boxed{f(x) = \sum_{n=0}^{\infty}[a_n\sin\frac{n\pi x}{L} + b_n\cos\frac{n\pi x}{L}], \quad -L < x < L}, \tag{6.19}$$

where

$$\boxed{\begin{aligned} a_n &= \frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}dx \\ b_0 &= \frac{1}{2L}\int_{-L}^{L} f(x)dx \\ b_n &= \frac{1}{L}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}dx, \quad n = 1, 2, 3, \ldots. \end{aligned}}$$

Notes: (i) If $f(x)$ is an odd function of x, i.e.

$$f(-x) = -f(x), \quad -L < x < L,$$

then all the cosine coefficients b_n are zero, and the Fourier series (6.19) becomes a sine series:

$$f(x) = \sum_{n=1}^{\infty} a_n \sin\frac{n\pi x}{L}, \quad -L < x < L,$$

where

$$a_n = \frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}dx = \frac{2}{L}\int_{0}^{L} f(x)\sin\frac{n\pi x}{L}dx$$

(ii) If $f(x)$ is an even function of x, i.e.

$$f(-x) = f(x),$$

then all the sine coefficients a_n are zero. The Fourier series (6.19) becomes a cosine series:

$$f(x) = \sum_{n=0}^{\infty} b_n \cos\frac{n\pi x}{L}, \quad -L < x < L,$$

where

$$b_n = \frac{1}{L}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}dx = \frac{2}{L}\int_{0}^{L} f(x)\cos\frac{n\pi x}{L}dx$$
$$b_0 = \frac{1}{2L}\int_{-L}^{L} f(x)dx = \frac{1}{L}\int_{0}^{L} f(x)dx.$$

(iii) The above discussion suggests a second way for obtaining the coefficients of the Fourier series (6.19). Since any function $f(x)$ can be written as

$$f(x) = f_{sym}(x) + f_{anti}(x), \tag{6.20}$$

where $f_{sym}(x) \equiv \frac{1}{2}(f(x) + f(-x))$ is symmetric about $x = 0$, and

$$f_{anti}(x) \equiv \frac{1}{2}(f(x) - f(-x))$$

is antisymmetric about $x = 0$.

Now, the symmetric function can be represented by a cosine series in $-L < x < L$:

$$f_{sym}(x) = \sum_{n=0}^{\infty} b_n \cos \frac{n\pi x}{L}, \tag{6.21}$$

where, from (5.4),

$$b_n = \frac{2}{L}\int_0^L f_{sym}(x) \cos \frac{n\pi x}{L} dx = \frac{1}{L}\int_{-L}^L f_{sym}(x) \cos \frac{n\pi x}{L} dx = \frac{1}{L}\int_{-L}^L f(x) \cos \frac{n\pi x}{L} dx$$

and

$$b_0 = \frac{1}{L}\int_0^L f_{sym}(x) dx = \frac{1}{2L}\int_{-L}^L f_{sym}(x) dx = \frac{1}{2L}\int_{-L}^L f(x) dx.$$

Similarly, the antisymmetric function can be represented by a sine series in $-L < x < L$:

$$f_{anti}(x) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L}, \tag{6.22}$$

where from (4.5),

$$\begin{aligned} a_n &= \frac{2}{L}\int_0^L f_{anti}(x) \sin \frac{n\pi x}{L} dx = \frac{1}{L}\int_{-L}^L f_{anti}(x) \sin \frac{n\pi x}{L} dx \\ &= \frac{1}{L}\int_{-L}^L f(x) \sin \frac{n\pi x}{L} dx. \end{aligned}$$

Combining (6.21) and (6.22) into (6.20) then yields (6.19).

6.4 Examples

6.4.1

(a) Represent $f(x) = 1$, as a Fourier sine series in $0 < x < L$. We let

$$\begin{aligned} f_s(x) &\equiv \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L}, \\ a_n &= \frac{2}{L}\int_0^L f(x) \sin \frac{n\pi x}{L} dx = \frac{2}{n\pi}[1 - \cos n\pi]. \end{aligned}$$

The Fourier sine series representation, obtained by combining sines with coefficients determined above is an antisymmetric function and so looks like:

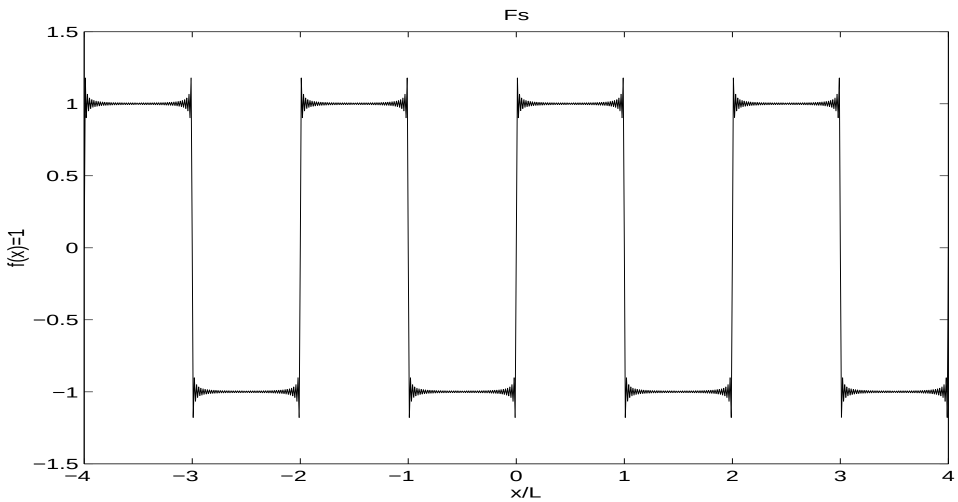


Figure 6.1 Fourier series representation of $f(x) = 1$, as a function of x/L; 50 terms used in the sum.

Thus, $f_s(x)$ looks like $f(x)$ only in the interval $0 < x < L$. It is antisymmetric about $x = 0$ and periodic with period $2L$.

(b) Represent $f(x) = 1$ as a Fourier cosine series in $0 < x < L$. We let

$$\begin{aligned} f_c(x) &\equiv \sum_{n=0}^{\infty} b_n \cos\frac{n\pi x}{L}, \\ b_n &= \frac{2}{L}\int_0^L f(x)\cos\frac{n\pi x}{L}dx = 0, \quad n \neq 0 \\ b_0 &= \frac{1}{L}\int_0^L 1dx = 1. \end{aligned}$$

$f_c(x) = b_0$ is actually a one-term cosine series. With $b_0 = 1$ it is a perfect representation of $f(x)$ in $0 < x < L$.

(c) Represent $f(x) = 1$ as a Fourier series in $-L < x < L$. We let

$$f_{sc}(x) \equiv \sum_{n=0}^{\infty}[a_n \sin\frac{n\pi x}{L} + b_n \cos\frac{n\pi x}{L}],$$
$$a_n = \frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}dx = 0$$
$$b_n = \frac{1}{L}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}dx = 0$$
$$b_0 = \frac{1}{2L}\int_{-L}^{L} f(x)dx = 1.$$

In this case $f_{sc}(x) = f_c(x) = f(x)$ in $-L < x < L$.

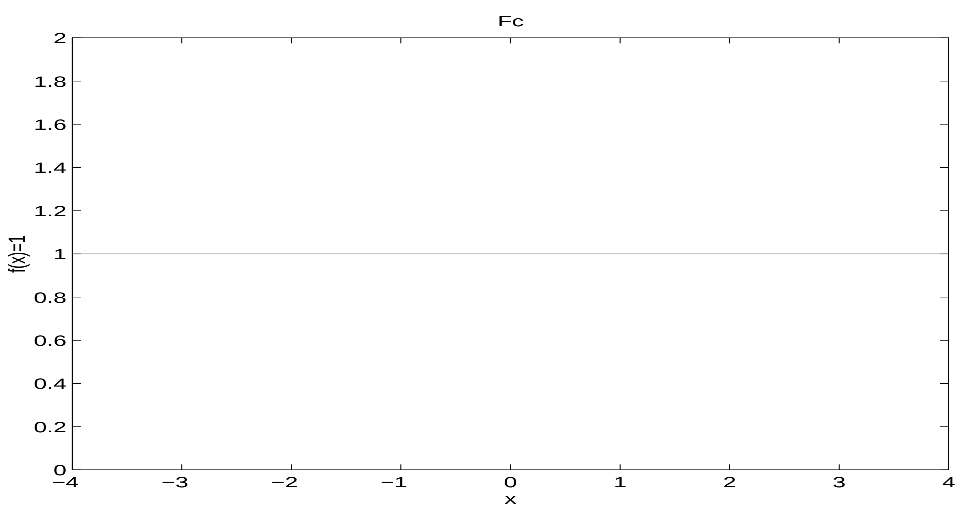


Figure 6.2 Fourier series representation of $f(x) = 1$.

6.4.2

(a) Represent $f(x) = 1 + x$ as a Fourier sine series in $0 < x < 1$.

The sine series representation, $f_s(x)$, is plotted in Figure 6.3, for all x.

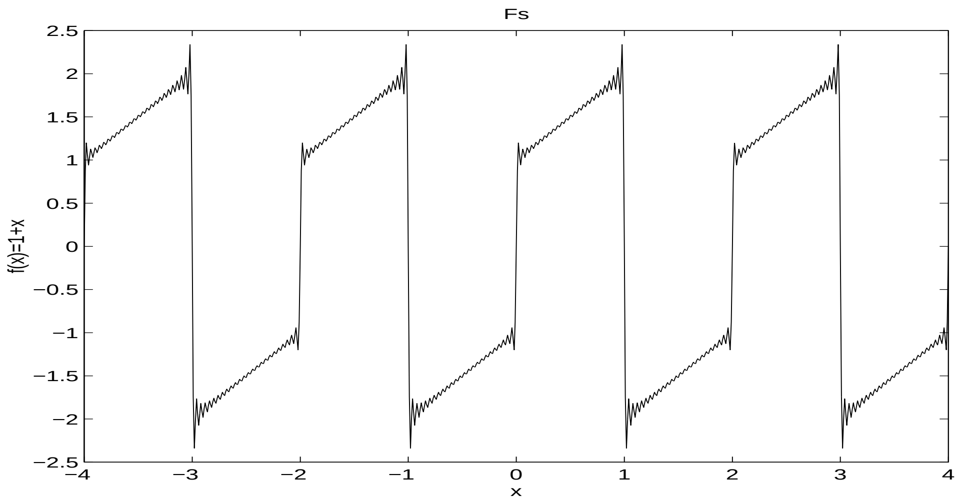


Figure 6.3 Fourier sine series representation of $f(x) = 1 + x$; 50 terms used in the sum.

(b) Represent $f(x) = 1 + x$ as a Fourier cosine series in $0 < x < 1$. The cosine series representation, $f_c(x)$, is plotted in Figure 6.4 for all x.

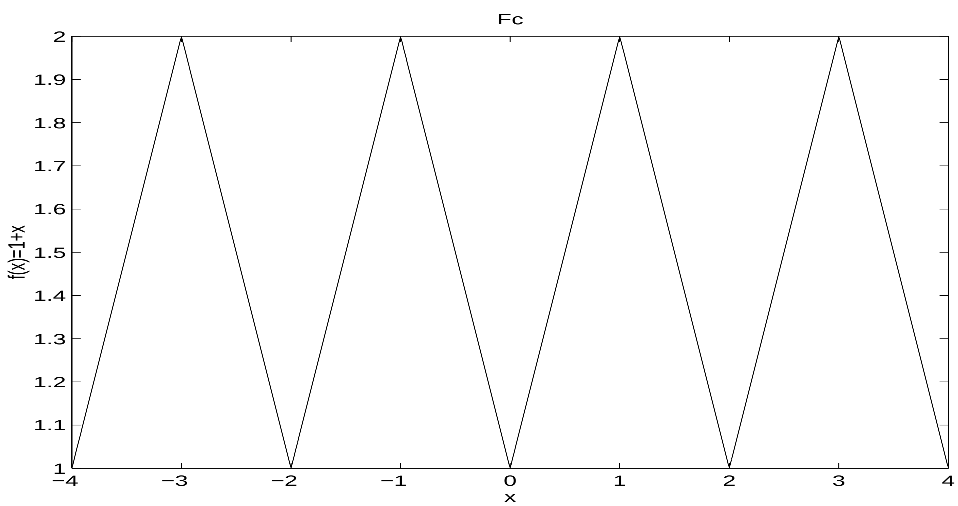


Figure 6.4 The Fourier cosine series representation of $f(x) = 1 + x$; using 50 terms in the sum.

(c) Represent $f(x) = 1 + x$ as a Fourier series in $-1 < x < 1$. $f_{sc}(x)$ is plotted in Figure 6.5 for all x. Notice that $f_{sc}(x)$ is different rom $f_c(x)$ or $f_s(x)$ beyond the interval $0 < x < 1$.

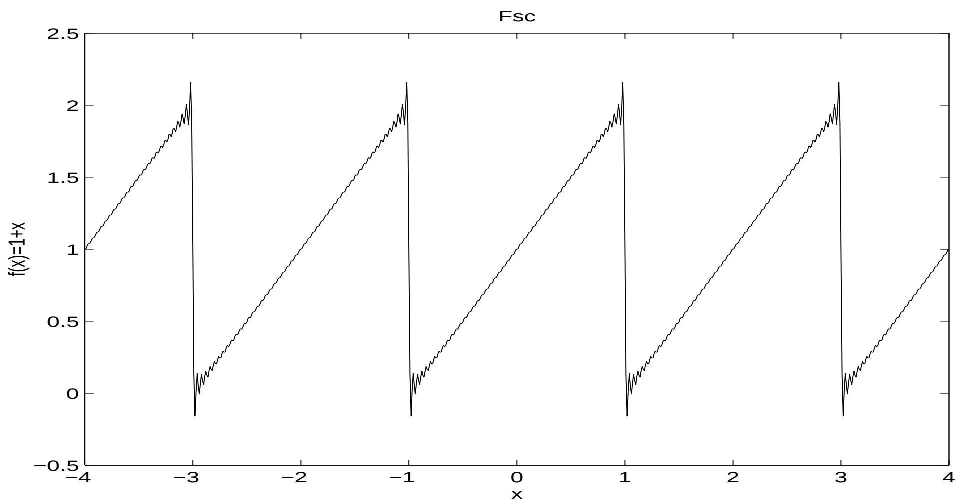


Figure 6.5 Fourier series representation of $f(x) = 1 + x$; 50 terms used in the sum.

6.4.3

(a) Represent $f(x) = e^x$ as a Fourier sine series in $0 < x < 1$. $f_s(x)$ is plotted for all x in Figure 6.6

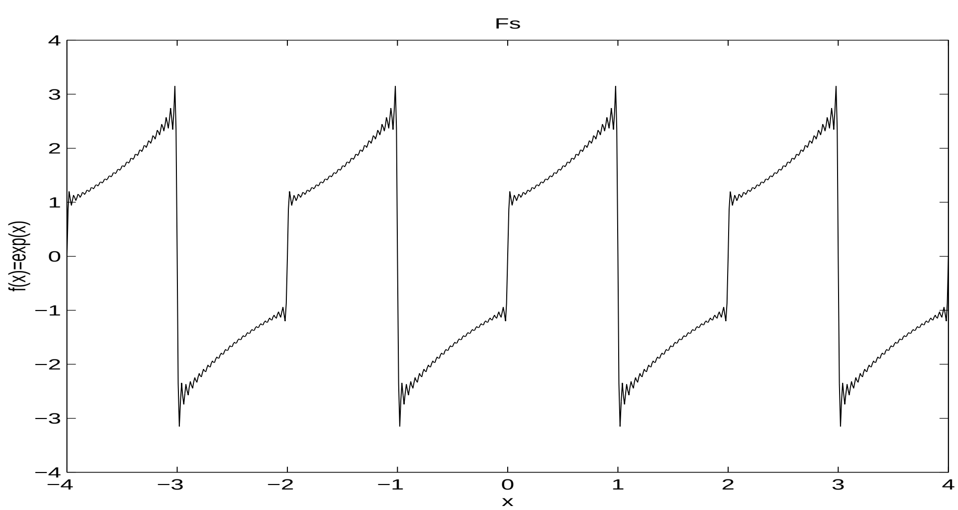


Figure 6.6 Fourier sine series representation of $f(x) = e^x$; 50 terms used in the sum.

(b) Represent $f(x) = e^x$ as a Fourier cosine series in $0 < x < 1$. $f_c(x)$ is plotted for all x in Figure 6.7

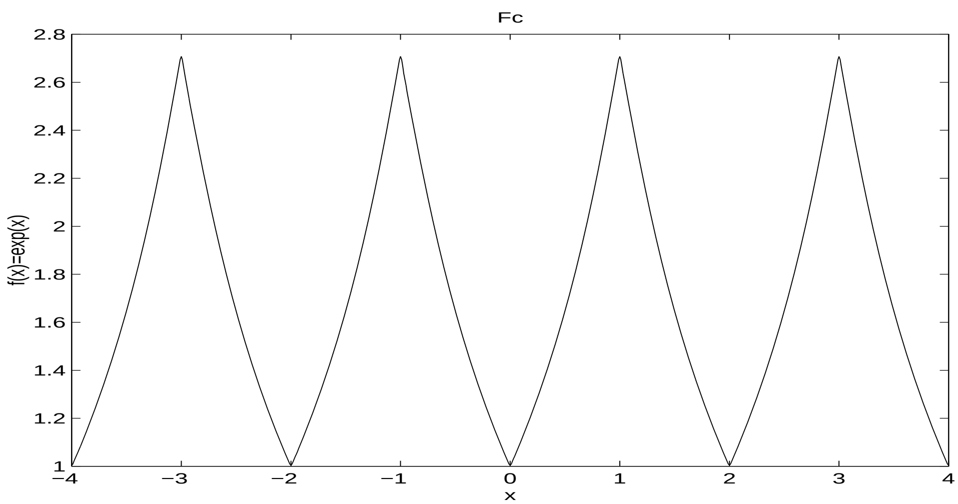


Figure 6.7 Fourier cosine series representation of $f(x) = e^x$; 50 terms used in the sum.

(c) Represent $f(x) = e^x$ as a Fourier series in $-1 < x < 1$. $f_{sc}(x)$ is plotted for all x in Figure 6.8.

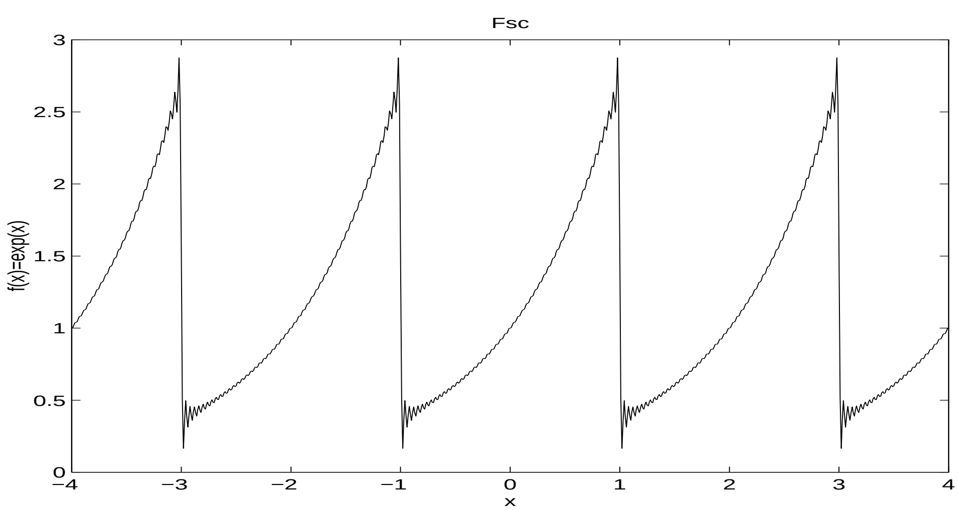


Figure 6.8 Fourier series representation of $f(x) = e^x$; 50 terms used in the sum.

6.5 Complex Fourier series

In this section we will discuss other forms of Fourier series (6.19).

In (6.19), the Fourier coefficients are

$$\begin{aligned} a_n &= \frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}dx \\ b_n &= \frac{1}{L}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}dx, \quad n = 1, 2, 3, \ldots \\ b_0 &= \frac{1}{2L}\int_{-L}^{L} f(x)dx. \end{aligned}$$

If we change n to $-n$ in the above definition for a_n and b_n, we will find

$$a_{-n} = -a_n, \quad b_{-n} = b_n.$$

Therefore we can rewrite the sum in (6.19) as

$$f(x) = \frac{1}{2}\sum_{n=-\infty}^{\infty}[a_n \sin\frac{n\pi x}{L} + b_n \cos\frac{n\pi x}{L}], \quad -L < x < L, \tag{6.23}$$

where now, for $n = 0, \pm 1, \pm 2, \pm 3, \ldots$

$$\begin{aligned} a_n &= \frac{1}{L}\int_{-L}^{L} f(x)\sin\frac{n\pi x}{L}dx, \\ b_n &= \frac{1}{L}\int_{-L}^{L} f(x)\cos\frac{n\pi x}{L}dx, \end{aligned}$$

[Note that b_0 defined this way is twice as big as the definition obtained in (6.19). This is an advantage, since b_0 now has the same form as the rest of the b_n's.]

The form (6.23) is equivalent to (6.19) but is sometimes preferred because the coefficients are easier to remember.

(6.23) can be further written more compactly using the complex notation:

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{-in\pi x/L}, \quad -L < x < L, \tag{6.24}$$

where

$$c_n = \frac{1}{2L}\int_{-L}^{L} f(x)e^{in\pi x/L}dx.$$

To show this, we use Euler's identity

$$e^{i\theta} = \cos\theta + i\sin\theta.$$

Changing θ to $-\theta$ gives

$$e^{-i\theta} = \cos\theta - i\sin\theta.$$

Adding yields

$$\cos\theta = \frac{1}{2}(e^{i\theta} + e^{-i\theta}).$$

Subtracting yields

$$\sin\theta = \frac{1}{2i}(e^{i\theta} - e^{-i\theta}).$$

We now also rewrite $\sin\frac{n\pi x}{L}$ and $\cos\frac{n\pi x}{L}$ in terms of $e^{\pm in\pi x/L}$. (6.23) becomes

$$\begin{aligned} f(x) &= \frac{1}{2}\sum_{n=-\infty}^{\infty}[b_n\frac{1}{2}(e^{in\pi x/L} + e^{-in\pi x/L}) \\ &\quad + a_n\frac{1}{2i}(e^{in\pi x/L} - e^{-in\pi x/L})] \\ &= \frac{1}{2}\sum_{n=-\infty}^{\infty}\frac{1}{2}(b_n - ia_n)e^{in\pi x/L} + \frac{1}{2}\sum_{n=-\infty}^{\infty}\frac{1}{2}(b_n + ia_n)e^{-in\pi x/L}. \end{aligned}$$

In the first sum we change n to $-n$, which is permitted since n is a dummy variable. We then see that the first sum is exactly the same as the second sum. Thus,

$$\boxed{f(x) = \sum_{n=-\infty}^{\infty} c_n e^{-in\pi x/L}, \quad -L < x < L}, \tag{6.25}$$

where

$$c_n = \frac{1}{2}(b_n + ia_n) = \frac{1}{2}\left\{\frac{1}{L}\int_{-L}^{L} f(x)(\cos\frac{n\pi x}{L} + i\sin\frac{n\pi x}{L})dx\right\}.$$

Thus,

$$\boxed{c_n = \frac{1}{2L}\int_{-L}^{L} f(x)e^{in\pi x/L}dx, \quad n = 0,\ \pm1,\ \pm2, \dots}. \tag{6.26}$$

The complex form (6.25) appears to be the most convenient to use. (6.26) can also be obtained directly from (6.25), by multiplying it by $e^{im\pi x/L}$, integrating from $-L$ to L, and utilizing the orthogonality relation:

$$\frac{1}{2L}\int_{-L}^{L} e^{im\pi x/L}e^{-in\pi x/L}dx = \delta_{mn}.$$

This relation can be obtained by direct integration (the integrand is just $e^{i(m-n)\pi x/L}$.

6.6 Example, Laplace's equation in a circular disk

Consider again the solution of Laplace's equation in a region bounded by a circle of radius a:

$$\begin{aligned} \text{PDE:} \quad & \nabla^2 u = 0, \quad 0 \le r < a \\ \text{BC:} \quad & u(r,\theta) = f(\theta) \text{ for } r = a \end{aligned}$$

and is periodic in θ with period 2π. In polar coordinates, the Laplace operator is

$$\nabla^2 = \frac{\partial^2}{\partial r^2} + \frac{1}{r}\frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2},$$

where θ is the angle and r is the radius.

Since $f(\theta)$ is periodic with period 2π, we can expand it in a periodic Fourier series:

$$f(\theta) = \sum_{n=-\infty}^{\infty} c_n e^{-in\theta},$$

with c_n given by (from 6.26)

$$c_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\theta) e^{in\theta} d\theta.$$

Since the solution $u(r,\theta)$ should also be periodic with period 2π, it too can be expanded in a periodic Fourier series:

$$u(r,\theta) = \sum_{n=-\infty}^{\infty} R_n(r) e^{-in\theta}.$$

Substituting this assumed form for u into the PDE yields:

$$R_n''(r) + \frac{1}{r}R_n'(r) - \frac{n^2}{r^2}R_n(r) = 0.$$

This ODE belongs to the "equi-dimensional type" and the solution is of the form r^b. Substituting this assumed form into the ODE we find that $b = \pm n$. Thus the solution is

$$R_n(r) = \alpha_n r^n + \beta_n r^{-n}$$

In order that $R_n(r)$ be finite at $r = 0$, we set $\beta_n = 0$ for $n > 0$ and set $\alpha_n = 0$ for $n < 0$. Also to satisfy the BC at $r = a$, we want $R_n(a) = c_n$. Thus

$$R_n(r) = c_n(r/a)^{|n|}, \quad n = 0, \pm 1, \pm 2, \pm 3, \ldots$$

Finally the solution to the PDE, satisfying all BCs, is:

$$u(r,\theta) = \sum_{n=-\infty}^{\infty} c_n (r/a)^{|n|} e^{-in\theta}$$

where

$$c_n = \frac{1}{2\pi}\int_{-\pi}^{\pi} f(\theta) e^{in\theta} d\theta.$$

As an example, suppose the specified boundary value is

$$u(a,\theta) = f(\theta) = \sin^2\theta = [\frac{1}{2i}(e^{i\theta} - e^{-i\theta})]^2$$

Then

$$\begin{aligned} c_n &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \sin^2\theta \cdot e^{in\theta} = -\frac{1}{4}\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{2i\theta}e^{in\theta} - \frac{1}{4}\frac{1}{2\pi}\int_{-\pi}^{\pi} e^{-2i\theta}e^{in\theta}d\theta + \frac{1}{2} \\ &= -\frac{1}{4}\delta_{2n} - \frac{1}{4}\delta_{-2n} + \frac{1}{2}\delta_{0n}. \end{aligned}$$

Thus

$$c_2 = -\frac{1}{4}, \quad c_{-2} = -\frac{1}{4}, c_0 = \frac{1}{2}, \quad \text{and} \quad c_n = 0 \quad \text{for other } n\text{'s}.$$

Finally:

$$u(r,\theta) = \frac{1}{2} - \frac{1}{2}(r/a)^2 \cos 2\theta.$$

An alternative method would be to use the real form of the Fourier series, which turns out to be a little easier.

Chapter 7

Fourier Series, Fourier Transform and Laplace Transform

7.1 Introduction

In the previous chapter, we discussed the Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{-in\pi x/L}, \quad -L < x < L, \tag{7.1}$$

for $f(x)$ in the interval $-L < x < L$ where

$$c_n = \frac{1}{2L} \int_{-L}^{L} f(x) e^{in\pi x/L} dx. \tag{7.2}$$

Previously, when sine and cosine series were discussed, we alluded to *Dirichlet's Theorem*, which tells us conditions under which Fourier series is a satisfactory representation of the original function $f(x)$. The full Dirichlet's Theorem is stated below.

7.2 Dirichlet Theorem

If $f(x)$ is a bounded and piecewise continuous function in $-L < x < L$, its Fourier series representation converges to $f(x)$ at each point x in the interval where $f(x)$ is continuous, and to the average of the left- and right-hand limits of $f(x)$ at those points where $f(x)$ is discontinuous. If $f(x)$ is periodic with period $2L$, the above statement applies throughout $-\infty < x < \infty$.

This theorem is easy to understand. The Fourier series, consisting of sines and cosines of period $2L$, has period $2L$. If $f(x)$ itself is also has the same period, then the Fourier series can be a good representation of $f(x)$ over the whole real axis $-\infty < x < \infty$. If on the other hand, $f(x)$ is either not periodic, or not defined beyond the interval $-L < x < L$, the Fourier series gives a good representation of $f(x)$ only in the stated interval. Beyond $-L < x < L$, the Fourier series is periodic and so simply repeats itself, but $f(x)$ may or may not be so. The above statements apply where $f(x)$ is continuous. When $f(x)$ takes a jump at a point, say x_0, the value of $f(x)$ at x_0 is not defined. The value which the Fourier seris of $f(x)$ converges to is the average of the value immediately to the left of x_0 and to the right of x_0, i.e. to $\lim_{\epsilon\to 0}\frac{1}{2}(f(x_0-\epsilon)+\frac{1}{2}f(x_0+\epsilon))$. We have already demonstrated this with the Fourier sine series. The same behavior applies to the full Fourier series.

7.3 Fourier integrals

Unless $f(x)$ is periodic, the Fourier series representation of $f(x)$ is an appropriate representation of $f(x)$ only over the interval $-L < x < L$. Question: Can we take $L \to \infty$, so as to obtain a good representation of $f(x)$ over the whole interval $-\infty < x < \infty$? The positive answer leads to the Fourier integral, and hence the Fourier transform, provided $f(x)$ is "integrable" over the whole domain.

We first rewrite (7.1) as a Riemann sum by letting

$$\Delta\omega = \pi/L \quad \text{and} \quad \omega_n = n\pi/L.$$

Thus, (7.1) becomes

$$f(x) = \frac{1}{2\pi}\sum_{n=-\infty}^{\infty} \Delta\omega F_n \cdot e^{-i\omega_n x}, \tag{7.3}$$

where

$$F_n \equiv (2Lc_n) = \int_{-L}^{L} f(x')e^{i\omega_n x'}dx'. \tag{7.4}$$

[We have changed the dummy variable in (7.4) from x to x', to avoid confusion later.]

In the limit $L \to \infty$, ω_n becomes ω, which takes on continuous values in $-\infty < \omega < \infty$. So $F_n \to F(\omega)$, where

$$F(\omega) = \int_{-\infty}^{\infty} f(x')e^{i\omega x'}dx', \tag{7.5}$$

and (7.3) becomes the integral:

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{-i\omega x}d\omega. \tag{7.6}$$

Substituting (7.5) into (7.6) leads to the *Fourier integral formula*:

$$\boxed{f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty}\left[\int_{-\infty}^{\infty} f(x')e^{i\omega x'}dx'\right]e^{-i\omega x}d\omega}\,. \tag{7.7}$$

The validity of the formula (7.7) is subject to the integrability of the function $f(x)$ in (7.5). Furthermore, the left-hand side of (7.7) must be modified at points of discontinuity of $f(x)$ to be the average of the left- and right-hand limits at the discontinuity, because the Fourier series, upon which the (7.7) is based, has this property.

The formula shows that the operation of integrating $f(x)e^{i\omega x}$ over all x is "reversible", by multiplying it by $e^{-i\omega x}$ and integrating over all ω. (7.7) allows us to define Fourier transforms and inverse transforms.

7.4 Fourier transform and inverse transform

Let the Fourier transform of $f(x)$ be denoted by $\mathcal{F}[f(x)]$. We should use (7.5) for a definition of such an operation:

$$\boxed{F(\omega) = \mathcal{F}[f(x)] \equiv \int_{-\infty}^{\infty} f(x)e^{i\omega x}dx}\,. \tag{7.8}$$

Let $\mathcal{F}^{-1}$ be the inverse Fourier transform, which recovers the original function $f(x)$ from $F(\omega)$. (7.6) tells us that the inverse transform is given by

$$\boxed{f(x) = \mathcal{F}^{-1}[F(\omega)] \equiv \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{-i\omega x}d\omega}\,. \tag{7.9}$$

Equations (7.8) and (7.9) form the transform pair. Not too many integrals can be "reversed". Take for example

$$\int_{-\infty}^{\infty} f(x)dx.$$

Once integrated, the information about $f(x)$ is lost and cannot be recovered. Therefore the relationships such as (7.8) and (7.9) are rather special and have wide application in solving PDEs.

Note that our definition of the Fourier transform and inverse transform is not unique. One could, as in some textbooks, put the factor $\frac{1}{2\pi}$ in (7.8) instead of in (7.9), or split it as $\frac{1}{\sqrt{2\pi}}$ in (7.8) and $\frac{1}{\sqrt{2\pi}}$ in (7.9). The only thing that matters is that in the Fourier integral formula there is the factor $\frac{1}{2\pi}$ when the two integrals are both carried out. Also, in (7.7), we can change ω to $-\omega$ without changing the form of (7.7). So, the Fourier transform in (7.8) can alternatively be defined with a negative sign in front of ω in the exponent, and the inverse transform in (7.9) with a positive sign in front of ω in the exponent. It does not matter to the final result as long as the transform and inverse transform have opposite signs in front of ω in their exponents.

7.5 Laplace transform and inverse transform

The Laplace transform is often used to transform a function of time, $f(t)$ for $t > 0$. It is defined as

$$\boxed{\mathcal{L}[f(t)] = \int_0^\infty f(t)e^{-st}dt \equiv \tilde{f}(s)}\,. \tag{7.10}$$

Mathematically, it does not matter whether we denote our independent variable by the symbol t or x; nor does it matter whether we call t time and x space or vice versa. What does matter for Laplace transforms is the integration ranges only over a semi-infinite interval, $0 < t < \infty$. We do not consider what happens before $t = 0$. In fact, as we will see, we need to take $f(t) = 0$ for $t < 0$.

Functions which are zero for $t < 0$ are called one-sided functions. For one-sided $f(t)$, we see that the Laplace transform (7.10) is the same as the Fourier transform (7.8) if we replace x by t and ω by is. That is, from (7.8)

$$\begin{aligned} F(is) &= \int_{-\infty}^\infty f(t)e^{-st}dt = \int_0^\infty f(t)e^{-st}dt \\ &\equiv \tilde{f}(s). \end{aligned} \tag{7.11}$$

Since the Laplace transform is essentially the same as the Fourier transform, we can use the Fourier inverse transform (7.9) to recover $f(t)$ from its Laplace transform $\tilde{f}(s)$. Let

$$f(t) = \mathcal{L}^{-1}[\tilde{f}(s)].$$

Then the operation $\mathcal{L}^{-1}$, giving the inverse Laplace transform, must be defined by

$$f(t) = \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \tilde{f}(s)e^{st}ds. \tag{7.12}$$

This is because

$$\begin{aligned} f(t) = \mathcal{F}^{-1}[F(\omega)] &= \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{-i\omega t}d\omega \\ &= \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \tilde{f}(s)e^{st}ds \end{aligned}$$

through the change from ω to is. Since the inverse Laplace transform involves an integration in the complex plane, it is usually not discussed in elementary mathematics courses which deal with real integrals. Tables of Laplace transforms and inverse transforms are used instead. Our purpose here is simply to point out the connection between Fourier and Laplace transform, and the origin of both in Fourier series.

Note: The inverse Laplace transform formula in (7.12) was obtained from the Fourier integral formula, which applies only to integrable functions. For "nonintegrable", but one-sided $f(t)$, (7.12) should be modified, with the limits of integration changed to $\alpha - i\infty$ and $\alpha + i\infty$, where α is some positive real constant bounding the exponential growth of f allowed.

To show this, suppose $f(t)$ is not integrable because it grows as $t \to \infty$. Suppose that for some positive α the product

$$g(t) \equiv f(t)e^{-\alpha t} \to 0 \text{ as } t \to \infty$$

and is thus integrable. We proceed to find the Laplace transform of $g(t)$:

$$\begin{aligned} \widetilde{g}(s) \equiv \mathcal{L}[g(t)] &= \int_0^{\infty} f(t)e^{-\alpha t}e^{-st}d\tau \\ &= \int_0^{\infty} f(t)e^{-(\alpha+s)t}dt. \end{aligned}$$

Thus if

$$\widetilde{f}(s) = \mathcal{L}[f(t)] = \int_0^{\infty} f(t)e^{-st}dt,$$

then

$$\widetilde{g}(s) = \widetilde{f}(\alpha + s).$$

The inverse of $\widetilde{g}(s)$ is

$$\begin{aligned} g(t) = \mathcal{L}^{-1}[\widetilde{g}(s)] &= \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \widetilde{g}(s)e^{st}ds \\ &= \frac{1}{2\pi i}\int_{-i\infty}^{i\infty} \widetilde{f}(\alpha+s)e^{st}ds \\ &= \frac{1}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty} \widetilde{f}(s')e^{-\alpha t}e^{s't}ds' \end{aligned}$$

where we have made the substitution $s' = \alpha + s$. Since $g(t) \equiv f(t)e^{-\alpha t}$, we obtain, on cancelling out the $e^{-\alpha t}$ factor:

$$f(t) = \frac{1}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty} \widetilde{f}(s')e^{s't}ds'.$$

This is a modified, and more general, formula for Laplace transform of a one-sided function $f(t)$, whether or not it decays as $t \to \infty$, as long as $f(t)e^{-\alpha t}$ is integrable.

$$\begin{aligned} \widetilde{f}(s) = \mathcal{L}[f(t)] &= \int_0^\infty f(t)e^{-st}dt, \;\; \mathrm{Re}\; s \geq \alpha \\ f(t) = \mathcal{L}^{-1}[\widetilde{f}(s)] &= \frac{1}{2\pi i}\int_{\alpha-i\infty}^{\alpha+i\infty} \widetilde{f}(s)e^{st}ds. \end{aligned}$$

7.6 Parseval's Theorem

7.6.1 Parseval's Theorem

$$\int_{-\infty}^{\infty} f(x)g(x)^*dx = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)G(\omega)^*d\omega, \tag{7.13}$$

where

$$F(\omega) = \mathcal{F}[f(x)] \quad \text{and} \quad G(\omega = \mathcal{F}[g(x)]$$

Proof: since

$$\begin{aligned} g(x) = \mathcal{F}^{-1}[G(\omega)] &= \frac{1}{2\pi}\int_{-\infty}^{\infty} G(\omega)e^{-i\omega x}d\omega \\ \int_{-\infty}^{\infty} f(x)g(x)^*dx &= \frac{1}{2\pi}\int_{-\infty}^{\infty} f(x)\int_{-\infty}^{\infty} G(\omega)^*e^{i\omega x}d\omega dx. \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(x)e^{i\omega x}dxG(\omega)^*d\omega \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)G(\omega)^*d\omega. \end{aligned}$$

7.6.2 Placherel's Theorem

$$\int_{-\infty}^{\infty} |f(x)|^2 dx = \frac{1}{2\pi} \int_{-\infty}^{\infty} |F(\omega)|^2 d\omega \tag{7.14}$$

Proof: Let $g(x) = f(x)$ in Parseval's Theorem.

7.7 Cauchy-Schwarz inequality:

$$|\int_{-\infty}^{\infty} f(x)g(x)^* dx|^2 \leq \int_{-\infty}^{\infty} |f|^2 dx \cdot \int_{-\infty}^{\infty} |g(x)|^2 dx \tag{7.15}$$

This inequality is equivalent to the inner product:

$$(f, g) \equiv \int_{-\infty}^{\infty} f(x) g^*(x) dx \quad \text{between two "vectors" } f \text{ and } g$$

being no greater than the product of the magnitudes of f and g

$$\|f\| \equiv \left(\int_{-\infty}^{\infty} |f|^2 dx \right)^{1/2}, \quad \|g\| \equiv \left(\int_{-\infty}^{\infty} |g|^2 dx \right)^{1/2}.$$

That is

$$|f, g|^2 \leq \|f\|^2 \cdot \|g\|^2.$$

Proof: For all t,

$$0 \leq \|f + tg\|^2 = \|f\|^2 + |t|^2 \|g\|^2 + 2 \operatorname{Re}\{t(f, g)\}$$

Take $t = -(f, g)^*/\|g\|^2$, $|t| = |(f, g)|/\|g\|^2 = r/\|g\|^2$, where we have written $(f, g) = re^{i\theta}$.

$$\begin{aligned} \operatorname{Re}\{t(f, g)\} &= -\operatorname{Re}\{\frac{|(f, g)|^2}{\|g\|^2}\} = -r^2/\|g\|^2 \\ 0 &\leq \|f\|^2 + r^2/\|g\|^2 - 2r^2\|g\|^2 \\ &= \|f\|^2 - r^2/\|g\|^2 \\ &= \{\|f\|^2\|g\|^2 - |(f, g)]|^2\}/\|g\|^2 \end{aligned}$$

This if $\|g\|^2 \neq 0$, we have

$$|(f, g)|^2 \leq \|f\|^2 \cdot \|g\|^2.$$

7.8 The Uncertainty Principle

7.8.1 Mathematical Uncertainty Principle

Let

$$\Delta_a f(x) \equiv \int_{-\infty}^{\infty} (x-a)^2 |f(x)|^2 dx \Big/ \int_{-\infty}^{\infty} |f(x)|^2 dx$$

be the uncertainty of $f(x)$ about a point $x = a$, and

$$\Delta_\alpha F(\omega) \equiv \int_{-\infty}^{\infty} (\omega-\alpha)^2 |F(\omega)|^2 d\omega \Big/ \int_{-\infty}^{\infty} |F(\omega)|^2 d\omega$$

be the "uncertainty" of $F(\omega)$ about a wavenumber $\omega = \alpha$.

The mathematical uncertainty principle is:

$$\Delta_a f(x) \cdot \Delta_\alpha F(\omega) \geq \frac{1}{4}. \tag{7.16}$$

Proof: Let's first do it for $a = 0$, $\alpha = 0$. The more general case of $a \neq 0$, $\alpha \neq 0$ can be obtained by shifting the axes.

Consider

$$\begin{aligned} f(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) e^{-i\omega x} d\omega \\ f'(x) &= \frac{1}{2\pi} \int_{-\infty}^{\infty} -i\omega F(\omega) e^{-i\omega x} d\omega \end{aligned}$$

That is, $-i\omega F(\omega)$ is the Fourier transform of $f'(x)$.

Using $f'(x)$ in Plancherel's Theorem then yields

$$\begin{aligned} \int_{-\infty}^{\infty} |f'(x)|^2 dx &= \frac{1}{2\pi} \int_{-\infty}^{\infty} |\omega F(\omega)|^2 d\omega \\ &= \Delta_\alpha F(\omega) \cdot \frac{1}{2\pi} \int_{-\infty}^{\infty} |F(\omega)|^2 d\omega \\ &= \Delta_\alpha F(\omega) \cdot \int_{-\infty}^{\infty} |f(x)|^2 dx. \end{aligned} \tag{7.17}$$

Plancherel's Theorem has been used in the last step.

Now consider the following integration by parts:

$$\int_{-\infty}^{\infty} f'(x) [x f(x)]^* dx$$

$$= x|f(x)|^2 \Big|_{-\infty}^{\infty} - \int_{-\infty}^{\infty} [|f(x)|^2 + xf(x)f'(x)^*]dx$$

Assuming that $x|f(x)|^2 \to 0$ as $x \to \pm\infty$, we have

$$\begin{aligned}
\int_{-\infty}^{\infty} |f(x)|^2 dx &= -\int_{-\infty}^{\infty} \{xf(x) \cdot [f'(x)]^* + f'(x)[xf(x)]^*\} dx \\
&= -2 \int_{-\infty}^{\infty} \mathrm{Re}\,\{xf(x) \cdot [f'(x)]^*\} dx
\end{aligned}$$

Since Re $z \le |z|$, we have

$$\begin{aligned}
\left(\left| \int_{-\infty}^{\infty} |f(x)|^2 dx \right| \right)^2 &= 4 \left(\left| \int_{-\infty}^{\infty} \mathrm{Re}\,\{xf(x) \cdot [f'(x)]^*\} dx \right| \right)^2 \\
&\le 4 \left(\left| \int_{-\infty}^{\infty} |xf(x)||f'(x)| dx \right| \right)^2 \\
&\le 4 \int_{-\infty}^{\infty} |xf(x)|^2 dx \cdot \int_{-\infty}^{\infty} |f'(x)|^2 dx \qquad (7.18)
\end{aligned}$$

using the Cauchy-Schwarz inequality in the last step.

This inequality (7.18) is

$$\frac{\int_{-\infty}^{\infty} x^2 |f(x)|^2 dx}{\int_{-\infty}^{\infty} |f(x)|^2 dx} \cdot \frac{\int_{-\infty}^{\infty} |f'(x)|^2 dx}{\int_{-\infty}^{\infty} |f(x)|^2 dx} \ge \frac{1}{4} \tag{7.19}$$

Thus, using (7.17)

$$\Delta_a f(x) \cdot \Delta_\alpha F(\omega) \ge \frac{1}{4}. \tag{7.20}$$

Although this is proved only for $a = 0$ and $\alpha = 0$, it is easy to show that it remains true for $a \neq 0$, $\alpha \neq 0$, simply by shifting the x axis by a and the ω axis by α.

7.8.2 Quantum Mechanical Uncertainty Principle

This quantum mechanical uncertainty principle is due to Heisenberg. It states that there is a limit to how presicely one can determine a particle's position and momentum simultaneously. We will see that it is actually a mathematical result, with quantum mechanical interpretation added.

In quantum mechanics, the probability density of finding a particle in the interval between x and $x + dx$ is

$$|\psi(x,t)|^2,$$

where $\psi(x,t)$ is the wavefunction. Thus

$$\int_{-\infty}^{\infty} |\psi(x,t)|^2 dx = 1, \tag{7.21}$$

since the particle has to be located somewhere.

The uncertainty of finding a particle at $x = a$ is defined as

$$\begin{aligned}\Delta_{\text{position}} &\equiv \int_{-\infty}^{\infty} (x-a)^2 |\psi(x,t)|^2 dx \Big/ \int_{-\infty}^{\infty} |\psi(x,t)|^2 dx \\ &= \int_{-\infty}^{\infty} (x-a)^2 |\psi(x,t)|^2 dx. \end{aligned} \tag{7.22}$$

If you know for certain that the particle is at $x = 0$, then $|\psi(x,t)| = \delta(x)$, and Δ_{position} would be zero.

In quantum mechanics, the momentum of a particle is related to the wavenumber ω through the de Broglie formula:

$$p = \omega\hbar. \tag{7.23}$$

Let $\Psi(\omega,t)$ be the Fourier transform of $\psi(x,t)$, and consider:

$$\Delta_{\alpha/\hbar}\Psi(\omega,t) \equiv \int_{-\infty}^{\infty} (\omega - \alpha/\hbar)^2 |\Psi(\omega,t)|^2 d\omega \Big/ \int_{-\infty}^{\infty} |\Psi(\omega,t)|^2 d\omega$$

Through a change in variable: $\omega = p/\hbar$, this becomes

$$\Delta_{\alpha/\hbar}\Psi(\omega,t) = \frac{1}{\hbar^3} \int_{-\infty}^{\infty} (p-\alpha)^2 |\Psi(\frac{p}{\hbar},t)|^2 dp \Big/ \int_{-\infty}^{\infty} |\Psi(\omega,t)|^2 d\omega \tag{7.24}$$

Let the uncertainty in momentum about $p = \alpha$ be defined by:

$$\Delta_{\text{momentum}} \equiv \int_{-\infty}^{\infty} (p-\alpha^2) |\Psi(\frac{p}{\hbar},t)|^2 dp \Big/ \int_{-\infty}^{\infty} |\Psi(\frac{p}{\hbar},t)|^2 dp$$

Here $\Psi(\frac{p}{\hbar},t)$ is the unscaled probability density wave function for momentum p. Since

$$\begin{aligned}\int_{-\infty}^{\infty} |\Psi(\frac{p}{\hbar},t)|^2 dp &= \hbar \int_{-\infty}^{\infty} |\Psi(\frac{p}{\hbar},t)|^2 d(p/\hbar) \\ &= \hbar \int_{-\infty}^{\infty} |\Psi(\omega,t)|^2 d\omega,\end{aligned}$$

we have:

$$\Delta_{\text{momentum}} = \frac{1}{\hbar}\int_{-\infty}^{\infty}(p-\alpha)^2|\Psi(\frac{p}{\hbar},t)|^2 dp/\int_{-\infty}^{\infty}|\Psi(\omega,t)|^2 d\omega \tag{7.25}$$

And so from (7.24):

$$\Delta_{\alpha/\hbar}\Psi(\omega,t) = \frac{1}{\hbar^2}\Delta_{\text{momentum}} \tag{7.26}$$

Substituting (7.22) and (7.26) into the mathematical uncertainty principle (7.20), we arrive at Heisenberg's uncertainty principle:

$$\Delta_{\text{position}}\cdot\Delta_{\text{momentum}} \geq \frac{\hbar^2}{4} \tag{7.27}$$

To decrease the uncertainty of a particle's position about some point a causes an increase in the uncertainty of the momentum of the particle about all values α, and vice versa.

Chapter 8

Fourier Transform and Its Application to PDE

8.1 Introduction

We shall first practice taking the Fourier transform of some functions before applying it to solving PDEs in infinite domains.

8.2 Fourier transform of some simple functions

Example 1:

Take the Fourier transform of

$$f(x) = e^{-|x|}, \quad -\infty < x < \infty.$$

$$\begin{aligned}
F(\omega) = \mathcal{F}[e^{-|x||}] &= \int_{-\infty}^{\infty} e^{-|x|} e^{i\omega x} dx \\
&= \int_0^{\infty} e^{-x+i\omega x} dx + \int_{-\infty}^{0} e^{x+i\omega x} dx \\
&= \frac{1}{-(1-i\omega)} e^{-(1-i\omega)x}|_0^{\infty} + \frac{1}{(1+i\omega)} e^{(1+i\omega)x}|_{-\infty}^{0} \\
&= \frac{1}{1-i\omega} + \frac{1}{1+i\omega} = \frac{2}{1+\omega^2}.
\end{aligned}$$

Note its decay as $\omega \to \pm\infty$.

Example 2:

Take the Fourier transform of

$$f(x) = e^x, \quad -\infty < x < \infty.$$

$$\begin{aligned} F(\omega) = \mathcal{F}[e^x] &= \int_{-\infty}^{\infty} e^x e^{i\omega x} dx \\ &= \frac{1}{(1+i\omega)} e^{(1+i\omega)x}|_{-\infty}^{\infty}. \end{aligned}$$

The limit at $x = \infty$ blows up. We say the Fourier transform of e^x does not exist because the function $f(x) = e^x$ is not "integrable", i.e.

$$\int_{-\infty}^{\infty} |f(x)| dx = \int_{-\infty}^{\infty} e^x dx$$

does not have a finite value. [Draw a picture of e^x, and see that the area under the curve is infinitely large.]

Example 3:

Take the Fourier transform of

$$f(x) = e^{-x}, \quad -\infty < x < \infty.$$

This funciton is also not integrable, and so its Fourier transform does not exist. [Show this.]

Example 4:

Take the Fourier transform of

$$f(x) = e^{-x^2}, \quad -\infty < x < \infty.$$

The value of the function decreases rapidly when x is away from $x = 0$ in *both* the positive and negative x directions. There is a finite area under the curve e^{-x^2}, so this function is integrable. To find its Fourier transform, we need to perform the integral:

$$F(\omega) = \int_{-\infty}^{\infty} e^{-x^2} e^{i\omega x} dx.$$

You can either look up a table of integrals or by completing the square in the exponent to get

$$F(\omega) = \sqrt{\pi}e^{-\omega^2/4}.$$

[In case you are curious:

$$-x^2 + i\omega x = -(x - i\omega/2)^2 - \omega^2/4.$$

So $F(\omega) = e^{-\omega^2/4}\int_{-\infty}^{\infty} e^{-(x-i\omega)/2)^2}dx = e^{-\omega^2/4}\int_{-\infty}^{\infty} e^{-y^2}dy$, where we have made a change of variable $y = x - i\omega/2$ and also shifted the path of integration. The remaining integral is a standard one (Euler's integral) and is equal to $\sqrt{\pi}$. In general,

$$\int_{-\infty}^{\infty} e^{-(x+b)^2}dx = \sqrt{\pi}, \quad \text{and} \quad \int_{-\infty}^{\infty} e^{-p^2x^2 \pm qx}dx = \frac{\sqrt{\pi}}{p}e^{\frac{q^2}{4p^2}},\ p > 0.]$$

Example 5:

Take the inverse transform of

$$F(\omega) = \sqrt{\pi}e^{-\omega^2/4}, \quad -\infty < \omega < \infty.$$

$$\begin{aligned}\mathcal{F}^{-1}[F(\omega)] &= \frac{\sqrt{\pi}}{2\pi}\int_{-\infty}^{\infty} e^{-\omega^2/4 - i\omega x}d\omega \\ &= \frac{\sqrt{\pi}}{2\pi}e^{-x^2}\int_{-\infty}^{\infty} e^{-(\omega/2+ix)^2}d\omega \\ &= e^{-x^2}.\end{aligned}$$

We have thus recovered the original function $f(x)$ in *Example 4.*

Example 6:

Take the inverse transform of

$$F(\omega) = \frac{2}{1+\omega^2}$$

$$\mathcal{F}^{-1}[F(\omega)] = \frac{2}{2\pi}\int_{-\infty}^{\infty} \frac{1}{1+\omega^2}e^{-i\omega x}d\omega.$$

This integral can be done very easily if you know complex variables and residue calculus. Otherwise, just rely on Tables of Integrals to tell you that

$$f(x) = e^{-|x|}.$$

We have thus recovered the $f(x)$ in *Example 1.*

8.3 Application to PDEs

The usual difficulty with PDEs is that the solution involves more than one independent variable. The transform method allows us to reduce one independent variable. We commonly try to transform the x-dependence through a Fourier transform, provided that the domain is infinite, i.e. $-\infty < x < \infty$. We sometimes use Laplace transform in t instead of or in addition to the Fourier transform in x, provided that $0 < t < \infty$.

Consider a function $u(x,t)$, with $-\infty < x < \infty$, $t > 0$. Let

$$\boxed{U(\omega,t) = \mathcal{F}[u(x,t)] = \int_{-\infty}^{\infty} u(x,t)e^{i\omega x}dx} \tag{8.1}$$

be the Fourier transform of $u(x,t)$ with respect to x. The original function $u(x,t)$ can then be recovered from the Fourier inverse transform:

$$\boxed{u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} U(\omega,t)e^{-i\omega x}d\omega}\,. \tag{8.2}$$

[Note that in (8.1) and (8.2) t plays no role; it may be regarded as arbitrary.] This is very similar to our previous method of writing the solution in the form of an eigenfunction expansion when the domain is finite. With (8.2), taking derivatives with respect to x is now very easy:

$$\begin{aligned}
u_x(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} (-i\omega)U(\omega,t)e^{-i\omega x}d\omega \\
u_{xx}(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} (-i\omega)^2U(\omega,t)e^{-i\omega x}d\omega \qquad (8.3)\\
u_t(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} U_t(\omega,t)e^{-i\omega x}d\omega \\
u_{tt}(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} U_{tt}(\omega,t)e^{-i\omega x}d\omega, \qquad (8.4)
\end{aligned}$$

provided of course that these integrals exist. At this point, there is no need to worry about these mathematical issues of integrability because we don't even know what $U(\omega,t)$ is yet.

8.4 Examples

8.4.1. The wave equation in an infinite domain

$$\begin{aligned}
\text{PDE:}\quad & u_{tt} = c^2 u_{xx}, \quad -\infty < x < \infty, \quad t > 0 && (8.5)\\
\text{BCs:}\quad & u(x,t) \to 0 \quad \text{as} \quad x \to \pm\infty && (8.6)\\
\text{ICs:}\quad & u(x,0) = f(x), && (8.7)\\
& u_t(x,0) = 0, \quad -\infty < x < \infty. && (8.8)
\end{aligned}$$

We assume the solution to be of the form of an integral (8.2) which we substitute into the PDE (8.4). This yields, using (8.3),

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}(U_{tt}(\omega,t) + c^2\omega^2 U(\omega,t))e^{-i\omega x}d\omega = 0,$$

which is the same as

$$\mathcal{F}^{-1}[U_{tt} + c^2\omega^2 U] = 0, \tag{8.9}$$

so (by taking $\mathcal{F}$ of (8.9)):

$$U_{tt} + c^2\omega^2 U = 0. \tag{8.10}$$

This is an ODE; the partial derivatives $\frac{\partial^2}{\partial x^2}$ have been converted to $(-i\omega)^2$, an algebraic multiplication. The ODE in t is to be solved subject to the following ICs:

$$u_t(x,0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} U_t(\omega,0)e^{-i\omega x}d\omega = 0,$$

and

$$u(x,0) = \frac{1}{2\pi}\int_{-\infty}^{\infty} U(\omega,0)e^{-i\omega x}d\omega = f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{-i\omega x}d\omega.$$

These imply:

$$U_t(\omega,0) = 0 \tag{8.11}$$

and

$$U(\omega,0) = F(\omega), \tag{8.12}$$

where the Fourier transform $F(\omega)$ of $f(x)$ is known if $f(x)$ is known.

The general solution to the ODE (8.10) is

$$U(\omega,t) = A(\omega)\sin(c\omega t) + B(\omega)\cos(c\omega t).$$

The ICs (8.10) and (8.11) can be used to determine the constants A and B to be $B(\omega) = F(\omega)$ and $A(\omega) = 0$. Thus,

$$U(\omega, t) = F(\omega)\cos(c\omega t). \tag{8.13}$$

We recover $u(x,t)$ by subsituting (8.13) back into (8.2).

$$\begin{aligned} u(x,t) = \mathcal{F}^{-1}[U(\omega,t)] &= \frac{1}{2\pi}\int_{-\infty}^{\infty} U(\omega,t)e^{-i\omega x}d\omega \\ &= \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)\cos(c\omega t)e^{-i\omega x}d\omega. \end{aligned} \tag{8.14}$$

Typically one cannot perform the integral explicitly unless $F(\omega)$ is known. In the particular case of the wave equation however, progress can be made by noting that

$$\cos(c\omega t) = \frac{1}{2}(e^{ic\omega t} + e^{-ic\omega t}),$$

and so (8.14) can be rewritten as

$$\begin{aligned} u(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{1}{2}F(\omega)e^{-i\omega(x-ct)}d\omega + \frac{1}{2\pi}\int_{-\infty}^{\infty}\frac{1}{2}F(\omega)e^{-i\omega(x+ct)}d\omega \\ &= \frac{1}{2}f(x-ct) + \frac{1}{2}f(x+ct), \end{aligned} \tag{8.15}$$

since

$$f(x) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{-i\omega x}d\omega,$$

so

$$f(x-ct) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{-i\omega(x-ct)}d\omega$$

and

$$f(x+ct) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{-i\omega(x+ct)}d\omega.$$

The physical intepretation of the solution (8.15) to the wave equation (8.4) is that an initial displacement of $f(x)$ will split into two shapes for $t > 0$, each with half the amplitude of the original shape, one propagates to the left and one propagates to the right, both with speed c. The quantity c is therefore called the wave speed.

8.4.2. Diffusion equation in an infinite domain:

$$\text{PDE:}\quad u_t = \alpha^2 u_{xx}, \quad -\infty < x < \infty, \quad t > 0 \tag{8.16}$$

$$\text{BCs:}\quad u(x,t) \to 0 \quad \text{as} \quad x \to \pm\infty, \tag{8.17}$$

$$\text{IC:}\quad u(x,0) = f(x), \quad -\infty < x < \infty. \tag{8.18}$$

We assume a solution of the form of an integral (8.2) and substitute it into the PDE (8.16). This yields, using (8.3)

$$\frac{1}{2\pi}\int_{-\infty}^{\infty}(U_t + \alpha^2\omega^2 U)e^{-i\omega x}d\omega = 0,$$

which implies

$$U_t + \alpha^2\omega^2 U = 0. \tag{8.19}$$

The ODE (8.19) is solved subject to the IC

$$U(\omega,0) = F(\omega), \tag{8.20}$$

which is obtained by taking the Fourier transform of (8.18).

The solution is

$$U(\omega,t) = A(\omega)e^{-\alpha^2\omega^2 t} = F(\omega)e^{-\alpha^2\omega^2 t}. \tag{8.21}$$

The final solution is obtained by substituting (8.21) into (8.2)

$$\boxed{u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty}F(\omega)e^{-\alpha^2\omega^2 t - i\omega x}d\omega.} \tag{8.22}$$

For the special case of

$$f(x) = ae^{-(x/L)^2}, \quad -\infty < x < \infty,$$

we know from Section 8.2 that

$$F(\omega) = \mathcal{F}[f(x)] = aL\sqrt{\pi}e^{-(L\omega)^2/4}.$$

Then

$$u(x,t) = \frac{aL}{2\pi}\int_{-\infty}^{\infty}\sqrt{\pi}e^{-(L\omega)^2/4-\alpha^2\omega^2 t - i\omega x}d\omega,$$

can be evaluated by completing squares

$$\begin{aligned} u(x,t) &= \frac{aL}{2\sqrt{\pi}}\int_{-\infty}^{\infty}e^{-(\alpha^2 t + \frac{L^2}{4})\omega^2 - i\omega x}d\omega \\ &= \frac{aL}{\sqrt{4\alpha^2 t + L^2}}e^{-x^2/(4\alpha^2 t + L^2)}. \end{aligned} \tag{8.23}$$

The physical interpretation of the solution (8.23) is that an initial concentration near $x = 0$ an initial with width of approximately $2L$ spreads out into a wider and wider region while its amplitude at $x = 0$ decreases monotonically to zero. This is a typical behavior of solutions to the diffusion/heat equation. The underlying physical process reduces gradients and spreads any initial concentration/heat to wider regions.

8.5 The "drunken sailor" problem

In Chapter 2, the "drunken sailor" problem was derived. Here we shall solve it using Fourier transform:

$$\text{PDE:} \qquad \frac{\partial}{\partial t}u = D\frac{\partial^2}{\partial x^2}u, \quad -\infty < x < \infty,\ t > 0 \tag{8.24}$$

$$\text{BC:} \qquad u(x,t) = 0 \text{ as } x \to \pm\infty \tag{8.25}$$

$$\text{IC:} \qquad u(x,0) = f(x) = \delta(x), \quad -\infty < x < \infty. \tag{8.26}$$

By taking Fourier transform in x, we found, in (8.22), that the solution can be written as

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{\infty} F(\omega)e^{-D\omega^2 t - i\omega x}d\omega, \tag{8.27}$$

where $F(\omega)$ is the Fourier transform of the initial distribution $u(x,0) = f(x)$. With $f(x) = \delta(x)$,

$$\begin{aligned} F(\omega) &= \int_{-\infty}^{\infty} f(x)e^{i\omega x}dx \\ &= \int_{-\infty}^{\infty} \delta(x)e^{i\omega x}dx = e^{i\omega 0} = 1. \end{aligned}$$

Thus

$$\begin{aligned} u(x,t) &= \frac{1}{2\pi}\int_{-\infty}^{\infty} e^{-D\omega^2 t - i\omega x} \\ &= (4\pi D t)^{-1/2}\exp\{-\frac{x^2}{4Dt}\}. \end{aligned} \tag{8.28}$$

Also, since the delta function can be obtained from the limit

$$\lim_{L\to 0}\frac{1}{\sqrt{\pi}L}e^{-(x/L)^2} = \delta(x)$$

one can obtain the result in (8.28) by taking the limit of $L \to 0$ in (8.23), with $a = \frac{1}{\sqrt{\pi}L}$.

8.6 Laplace transform solution of the same problem (optional)

The "drunken sailor" problem was solved in 8.5 using the Fourier transform in x. The same problem can also be solved using Laplace transform in t. The second approach is more difficult, because the transformed equation is a second-order ordinary differential equation, while the first approach (of using Fourier transform on the independent variable with the highest derivatives) yields a simpler first-order ordinary differential equation

$$\begin{aligned}
\text{PDE:} \quad & \frac{\partial}{\partial t}u = D\frac{\partial^2}{\partial x^2}u, \quad -\infty < x < \infty, \quad 0 < t < \infty \\
\text{BC:} \quad & u(x,t) = 0 \text{ as } x \to \pm\infty \\
\text{IC:} \quad & u(x,0) = f(x) = \delta(x), \quad -\infty < x < \infty.
\end{aligned}$$

Let $\tilde{u}(x,s)$ be the Laplace transform of the solution:

$$\tilde{u}(x,s) = \int_0^\infty e^{-st}u(x,t)dt.$$

Taking the Laplace transform of the PDE yields

$$\mathcal{L}\left\{\frac{\partial}{\partial t}u\right\} = D\tilde{u}_{xx}.$$

Since

$$\begin{aligned}
\mathcal{L}\left\{\frac{\partial}{\partial t}u\right\} &= \int_0^\infty \frac{\partial}{\partial t}ue^{-st}dt = ue^{-st}\Big|_0^\infty + s\int_0^\infty ue^{-st}dt \\
&= s\tilde{u} - u(x,0),
\end{aligned}$$

we have the following ordinary differential equation to solve:

$$\tilde{u}_{xx} - \frac{s}{D}\tilde{u} = -\frac{1}{D}\delta(x).$$

For $x > 0$:

$$\tilde{u}_{xx} - \frac{s}{D}\tilde{u} = 0.$$

The solution which vanishes as $x \to \infty$ is:

$$\tilde{u}(x,s) = A(s)\exp\{-(s/D)^{1/2}x\}, \quad \text{Re } s^{1/2} > 0.$$

For $x < 0$:

$$\tilde{u}_{xx} - \frac{s}{D}\tilde{u} = 0.$$

The solution which vanishes as $x \to -\infty$ is:

$$\tilde{u}(x,s) = B(s)\exp\{(s/D)^{1/2}x\}, \quad \text{Re } s^{1/2} > 0.$$

Assuming that $\tilde{u}$ is continuous at $x = 0$ implies that $A = B$. Another matching condition at $x = 0$ is obtained by integrating the ordinary differential equation across $x = 0$:

$$\int_{0^-}^{0^+} (\tilde{u}_{xx} - \frac{s}{D}\tilde{u})dx = \int_{0^-}^{0^+} -\frac{1}{D}\delta(x)dx.$$

$$\tilde{u}_x|_{0^-}^{0^+} = -\frac{1}{D},$$

since $\int_{0^-}^{0^+} \delta(x)dx = 1$, and $\int_{0^-}^{0^+} \tilde{u}dx = 0$ if $\tilde{u}$ is finite. Since $\tilde{u}_x$ at 0^+ is $-(s/D)^{1/2}A$, and $\tilde{u}_x$ at 0^- is $(s/D)^{1/2}B$ we have

$$2(s/D)^{1/2}A = -\frac{1}{D}.$$

Thus we find:

$$\tilde{u}(x,s) = \frac{1}{2(Ds)^{1/2}}\exp\left\{-(\frac{s}{D})^{1/2}|x|\right\}.$$

$u(x,t)$ is then found via the inverse Laplace transform:

$$u(x,t) = \frac{1}{2\pi i}\int_L \frac{1}{2(Ds)^{1/2}}\exp\{st - (s/D)^{1/2}|x|\}ds,$$

where L is the vertical line in the complex-s plane to the right of all singularities. There is a branch point at $s = 0$. The branch with Re $s^{1/2} > 0$ is defined by $s = re^{i\theta}$, $s^{1/2} = r^{1/2}e^{i\theta/2}$, and so $\cos(\theta/2) > 0$. Thus $\theta/2$ should be between $-\pi/2$ and $\pi/2$, and so

$$-\pi < \theta < \pi.$$

This implies a branch cut from $s = 0$ along the negative real-s axis. A closed contour C can be constructed as

$$C = L + C_R + C_2 + C_3 + C_4.$$

There is no singularity inside C and so $\oint_C ds = 0$. $\int_{C_R} ds \to 0$ by Jordan's lemma as the radius of the semicircle goes to infinity. The integral over the small circle C_3 vanishes as its radius goes to zero. On the upper horizontal line C_2, $s = re^{i\pi^-}$, and so

$$\begin{aligned}\frac{1}{2\pi i}\int_{C_2} &= \frac{1}{2\pi i}\int_{\infty}^{0} e^{-rt-i(r/D)^{1/2}|x|}\frac{e^{i\pi}dr}{2i(Dr)^{1/2}} \\ &= -\frac{1}{4\pi D^{1/2}}\int_0^\infty \frac{e^{-rt-i(r/D)^{1/2}|x|}}{r^{1/2}}dr.\end{aligned}$$

On the lower horizontal line C_4, $s = re^{-i\pi^+}$, and so:

$$\begin{aligned}\frac{1}{2\pi i}\int_{C_4} &= \frac{1}{2\pi i}\int_{0}^{\infty} e^{-rt+i(r/D)^{1/2}|x|}\frac{e^{-i\pi}dr}{-2i(Dr)^{1/2}} \\ &= -\frac{1}{4\pi D^{1/2}}\int_0^\infty \frac{e^{-rt+i(r/D)^{1/2}|x|}}{r^{1/2}}dr.\end{aligned}$$

Since

$$\begin{aligned}u(x,t) &= \frac{1}{2\pi i}\int_L = \frac{1}{2\pi i}\left\{\oint_C - \int_{C_R} - \int_{C_2} - \int_{C_3} - \int_{C_4}\right\} \\ &= -\frac{1}{2\pi i}\left\{\int_{C_2} + \int_{C_4}\right\} \\ &= \frac{1}{4\pi D^{1/2}}\int_0^\infty \frac{dr}{r^{1/2}}e^{-rt}\left\{e^{i(r/D)^{1/2}|x|} + e^{-i(r/D)^{1/2}|x|}\right\}\end{aligned}$$

By setting $y = r^{1/2}$, this becomes

$$\begin{aligned}u(x,t) &= \frac{1}{4\pi D^{1/2}}\int_0^\infty 2dye^{-y^2t}\{e^{i(|x|/D^{1/2})y} + e^{-i(|x|/D^{1/2})y}\} \\ &= \frac{1}{2\pi D^{1/2}}\int_{-\infty}^{\infty} e^{-ty^2+i\frac{|x|}{D^{1/2}}y}dy \\ &= \frac{1}{(4\pi Dt)^{1/2}}\exp\{-\frac{x^2}{4Dt}\}.\end{aligned}$$

This is the same as previously found using Fourier transform in x.

8.7 Wave equation in 3-D (optional)

$$\text{PDE:}\frac{\partial^2}{\partial t^2}u = c^2\nabla^2 u,\ \nabla^2 \equiv \frac{\partial^2}{\partial x_1^2} + \frac{\partial^2}{\partial x_2^2} + \frac{\partial^2}{\partial x_3^2}$$
$$\text{BC:}u \to 0 \text{ as } x^2 + y^2 + z^2 \to \infty$$
$$\text{IC:}u(\mathbf{x}, t) = u_0(r)$$
$$u_t(\mathbf{x}, t) = 0$$

where $r = (x_1^2+x_2^2+x_3^2)^{1/2}$. The initial u is assumed to have radial symmetry about the origin, and hence is a function of r only.

We apply Fourier transform to each space dimension by letting

$$\begin{aligned} U(\boldsymbol{\lambda}, t) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} u(\mathbf{x}, t)e^{i(\lambda_1 x_1+\lambda_2 x_2+\lambda_3 x_3)}dx_1 dx_2 dx_3 \\ &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} u(\mathbf{x}, t)e^{i\boldsymbol{\lambda}\cdot\mathbf{x}}d\mathbf{x}. \end{aligned}$$

It is understood that

$$d\mathbf{x} = dx_1 dx_2 dx_3, \mathbf{x} = (x_1, x_2, x_3), \boldsymbol{\lambda} = (\lambda_1, \lambda_2, \lambda_3).$$

If we take the 3-D transform of the PDE we will get

$$\frac{\partial^2}{\partial t^2}U = -c^2\lambda^2 U,$$

where $\lambda^2 \equiv \lambda_1^2 + \lambda_2^2 + \lambda_3^2$. The solution to the ODE is

$$U(\boldsymbol{\lambda}, t) = A(\boldsymbol{\lambda})\cos c\lambda t + B(\boldsymbol{\lambda})\sin c\lambda t.$$

Applying the IC, we find $B(\boldsymbol{\lambda}) = 0$ and $A(\boldsymbol{\lambda}) = U(\boldsymbol{\lambda}, 0)$, where

$$\begin{aligned} U(\boldsymbol{\lambda}, 0) &= \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} u_0(r)e^{i\boldsymbol{\lambda}\cdot\mathbf{x}}d\mathbf{x} \\ &= \int_0^{\infty} dr \int_0^{\pi} r^2\sin\theta d\theta \int_0^{2\pi} d\varphi u_0(r)e^{i\lambda r\cos\theta} \end{aligned}$$

in spherical coordinates. [We have oriented the coordinate systems so that θ is the angle the vector $\mathbf{x}$ makes relative to a (fixed) vector $\boldsymbol{\lambda}$.]

$$\begin{aligned} U(\boldsymbol{\lambda}, 0) &= 2\pi\int_0^{\infty} dr r^2 u_0(r)\int_0^{\pi} d(-\cos\theta)e^{i\lambda r\cos\theta} \\ &= 2\pi\int_0^{\infty} dr r^2 u_0(r)(e^{i\lambda r\cos\theta}/(-i\lambda r))\Big|_0^{\pi} \\ &= 4\pi\int_0^{\infty} u_0(r)\frac{\sin\lambda r}{\lambda}r dr \equiv U_0(\lambda), \end{aligned}$$

which is a function of the magnitude of $\boldsymbol{\lambda}$ only. Thus

$$U(\boldsymbol{\lambda}, t) = U_0(\lambda) \cos c\lambda t.$$

The inverse Fourier transform is

$$\begin{aligned}
u(\mathbf{x}, t) &= \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_0(\lambda) \cos c\lambda t e^{-i\boldsymbol{\lambda}\cdot\mathbf{x}} d\boldsymbol{\lambda} \\
&= \frac{1}{(2\pi)^3} \int_0^{\infty} d\lambda \int_0^{\pi} 2\pi \sin\theta \lambda^2 U_0(\lambda) \cos(c\lambda t) e^{-i\lambda r \cos\theta} d\theta \\
&= \frac{2}{(2\pi)^2} \int_0^{\infty} \lambda d\lambda U_0(\lambda) \cos(c\lambda t) \sin\lambda r / r
\end{aligned}$$

Since $\sin\lambda r (\cos c\lambda t = \frac{1}{2}\sin\lambda(r - ct) + \frac{1}{2}\sin\lambda(r + ct)$ and

$$\begin{aligned}
u(\mathbf{x}, 0) = u_0(r) &= \frac{1}{(2\pi)^3} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} \int_{-\infty}^{\infty} U_0(\lambda) e^{-i\boldsymbol{\lambda}\cdot\mathbf{x}} d\boldsymbol{\lambda} \\
&= \frac{2}{(2\pi)^2} \int_0^{\infty} \lambda d\lambda U_0(\lambda) \sin\lambda r / r,
\end{aligned}$$

we have

$$\begin{aligned}
ru(\mathbf{x}, t) &= \frac{1}{(2\pi)^2} \int_0^{\infty} \lambda d\lambda U_0(\lambda) \sin\lambda(r - ct) \\
&\quad + \frac{1}{(2\pi)^2} \int_0^{\infty} \lambda d\lambda U_0(\lambda) \sin\lambda(r + ct) \\
&= \frac{1}{2}(r - ct) u_0(r - ct) + \frac{1}{2}(r + ct) u_0(r + ct).
\end{aligned}$$

Chapter 9

Numerical Fourier Transform and FFT

9.1 Introduction

Often the Fourier integrals cannot be evaluated analytically, and we need to resort to numerical approximation. It turns out that the numerical approximation of the Fourier integral is the same as a Fourier series. A fast way to compute the Fourier series is called Fast Fourier Transform (FFT).

9.2 Numerical evaluation of Fourier Transform

To numerically evaluate

$$F(\omega) = \int_{-\infty}^{\infty} f(x) e^{i\omega x} dx \tag{9.1}$$

we first truncate the infinite integral to $(-L, L)$, taking L to be as large as computationally feasible. The assumption is that since $|f(x)| \to 0$ as $|x| \to \infty$, the integrand should be small in the part of the domain truncated away.

$$F(\omega) \approx \int_{-L}^{L} f(x) e^{i\omega x} dx. \tag{9.2}$$

If $F(\omega)$ is evaluated at discrete points:

$$\omega = \omega_n = \frac{2\pi n}{2L}, \quad n \text{ an integer}$$

then the integral in (2) is simply $2L$ times c_n, the Fourier coefficient:

$$F(\omega_n) \approx \int_{-L}^{L} f(x) e^{in\pi x/L} dx = 2Lc_n, \tag{9.3}$$

where

$$c_n = \frac{1}{2L} \int_{-L}^{L} f(x) e^{in\pi x/L} dx \tag{9.4}$$

is the Fourier coefficient for the Fourier series

$$f(x) = \sum_{n=-\infty}^{\infty} c_n e^{-in\pi x/L}, \quad -L < x < L \tag{9.5}$$

In practice this infinite sum is performed by truncating it to a finite sum of $2N$ terms:

$$f(x) \approx \sum_{n=-N}^{N-1} c_n e^{-in\pi x/L}, \quad -L < x < L. \tag{9.6}$$

The integral defining c_n can be evaluated by turning it into a Riemann sum:

$$\begin{aligned} F(\omega_n) = (2Lc_n) &= \int_{-L}^{L} f(x) e^{in\pi x/L} dx \\ &= \Delta x \sum_{j=-N}^{N-1} f(x_j) e^{in\pi x_j/L}. \end{aligned}$$

By choosing

$$x_j = j\Delta x, \quad \Delta x = \frac{2L}{2N},$$

we obtain:

$$F(\omega_n) \approx \frac{L}{N} \sum_{j=-N}^{N-1} f(x_j) e^{i\pi jn/N} = 2Lc_n \tag{9.7}$$

and

$$f(x_j) \approx \sum_{n=-N}^{N-1} c_n e^{-i\pi jn/N}, \tag{9.8}$$

with $x_j = j\frac{2L}{2N}$, $\omega_n = \frac{2\pi n}{2L}$.

To obtain $f(x)$ at a single location x_j requires $2N$ complex multiplications (not counting the additions, which take relatively little time). There are $2N$ such x locations. Therefore there is a total of $(2N)^2$ operations. By judiciously combining the terms in the sum, considerable reduction in the number of operations can be achieved.

9.3 Fast Fourier Transform (FFT)

The inverse Fourier transform can be evaluated numerically from the sum:

$$f(x_j) \approx \sum_{n=-N}^{N-1} c_n e^{-ij\pi n/N}$$

The evaluation of the sum on the right-hand side requires $2N$ complex multiplications. The number of such multiplications can be reduced by half by combining the positive and negative n's.

$$\begin{aligned} f(x_j) &\cong \sum_{n=0}^{N-1} c_n e^{-ij\pi n/N} + \sum_{n=0}^{N-1} c_{n-N} e^{-ij\pi(n-N)/N} \\ &= \sum_{n=0}^{N-1} \alpha_n e^{-ij\pi n/N}, \end{aligned}$$

where $\alpha_n = c_n + c_{n-N} e^{ij\pi N/N} = c_n + c_{n-N}(-1)^j$.

This last sum has only N terms and its evaluation requires only N (half the orginal $2N$) complex multiplications, not counting the multiplication by -1 and the additions.

The process can be continued if N is even, $N = 2N_1$:

$$\begin{aligned} f(x_j) &= \sum_{n=0}^{N_1-1} \alpha_n e^{-ij\pi n/N} + \sum_{n=0}^{N_1-1} \alpha_{n+N_1} e^{-ij\pi(n+N_1)/N} \\ &= \sum_{n=0}^{N_1-1} \beta_n e^{-ij\pi n/N}, \end{aligned}$$

where $\beta_n = \alpha_n + \alpha_{n+N_1}(-i)^j$.

The number of terms in the sum is now $N/2$, one-fourth the orignal $2N$. There is a one-time overhead of computing β_n from α_n.

For $2N$ being a power of 2, say, $2N = 2^p$, where p is a positive integer, this process can be repeated until there is only one term left in the sum. The number of operations is simply p overheads.

To obtain $2N$ values of $f(x)$ at $2N$ x_j points requires a total of

$$2Np = (2N)(\log_2 2N)$$

operations, a substantial reduction from $(2N)^2$. For example, if $2N = 1,024$ points, $(2N)^2 \sim 1$ million, while $(2N)\log_2(2N) = 10,240$, a factor of 100 reduction.

FFT routines are now widely available. Note that you do not need a separate routine for Fourier transforms and inverse Fourier transforms. The same routine can be used for either by changing the sign of n or j in (7) or (8).

9.4 Discrete Fourier Transform

Discrete Fourier transform and its inverse is an exact mathematical result, and should not be viewed as a numerical approximation of the continuous Fourier transform, which have been discussed in section 2. Its derivation starts with the following interesting identity:

For j, $n = 0, 1, 2, \ldots, N-1$,

$$\frac{1}{N}\sum_{k=0}^{N-1} e^{2\pi ik\frac{(j-n)}{N}} = \delta_{jn} \equiv \begin{cases} 0 & \text{if } j \neq n \\ 1 & \text{if } j = n. \end{cases} \tag{9.9}$$

Note first that for $j = k$, each term in the sum is 1. So the N-term sum of 1 is N. Thus $\frac{1}{N}\sum_{k=0}^{N-1}(1) = 1$. For $j \neq n$, let

$$z = e^{2\pi i\frac{j-n}{N}}.$$

It is seen that the sum is a geometric series of N terms. So

$$\sum_{k=0}^{N-1} z^k = \frac{1-z^N}{1-z} = 0$$

since $z^N = e^{2\pi i(j-n)} = 1$, and $z \neq 1$ if $j \neq n$. Thus (9) is proved.

Let $\{g_n\}$ be a sequence of numbers, e.g. $g_n = g(x_n)$. That is, it could be the value of a function evaluated at discrete points x_n. Since

$$\begin{aligned} g_n &= \sum_{j=0}^{N-1} g_j \delta_{jn} \\ &= \sum_{j=0}^{N-1} g_j \frac{1}{N} \sum_{k=0}^{N-1} e^{2\pi ik(j-n)/N} \\ &= \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} \left\{ \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} g_j e^{2\pi ijk/N} \right\} e^{-2\pi ink/N} \\ &= \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} G_k e^{-2\pi ink/N}, \end{aligned} \tag{9.10}$$

where we have defined

$$G_k = \mathcal{F}_N[x] \equiv \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} g_j e^{2\pi ijk/N} \tag{9.11}$$

to be the N-point discrete Fourier transform (DFT) of $\{g_j\}$.

Equation (19) then is the inverse DFT of $\{G_n\}$:

$$g_n = \mathcal{F}_N^{-1}[G] \equiv \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} G_k e^{-2\pi ink/N} \tag{9.12}$$

Note that this result is exact. There has been no assumptions. DFT's are not the numerical approximations of FT's, although they can be shown to be related (approximately).

9.5 Relation between FT and DFT

The Fourier transform of $f(x)$ is:

$$\begin{aligned} F(\omega) &= \sum_{-\infty}^{\infty} f(x)e^{i\omega x}dx, \quad -\infty < \omega < \infty \\ &\approx \int_{-L}^{L} f(x)e^{i\omega x}dx; \end{aligned}$$

The integral is truncated. L is chosen to be very large.

$$\begin{aligned} F(\omega) &\approx \int_0^L + \int_{-L}^0 f(x)e^{i\omega x}dx \\ &= \int_0^L + \int_L^{2L} f(x-2L)e^{i\omega(x'-2L)}dx. \end{aligned}$$

In the second integral we made the change in variable from x to $x' = x+2L$. The prime over x can be dropped later.

If we evaluate $F(\omega)$ at $\omega_k = \frac{2\pi k}{2L}$, k an integer, then $e^{i\omega 2L} = e^{i2\pi k} = 1$, and

$$\begin{aligned} F(\omega_k) &\cong \int_0^L + \int_L^{2L} f(x-2L)e^{i\omega_k x}dx \\ &= \int_0^{2L} g(x)e^{i\omega_k x}dx \end{aligned}$$

where we have defined a function $g(x)$ to be

$$g(x) = \begin{cases} 0 & \text{if } x < 0 \\ f(x) & \text{if } 0 \le x \le L \\ f(x-2L) & \text{if } L \le x \le 2L \\ 0 & \text{if } x > 2L. \end{cases}$$

The integral is next approximated by a Riemann sum of N terms:

$$\begin{aligned} \int_0^{2L} g(x) e^{i\omega_k x} dx &= \sum_{j=0}^{N-1} g(x_j) e^{i\omega_k x_j} \Delta x \\ &= \frac{L}{N} \sum_{j=0}^{N-1} g_j e^{i2\pi kj/N} = \frac{2L}{\sqrt{N}} G_k \end{aligned}$$

by choosing $\Delta x = \frac{2L}{N}$, $x_j = j\Delta x$, $j = 0, \ldots, N-1$. G_k is the DFT of g_j defined in (11). Therefore the FT of $f(x)$ is related to the DFT by

$$F(\omega_k) \cong \frac{2L}{\sqrt{N}} G_k, \quad \omega_k = \frac{2\pi k}{2L}.$$

$$G_k \equiv \frac{1}{\sqrt{N}} \sum_{j=0}^{N-1} g(x_j) e^{2\pi ijk/N} \tag{9.13}$$

To recover $g(x_j)$, we use the formula for the inverse DFT (12):

$$g(x_n) = \frac{1}{\sqrt{N}} \sum_{k=0}^{N-1} G_k e^{-2\pi ink/N} \tag{9.14}$$

Note that the N used in this section is twice the N used in the previous section.

9.6 Sampling Theorem

Often the inverse Fourier transform

$$f(x) = \frac{1}{2\pi} \int_{-\infty}^{\infty} F(\omega) e^{-i\omega x} d\omega, \quad -\infty < x < \infty$$

cannot be evaluated analytically and we need to resort to numerical means. The first step of the numerical procedure is to replace the infinite integral by a finite integral:

$$f(x) \cong \frac{1}{2\pi}\int_{-W}^{W} F(\omega)e^{-i\omega x}d\omega, \tag{9.15}$$

assuming that $F(\omega)$ is negligible for ω outside $[-W, W]$. Mathematicians like to deal with exact relationships and so they define a class of function $f(x)$ called "band-limited" functions whose Fourier transform $F(\omega) = 0$ for $\omega > W$ and $\omega < -W$. W is called the "band width" of $f(x)$. For such functions, the inverse Fourier transform can be written exactly as:

$$f(x) = \frac{1}{2\pi}\int_{-W}^{W} F(\omega)e^{-i\omega x}d\omega \tag{9.16}$$

Ignoring for the moment the definition of $F(\omega)$ as the Fourier transform of $f(x)$, we seek an alternative representation of $F(\omega)$ as a Fourier series for ω between $-W$ and W. (We wouldn't have been able to represent $F(\omega)$ in a Fourier series from $-\infty < \omega < \infty$):

$$F(\omega) = \sum_{n=-\infty}^{\infty} c_n e^{in\pi\omega/W}, \quad -W < \omega < W, \tag{9.17}$$

with

$$c_n = \frac{1}{2W}\int_{-W}^{W} F(\omega)e^{-i(n\pi/W)\omega}d\omega. \tag{9.18}$$

[Note that we switched the signs in front of the complex exponentials, which is allowable as long as we switch both signs]. Comparing (18) with (16), we see

$$c_n = \frac{\pi}{W} f\left(\frac{n\pi}{W}\right). \tag{9.19}$$

This yields, from (17):

$$F(\omega) = \sum_{n=-\infty}^{\infty} \frac{\pi}{W} f\left(\frac{n\pi}{W}\right) e^{i(n\pi/W)\omega}. \tag{9.20}$$

(20) says that the Fourier transform of a "band-limited" function $f(x)$ can be constructed by sampling $f(x)$ over only a set of discrete points $x_n = \frac{n\pi}{W}$, $n = 0, \pm 1, \pm 2, \ldots$ in the x domain.

Substituting (20) into the inverse Fourier transform (16), we get

$$f(x) = \frac{1}{2W} \sum_{n=-\infty}^{\infty} f(x_n) \int_{-W}^{W} e^{ix_n\omega} e^{-ix\omega} d\omega$$

The integral can be evaluated:

$$\frac{1}{2W} \int_{-W}^{W} e^{i(x_n - x)\omega} d\omega = \frac{\sin(Wx - n\pi)}{Wx - n\pi}.$$

Finally

$$f(x) = \sum_{n=-\infty}^{\infty} f(x_n) \frac{\sin(Wx - n\pi)}{Wx - n\pi}, \tag{9.21}$$

where $x_n = \frac{n\pi}{W}$, $n = 0, \pm 1, \pm 2, \ldots$.

Equation (21) is quite interesting: it says that we can reconstruct the original function $f(x)$ in continuous variable $-\infty < x < \infty$ by "sampling" $f(x)$ only at discrete points x_n. This is possible of course only for band-limited functions; there is no useful information between gridpoints: $x_{n-1} - x_n = \frac{\pi}{W}$, if there is no oscillation with frequency higher than W.

9.6.1 Sampling Theorem

If $f(x)$ is band-limited with band width W, then for all x, $f(x)$ can be constructed completely from its sample values $f(\frac{n\pi}{W})$, $n = 0, \pm 1, \pm 2, \ldots$ as

$$f(x) = \sum_{n=-\infty}^{\infty} f(\frac{n\pi}{W}) \frac{\sin(Wx - n\pi)}{(Wx - n\pi)}.$$

Chapter 10

Some Special Functions

10.1 Introduction

In the next few chapters we will study partial differential equations in multi-dimensions. Instead of sines and cosines we encountered in one dimensions (and also in multi-dimensions in Cartesian geometry), we will often run into special functions, such as the Bessel function (in cylindrical coordinates), Legendre function and spherical harmonics (in spherical geometry). These special functions will be introduced here. We will make extensive use of the method of Frobenius.

10.2 Legendre differential equation

Legendre equation arises in polar coordinates, where $x = \cos\theta$:

$$\frac{d}{dx}[(1-x^2)\frac{d}{dx}y] + \mu y = 0 \tag{10.1}$$

This equation has singularities at $x = \pm 1$. We seek a series solution about $x = 0$, which is an ordinary point (not singular), and so the solution can be written in the form:

$$y(x) = \sum_{n=0}^{\infty} a_n x^n. \tag{10.2}$$

Differentiating:

$$\begin{aligned} y'(x) &= \sum n a_n x^{n-1} \\ y''(x) &= \sum n(n-1) a_n x^{n-1}. \end{aligned}$$

Substituting these series into (1) yields

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

Making the substitution $m = n-2$ in the first sum and $m = n$ in the other terms:

$$\sum_{m=-2}^{\infty} (m+2)(m+1)a_{m+2}x^m - \sum_{m=0}^{\infty} m(m-1)a_m x^m - 2\sum_{m=0}^{\infty} m a_m x^m + \mu \sum_{m=0}^{\infty} a_m x^m = 0$$

which is

$$\sum_{m=0}^{\infty} \{(m+2)(m+1)a_{m+2} - (m(m+1)-\mu)a_m\}x^m = 0. \tag{10.3}$$

Since (10.3) is to hold for all x in certain domain, the terms in $\{\quad\}$ must add up to zero. Thus

$$a_{m+2} = \frac{m(m+1)-\mu}{(m+2)(m+1)} a_m, \quad m = 0, 1, 2, 3\ldots \tag{10.4}$$

(10.4) is a second-order recurrent relationship. The coefficients a_m for m even will all be proportional to a_0:

$$a_2 = \frac{-\mu}{2}a_0, \quad a_4 = \frac{2\cdot 3-\mu}{4.3}a_2 = \frac{-(2\cdot 3-\mu)\mu}{4!}a_0$$

$$\ldots.$$

$$a_{2j} = \frac{-\mu(2\cdot 3-\mu)(4\cdot 5-\mu)\ldots((2j-2)(2j-1)-\mu)}{(2j)!}a_0$$

And the coefficients a_m for m odd will all be proportional to a_1:

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

$$\ldots.$$

$$a_{2j+1} = \frac{(1\cdot 2-\mu)(3\cdot 4-\mu)\ldots((2j-1)(2j)-\mu)}{(2j+1)!}a_1$$

The general solution is

$$y(x) = a_0\sum_{j=0}^{\infty}(a_{2j}/a_0)x^{2j} + a_1\sum_{j=0}^{\infty}(a_{2j+1}/a_1)x^{2j+1}$$

Both solutions converge at $x = 0$ and in its neighborhood as long as $|x| < 1$. This can be shown using the ratio test. For convergence, we must have

$$\lim_{m\to\infty}\left|\frac{a_{m+2}x^{m+2}}{a_m x^m}\right| < 1,$$

but from (10.4)

$$\lim_{m\to\infty}|a_{m+2}/a_m| = 1.$$

Therefore both series converge for $|x| < 1$. That the series diverges at $x = \pm 1$ is not surprising in view of the presence of a singularity there.

Notice however, that the series converge for any value of x if they terminate. This happens for one of the series when μ is equal to the product of two consecutive integers:

$$\mu = n(n+1), \quad n = \text{ integer}.$$

This fact can be used to find the following *eigenvalue* problem: Find the eigenvalue μ and the eigenfunction $y(x)$ such that

$$\frac{d}{dx}[(1-x^2)\frac{d}{dx}y] + \mu y = 0, \qquad -1 \leq x \leq 1$$

subject to the boundary condition:

$$y(x) \text{ bounded at } x = -1 \text{ and } x = 1. \tag{10.5}$$

[Later on we will show that $x = \pm 1$ corresponds to the north and south poles; and we don't want our solution to blow up there (or anywhere else).]

We construct the eigenfunction

$$y(x) = P_n(x)$$

corresponding to the eigenvalue

$$\mu = +n(n+1)$$

in the following way.

For $n = 0$, $\mu = 0$, the even series terminates after one term. We set $a_0 = 1$ and $a_1 = 0$ to get

$$P_0(x) = 1$$

For $n = 1$, $\mu = 2$, the odd series terminates after one term. We set $a_0 = 0$ and $a_1 = 1$ to get

$$P_1(x) = x$$

For $n = 2$, $\mu = 6$, we set $a_1 = 0$ and $a_0 = -\frac{1}{2}$:

$$P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}$$

For $n = 3$, $\mu = 12$, we set $a_0 = 0$, $a_1 = -\frac{3}{2}$:

$$P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x.$$

For general integer n:

$$P_n(x) = \sum_{k=0}^{[n/2]} (-1)^k \frac{(2n-2k)!}{2^n k!(n-k)!(n-2k)!} x^{n-2k}, \quad [n/2] \text{ greatest integer } \leq n/2$$

These solutions are known as the Legendre polynomials. The solution to (10.5) can simply be written as

$$y(x) = P_n(x), \quad \mu = n(n+1), \quad n = 0, 1, 2, 3, \ldots \tag{10.6}$$

The overall constant is chosen so that the eigenfunction is equal to 1 at $x = 1$, the north pole. The solution can be multiplied by any arbitrary constant.

There is a useful formula, called Rodrigue's Formula, which allows us to generate all P_n's simply:

$$P_n(x) = \frac{1}{2^n n!} \frac{d^n}{dx^n} (x^2 - 1)^n. \tag{10.7}$$

One can show by differentiation that (10.7) satisfies

$$\frac{d}{dx}[(1-x^2)\frac{d}{dx}P_n] + n(n+1)P_n = 0,$$

and that it is a polynomial of degree n. Therefore the function defined in (10.7) must be the same (within an overall constant) of the required eigenfunction defined in (10.6). It can be shown that both function has the normalization such that $P_n(1) = 1$. Thus (10.6) and (10.7) must be the same.

The Legendre polynomials are orthogonal to each other, i.e.:

$$\int_{-1}^{1} P_m(x)P_n(x)dx = \begin{cases} 0 & \text{if } m \neq n \\ \frac{2}{2n+1} & \text{if } m = n \end{cases} \tag{10.8}$$

Proof: [see later for an easier proof using Sturm-Liouville theory.]

To show the first part for $m \neq n$, we assume, without loss of generality, $m < n$. Let $f(x)$ be any function with at least n continuous derivatives in $-1 \leq x \leq 1$. Consider the integral

$$I \equiv \int_{-1}^{1} f(x) P_n(x) dx$$

Using Rodrigue's Formula:

$$I = \frac{1}{2^n n!} \int_{-1}^{1} f(x) \frac{d^n}{dx^n} (x^2-1)^n dx,$$

and an integration by parts, we find

$$I = \frac{1}{2^n n!} [f(x) \frac{d^{n-1}}{dx^{n-1}} (x^2-1)^n]_{-1}^{1} - \frac{1}{2^n n!} \int_{-1}^{1} f'(x) \frac{d^{n-1}}{dx^{n-1}} (x^2-1)^n dx$$

The boundary terms vanish, because after $(n-1)$ derivatives, there is still a (x^2-1) term left over undifferentiated. That term vanishes at $x = \pm 1$.

This integration by parts can be continued to give in the end:

$$I = \frac{(-1)^n}{2^n n!} \int_{-1}^{1} f^{(n)}(x) (x^2-1)^n dx.$$

If $f(x) = P_m(x)$, $m < n$, which is a polynomial of degree less than n, then its nth derivative, $f^{(n)}(x)$, must vanish. Thus $I = 0$ for $m < n$, (and also for $m > n$, by interchanging m and n in the above proof).

For $m = n$, $f(x) = P_n(x)$, we have, since

$$P_n^{(n)}(x) = (2n)!/2^n n!,$$

$$I = \frac{(2n)!}{2^{2n}(n!)^2} \int_{-1}^{1} (1-x^2)^n dx$$

This integral can be evaluated with a change of variable $x = \sin\theta$ and repeated integration of $\cos^{2n+1}\theta$:

$$\int_{-1}^{1} (1-x^2)^n dx = 2\int_{0}^{1} (1-x^2)^n dx = \int_{0}^{\pi/2} \cos^{2n+1}\theta d\theta = \frac{2^{2n+1}(n!)^2}{(2n)!(2n+1)}$$

Thus $I = \frac{2}{2n+1}$ when $m = n$.

10.3 Associated Legendre differential equation

The associated Legendre differential equation is

$$\frac{d}{dx}[(1-x^2)\frac{d}{dx}y] + [\mu - \frac{m^2}{1-x^2}]y = 0, \quad -1 \le x \le 1. \tag{10.9}$$

The case of $m = 0$ reduces to the Legendre differential equation. For physical reasons (to be discussed in the next chapter) we are interested only in the case where m is an integer

$$m = 0, \quad \pm 1, \quad \pm 2, \quad \pm 3, \ldots$$

Since the equation has a singular point at $x = \pm 1$, the general solution is probably not bounded at the boundaries $x = \pm 1$ of the domain in (10.9). The eigenvalue problem is to find μ such that the eigenfunctions $y(x)$ is bounded at $x = \pm 1$. The procedure for solving this eigenvalues problem is quite similar to that for the Legendre differential equation. The eigenvalue is found to be

$$\mu = n(n+1), \quad n = 0, 1, 2, 3, \ldots \tag{10.10}$$

and the eigenfunction is the associated Legendre functions:

$$y(x) = P_n^m(x). \tag{10.11}$$

They are related to the Legendre polynomials by, for $m \ge 0$:

$$P_n^m(x) = (x^2-1)^{m/2}\frac{d^m}{dx^m}P_n(x), \quad m \le n. \tag{10.12}$$

$$P_n^m(x) \equiv 0 \qquad \text{for } m > n$$

because $P_n(x)$ is a polynomial of degree n, and its mth derivative vanishes if $m > n$. (10.12) is also called Rodrigue's Formula. We will prove it in a moment.

The definition of $P_n^m(x)$ is extended to negative m's by this formula:

$$P_n^m(x) = (-1)^m \frac{(n+m)!}{(n-m)!} P_n^{-m}(x), \tag{10.13}$$

so that $P_n^m(x)$ is simply a scalar multiple of $P_n^{-m}(x)$.

For each n ($n = 0, 1, 2, 3, \ldots$) we have $2n+1$ associated Legendre functions $P_n^m(x)$, where m runs from $-n$ to n.

The first few of $P_n^m(x)$ are, with $x = \cos\theta$

$$P_1^1 = \sin\theta, \quad P_2^1 = \frac{3}{2}\sin 2\theta, \quad P_3^1 = \frac{3}{8}(\sin\theta + 5\sin 3\theta)$$
$$P_1^2 = 0, \quad P_2^2 = \frac{3}{2}(1-\cos 2\theta), \quad P_3^2 = \frac{15}{4}(\cos\theta - \cos 3\theta)$$

The associated Legendre functions are also orthogonal to each other:

$$\int_{-1}^{1} P_k^m(x)P_n^m(x)dx = \begin{cases} 0 & \text{if } k \neq n \\ \frac{2}{(2n+1)}\frac{(n+m)!}{(n-m)!} & \text{if } k = n. \end{cases} \tag{10.14}$$

10.4 Proof of Rodrigue's Formula

First we show that

$$P_n^m(x) = (-1)^m(1-x^2)^{m/2}\frac{d^m P_n(x)}{dx^m}$$

satisfies the associated Legendre differential equation

$$(1-x^2)y'' - 2xy' + [n(n+1) - \frac{m^2}{1-x^2}]y = 0, \quad -1 < x < 1.$$

It suffices to consider $m > 0$. We will start with the equation satisfied by $P_n^0 = P_n(x)$:

$$(1-x^2)P_n^{(2)} - 2xP_n^{(1)} + [n(n+1)]P_n = 0$$

and differentiate it m times to get (trust me!).

$$(1-x^2)P_n^{(m+2)} - 2(m+1)xP_n^{(m+1)} + (n-m)(n+m+1)P_n^{(m)} = 0,$$

where $P_n^{(m)} \equiv \frac{d^m}{dx^m}P_n(x)$. [If you don't believe me, you can prove this by induction. First show that it is true for $m = 1$, by simply differentiating the equation for P_n once to get

$$(1-x^2)P_n^{(3)} - 2\cdot 2\cdot xP_n^{(2)} + (n-1)(n+1+1)P_n^{(1)} = 0$$

Now assume that it is true for m, and show that it is also true for $m+1$. This is done by differentiating the equation for $P_n^{(m)}$ once, to yield

$$(1-x^2)P_n^{(m+3)} - 2(m+2)xP_n^{(m+2)} + (n-m-1)(n+m+2)P_n^{(m+1)} = 0$$

This is the same equation as that for $P_n^{(m+1)}$. So the result is proved.]

Therefore

$$w(x) \equiv P_n^{(m)}(x)$$

satisfies

$$(1-x^2)w'' - 2(m+1)xw' + (n-m)(n+m+1)w = 0$$

Now let

$$y = (-1)^m(1-x^2)^{m/2}w$$

(the $(-1)^m$ factor is immaterial).

Substituting

$$w = (-1)^m(1-x^2)^{-m/2}y(x)$$

into the w equation above shows that $y(x)$ satisfies the associated Legendre equation:

$$(1-x^2)y'' - 2xy' + [n(n+1) - \frac{m^2}{1-x^2}]y = 0.$$

Therefore the solution is

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

For $m > 0$, $y(x) = 0$ at $x = \pm 1$, and so are bounded there. Also, since $\frac{d^m}{dx^m}P_n(x)$ is the mth derivative of an nth order polynomial, it is also a polynomial (and therefore are bounded in $-1 \leq x \leq 1$).

For $m < 0$, $P_n^m(x)$ is not defined through the Rodrigues' Formula because $\frac{d^m}{dx^m}$ is not defined. $P_n^m(x)$ is then defined as a scalar multiple of $P_n^{-m}(x)$, which also satisfies the associated Legendre equation for negative m.

For m even, $P_n^m(x)$ is a polynomial. For m odd P_n^m is not a polynomial because of the factor $(1-x^2)^{m/2}$. $P_n^m(x)$ is even if $n+m$ is even and odd if $n+m$ is odd.

10.5 Bessel's differential equation

Bessel equation is one of the important special functions. It arises most commonly from separation of variables in cylindrical coordinates, and also in spherical coordinates, in the radial coordinate r:

$$r^2\frac{d^2R}{dr^2} + r\frac{d}{dr}R + (\lambda^2 r^2 - p^2)R = 0 \tag{10.15}$$

It can be put into a standard form by letting

$$R(r) = y(x), \quad x \equiv \lambda r.$$

Then,

$$x^2 \frac{d^2}{dx^2} y + x \frac{d}{dx} y + (x^2 - p^2) y = 0 \tag{10.16}$$

This is called Bessel equation of oder p. In cylindrical coordinates, p is usually an integer m, $m = 0, \pm 1, \pm 2, \ldots$. In spherical coordinates, p is usually a half integer, $p = n + \frac{1}{2}$, $n = 0, 1, 2, \ldots$.

The origin $x = 0$ is a regular singular point of the Bessel equation. A test with

$$y(x) \sim x^s$$

yields the indicial equation

$$s(s-1) + s - p^2 = 0$$

Thus the two indices are

$$s_1 = p \quad \text{and} \quad s_2 = -p.$$

In the application we will be dealing with, s_1 and s_2 differ by an integer. Frobenius method tells us that we will have one series solution, and another solution which blows up at $x = 0$.

The two solutions are denoted by $J_p(x)$ and $Y_p(x)$ and are called Bessel function of the first kind and the second kind, respectively. Near $x = 0$, they behave like, for $p = m$, an integer

$$J_m(x) \sim \frac{1}{2^m m!} x^m$$

$$Y_m(x) \sim \begin{cases} -2^m \frac{(m-1)!}{\pi} x^{-m}, & m > 0 \\ \frac{2}{\pi} \ell n x, & m = 0 \end{cases}$$

The general solution to (10.15) is, for $p = m$

$$R(r) = c_1 J_m(\lambda r) + c_2 Y_m(\lambda r).$$

Boundedness at $r = 0$ implies $c_2 = 0$. Thus (with $c_1 = 1$)

$$R(r) = J_m(\lambda r)$$

The boundary condition at $r = a$ is:

$$0 = R(a) = J_m(\lambda a)$$

Let z_{mn} be the nth zero of $J_m(x)$. The eigenvalue λ is then determined as

$$\lambda = \lambda_{mn} = \frac{z_{mn}}{a}$$

The values of the zeros of $J_m(x)$ (i.e. $J_m(z_{mn}) = 0$) are tabulated.

10.5.1 Frobenius solution to the Bessel equation

$$x^2y''(x) + xy'(x) + (x^2 - p^2)y(x) = 0$$

Let's consider the series solution corresponding to the index $s_1 = p$:

$$\begin{aligned} y(x) &= x^p \sum_{n=0}^{\infty} a_n x^n = \sum_{n=0}^{\infty} a_n x^{n+p} \\ y'(x) &= \sum (n+p) a_n x^{n+p-1} \\ y''(x) &= \sum (n+p-1)(n+p) a_n x^{n+p-2}. \end{aligned}$$

Substituting these into the Bessel equation implies

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

We change the dummy index in the second sum to $n + 2 = m$

$$\sum_{n=0}^{\infty} a_n x^{n+p+2} = \sum_{m=2}^{\infty} a_{m-2} x^{m+p} = \sum_{n=2}^{\infty} a_{n-2} x^{n+p}.$$

So the equation becomes

$$\sum_{n=2}^{\infty} \{[(n+p)^2 - p^2] a_n + a_{n-2}\} x^{n+p} + 0 \cdot a_0 + (2p+1) a_1 x^{1+p} = 0$$

Therefore we have, by equating the coefficient of each power of x to zero:

$$a_0 = \text{arbitrary}, \quad a_1 = 0$$

and

$$a_n = -\frac{a_{n-2}}{n(2p+n)}, \quad n = 2, 3, 4, \ldots.$$

All $a_n = 0$ for n odd.

$$\begin{aligned} a_2 &= -\frac{a_0}{2(2p+2)} \\ a_4 &= -\frac{a_2}{4(2p+4)} = \frac{a_0}{2 \cdot 4(2p+2)(2p+4)} \\ a_6 &= -\frac{a_4}{6(2p+6)} = -\frac{a_0}{2 \cdot 4 \cdot 6(2p+2)(2p+4)(2p+6)}, \end{aligned}$$

$$\begin{aligned}
y(x) &= a_0 x^p [1 - \frac{x^2}{2^2(p+1)} + \frac{x^4}{2^4 2!(p+1)(p+2)} \\
&\quad - \frac{x^6}{2^6 3!(p+1)(p+2)(p+3)} + \ldots] \\
&= a_0 x^p \sum_{n=0}^{\infty} (-1)^n \frac{x^{2n}}{2^{2n} n!(p+1)\ldots(p+n)}
\end{aligned}$$

The Bessel function of the first kind of order p, denoted by $J_p(x)$, is defined with $a_0 = \frac{1}{2^p \Gamma(p+1)}$

$$J_p(x) = \sum_{n=0}^{\infty} \frac{(-1)^n (x/2)^{2n+p}}{n!\Gamma(p+1+n)},$$

where the gamma function is defined by: $\Gamma(z+1) = z\Gamma(z)$, and so $\Gamma(1+p) \cdot [(1+p)(2+p)\ldots(n+p)] = \Gamma(2+p) \cdot [(2+p)\ldots(n+p)] = \Gamma(3+p) \cdot [(3+p)\ldots(n+p)] = \ldots = \Gamma(n+p+1)$. For $p = m$, a positive integer, $\Gamma(m+1+n) = (n+m)!$. For $p = -m$, a negative integer, $1/\Gamma(n+1-m) = 0$, for $n > m$.

10.5.2 Some identities

The Bessel function $J_p(x)$ is defined for any real number p by

$$\boxed{J_p(x) = \sum_{n=0}^{\infty} (-1)^n \frac{(x/2)^{2n+p}}{n!\Gamma(p+1+n)}}.$$

Some useful identities follow from this definition:

$$\begin{aligned}
\frac{d}{dx}[x^p J_p(x)] &= \frac{d}{dx} \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+2p}}{2^{2n+p} n!\Gamma(p+1+n)} \\
&= \sum_{n=0}^{\infty} \frac{(-1)^n x^{2n+2p-1}}{2^{2n+p-1} n!\Gamma(p+n)} \\
&= x^p \sum_{n=0}^{\infty} \frac{(-1)^n (x/2)^{2n+p-1}}{n!\Gamma(p+n)} \\
&= x^p J_{p-1}(x).
\end{aligned}$$

Therefore we have the identity:

$$\boxed{\frac{d}{dx}[x^p J_p(x)] = x^p J_{p-1}(x)}$$

Similarly, we can show that

$$\boxed{\frac{d}{dx}[x^{-p}J_p(x)] = -x^{-p}J_{p+1}(x)}$$

Combining the last two formula, we have

$$2\frac{d}{dx}J_p(x) = J_{p-1}(x) - J_{p+1}(x).$$

10.5.3 Linear independence

If p is not an integer, a second independent solution to the Bessel's equation is given by

$$J_{-p}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n (x/2)^{2n-p}}{n!\Gamma(-p+1+n)}.$$

When $p = m$ an integer, howeover, $J_m(x)$ and $J_{-m}(x)$ cease to be linearly independent because it can be shown that

$$J_{-m}(x) = (-1)^m J_m(x), \quad m \text{ integer} \geq 0.$$

To show this, we start with

$$J_{-m}(x) = \sum_{n=0}^{\infty} \frac{(-1)^n (x/2)^{2n-m}}{n!\Gamma(n-m+1)}$$

and note that for the factorial $1/\Gamma(n-m+1) = 0$ if $n < m$. $\Gamma(n-m+1) = (n-m)!$ for $n > m$. Thus

$$J_{-m}(x) = \sum_{n=m}^{\infty} \frac{(-1)^n (x/2)^{2n-m}}{n!(n-m)!}$$

Let $k = n - m$,

$$\begin{aligned} J_{-m}(x) &= \sum_{k=0}^{\infty} \frac{(-1)^{k+m} (x/2)^{2k+m}}{(k+m)!k!} = (-1)^m \sum_{n=0}^{\infty} \frac{(-1)^n (x/2)^{2n+m}}{n!(n+m)!} \\ &= (-1)^m J_m(x). \end{aligned}$$

Since $J_m(x)$ and $J_{-m}(x)$ are not linearly independent, the general solution of the Bessel's equation should be

$$y(x) = AJ_p(x) + BJ_{-p}(x) \text{ if } p \text{ is not an integer}$$

but

$$y(x) = AJ_p(x) + B(Y_m(x) \text{ if } p = m \text{ an integer}$$

10.5.4 Generating function

We multiply $J_m(z)$ by t^m for another variable t, and form the following infinite series:

$$\sum_{m=-\infty}^{\infty} J_m(z)t^m \equiv \varphi(z,t)$$

We called this series $\varphi(z,t)$ above. We note that $\varphi(0,t)=1$. Assuming that this series converges, we can differentiate it

$$\begin{aligned}\frac{\partial}{\partial z}\varphi(z,t) &= \sum_{m=-\infty}^{\infty} J'_m(z)t^m \\ &= \sum_{m=-\infty}^{\infty} \frac{1}{2}(J_{m-1}(z) - J_{m+1}(z_1)t^m,\end{aligned}$$

using the formula derived in 10.5.2 for the derivative.

We can rewrite the series by letting $n=m-1$ in the first and $n=m+1$ in the second, to yield

$$\frac{\partial}{\partial z}\varphi(z,t) = \sum_{n=-\infty}^{\infty} \frac{1}{2}(t-\frac{1}{t})J_n(z)t^n.$$

So the function $\varphi(z,t)$ satisfies the ordinary differential equation

$$\frac{\partial}{\partial z}\varphi(z,t) = \frac{1}{2}(t-\frac{1}{t})\varphi(z,t).$$

Treating t as a "constant" as far as the z-derivative is concerned, we find the solution to this first order ordinary differential equation as an exponential:

$$\varphi(z,t) = f(t)e^{\frac{1}{2}(t-1/t)z},$$

where $f(t)$ is an arbitrary "constant". Setting $z=0$ we see that $f(t)=1$.

Finally we obtained the so-called generating function for Bessel functions:

$$e^{\frac{1}{2}z(t-\frac{1}{t})} = \sum_{n=-\infty}^{\infty} J_n(z)t^n$$

Some useful forms can also be derived. We let $t=e^{i\theta}$, $-\pi \le \theta \le \pi$:

$$e^{z(e^{i\theta}-e^{-i\theta})/2} = \sum_{n=-\infty}^{\infty} J_n(z)e^{in\theta}$$

Therefore

$$e^{iz\sin\theta} = \sum_{n=-\infty}^{\infty} J_n(z)e^{in\theta}, \quad -\pi \le \theta \le \theta$$

which is in the form of a Fourier series. So $J_n(z)$ must be the Fourier series coefficient c_n of the function $e^{iz\sin\theta}$

$$\begin{aligned} J_n(z) = c_n &= \frac{1}{2\pi}\int_{-\pi}^{\pi} e^{iz\sin\theta}e^{-in\theta}d\theta \\ &= \frac{1}{2\pi}\left[\int_0^{\pi} + \int_{-\pi}^{0}\right] \\ &= \frac{1}{2\pi}\int_0^{\pi}[e^{-i(n\theta - z\sin\theta)} + e^{i(n\theta - z\sin\theta)}]d\theta \end{aligned}$$

after making the switch of θ to $-\theta$ in the second integral. Finally,

$$\boxed{J_n(z) = \frac{1}{\pi}\int_0^{\pi} \cos(n\theta - z\sin\theta)d\theta,}$$

which is called Bessel's integral.

An immediate consequence of this formula is that

$$|J_n(x)| \le 1 \text{ for all real } x$$

10.5.5 Qualitative properties of Bessel functions

We have enough information now to derive some asymptotic results for the Bessel functions. For large x, $J_m(x)$ and $Ym(x)$ are like cosines and sines, except with a decaying amplitude (we will show in a moment):

$$\begin{aligned} J_m(x) &\sim \sqrt{\frac{2}{\pi x}}\cos(x - \frac{\pi}{4} - m\pi/2) \\ Y_m(x) &\sim \sqrt{\frac{2}{\pi x}}\sin(x - \frac{\pi}{4} - m\pi/2), \quad \text{for } |x| \gg 1 \end{aligned}$$

From this expression, we know that the kth zero of $J_m(x)$ is, approximately

$$z_{mk} \cong m\pi/2 - \pi/4 + k\pi.$$

For small x, we know already (from the Frobenius solution)

$$\begin{aligned}
&J_0(x) \cong 1, \quad Y_0(x) \cong \frac{2}{\pi}\ell n x \\
&J_1(x) \cong \frac{1}{2}x, \quad Y_1(x) \cong -\frac{2}{\pi}x^{-1} \\
&J_2(x) \cong \frac{1}{8}x^2, \quad Y_2(x) \cong -\frac{\pi}{4}x^{-2}, \qquad \text{for } |x| \ll 1
\end{aligned}$$

These are sufficient for us to obtain a sketch of these functions.

Method of stationary phase

To obtain the asymptotic behavior of the Bessel functions for large values of x, we start with the integral representation of $J_m(x)$:

$$J_m(x) = \frac{1}{\pi}\int_0^\pi \cos\phi(\theta)d\theta,$$

where $\phi(\theta) \equiv x\sin\theta - m\theta$ is the phase of the oscillation in the integrand. When x is large, the oscillation is rapid, with positive and negative values of $\cos\phi$ cancels themselves out when integrated. The only place where there is no cancellation is where $\phi(\theta)$ does not vary with θ. This occurs at *stationary phase* points, θ_0, given by

$$\phi'(\theta_0) = x\cos\theta_0 - m = 0.$$

This is

$$\cos\theta_0 = m/x \cong 0, \quad \text{for large } x.$$

Therefore

$$\theta_0 \cong \pi/2, \quad \phi(\theta_0) = x - m\pi/2$$

since we are only interested in values of θ_0 inside $0 < \theta < \pi$ of the integral. In the neighborhood of this point, $\phi(\theta)$ can be approximated in a Taylor series by:

$$\phi(\theta) \cong \phi(\theta_0) + \frac{1}{2}\phi''(\theta_0)(\theta - \theta_0)^2,$$

where

$$\phi''(\theta_0) = -x\sin\theta_0 \cong -x$$

The integral is approximated by

$$\begin{aligned}
J_m(x) &\cong \frac{1}{\pi}\int_0^\pi \cos(\phi(\theta_0) + \frac{1}{2}\phi''(\theta_0)(\theta-\theta_0)^2)d\theta \\
&\cong \frac{1}{\pi}\int_{-\infty}^\infty \cos(\phi(\theta_0) + \frac{1}{2}\phi''(\theta_0)(\theta-\theta_0)^2)d\theta
\end{aligned}$$

Since the integrand does not contribute much to the integral for θ away from $\theta_0 \cong \pi/2$, we are making only a small error by extending the integral to $\pm\infty$. This latter integral can be performed exactly, since from table of integrals:

$$\int_0^\infty \sin ax^2 dx = \int_0^\infty \cos ax^2 dx = \frac{1}{2}\sqrt{\frac{\pi}{2|a|}}, \quad a > 0.$$

$$\begin{aligned}
J_m(x) &\cong \frac{1}{\pi}\int_{-\infty}^{\infty} \cos(\phi(\theta_0) + \frac{1}{2}\phi''(\theta_0)\theta^2)d\theta \\
&= \frac{2}{\pi}\int_0^\infty \cos(\phi(\theta_0) + \frac{1}{2}\phi''(\theta_0)\theta^2)d\theta \\
&= \frac{2}{\pi}\int_0^\infty \cos(\phi(\theta_0))\cos(\frac{1}{2}|\phi''(\theta_0)|\theta^2)d\theta \\
&\quad + \frac{2}{\pi}\int_0^\infty \sin(\phi(\theta_0))\sin(\frac{1}{2}|\phi''(\theta_0)|\theta^2)d\theta \\
&= \sqrt{\frac{1}{|\phi''(\theta_0)|\pi}}[\cos(\phi(\theta_0)) + \sin(\phi(\theta_0))] \\
&= \sqrt{\frac{2}{\pi|\phi''(\theta_0)|}}\cos[\phi(\theta_0) - \frac{\pi}{4}] \\
&= \sqrt{\frac{2}{\pi x}}\cos(x - m\pi/2 - \pi/4).
\end{aligned}$$

Chapter 11

The Helmholtz equation in three dimensions

11.1 Introduction

Many classical equations arising from physical contexts contain the Laplacian operator

$$\nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}.$$

Some examples are:

The wave equation:

$$\frac{\partial^2}{\partial t^2} u = c^2 \nabla^2 u.$$

The Laplace equation:

$$\nabla^2 u = 0$$

The Schrödinger equation in quantum mechanics also involves this operator for the space derivatives:

$$i\hbar \frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2\mu}\nabla^2 \psi.$$

In previous chapters, we considered the one-dimensional problems, for which $\nabla^2 = \frac{\partial^2}{\partial x^2}$. Here we shall treat the problem in higher dimensions. Separating out the time dependence will result in the Helmoltz's eigenvalue problem for all the cases listed above. This problem is to solve:

$$\nabla^2 u = -\lambda^2 u \tag{11.1}$$

subject to appropriate homogeneous boundary conditions, and determine the eigenvalue λ^2 in the process. Laplace's equation is simply (11.1) with $\lambda^2 = 0$. It has the trivial solution unless the boundary conditions are non-homogeneous.

11.2 An example: An electron in a box

Consider the case of an electron of mass μ contained in a cubic box with infinite potentials on all sides. This situation is described by the Schrödinger's equation

$$\begin{aligned}
\text{PDE:} \quad & i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2\mu}\nabla^2\psi, && 0 < x < L \\
& && 0 < y < L \\
& && 0 < z < L \\
\text{BC:} \quad & \psi = 0 \text{ at } x = 0 \text{ and } x = L \\
& \psi = 0 \text{ at } y = 0 \text{ and } y = L \\
& \psi = 0 \text{ at } z = 0 \text{ and } z = L.
\end{aligned}$$

Separation of variables involves first assuming

$$\psi(x, y, z, t) = T(t)u(x, y, z).$$

This results:

$$\frac{i\hbar T'(t)}{T(t)} = -\frac{\hbar^2}{2\mu}\frac{\nabla^2 u}{u} = \text{const} \equiv E \tag{11.2}$$

From the solution of the $T(t)$ equation:

$$\frac{i\hbar T'(t)}{T(t)} = E,$$

$$T(t) = T(0)e^{-i(E/\hbar)t},$$

the separation constant E is interpreted as the energy of the electron (since $E/\hbar$ is the frequency and frequency times $\hbar$ is the energy in quantum mechanics).

From (11.2), the space dependence of ψ satisfies the Helmoltz equation:

$$\nabla^2 u = -\lambda^2 u, \qquad \nabla^2 = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}$$

where $\lambda^2 \equiv 2\mu E/\hbar^2$. By determing the eigenvalue λ^2 in the solution process we will be able to determine the energy of the electron. It will turn out to be quantized.

Further separation of variables:

$$u(x,y,z) = X(x)Y(y)Z(y)$$

leads to

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} = -\lambda^2.$$

We can argue that since

$$\frac{X''(x)}{X(x)} = -\frac{Y''(y)}{Y(y)} - \frac{Z''(z)}{Z(z)} - \lambda^2, \tag{11.3}$$

the left-hand side, which is a function of x only, can equal to the right-hand side, which is not a function of x, only if each side is equal to a constant. Setting that separation constant to $-a^2$, we will have, from (11.2)

$$\frac{X''(x)}{X(x)} = -a^2 \tag{11.4}$$

and

$$-\frac{Y''(y)}{Y(y)} - \frac{Z''(z)}{Z(z)} - \lambda^2 = -a^2 \tag{11.5}$$

Equation (11.4) is to be solved subject to the boundary condition

$$X(0) = 0, \quad X(L) = 0.$$

This yields

$$X(x) = X_n(x) \equiv \sin\frac{n\pi x}{L},$$

$$a = a_n \equiv \frac{n\pi}{L}, \quad n = 1, 2, 3, \ldots.$$

Equation (11.5) can similarly be re-arranged to

$$\frac{Y''(y)}{Y(y)} = -\frac{Z''(z)}{Z(z)} + a_n^2 - \lambda^2 = \text{const} \equiv -b^2 \tag{11.6}$$

Solving

$$\frac{Y''(y)}{Y(y)} = -b^2$$

subject to the boundary condition

$$Y(0) = 0, \quad Y(L) = 0,$$

yields

$$\begin{aligned} Y(y) = Y_m(y) &\equiv \sin\frac{m\pi y}{L} \\ b = b_m &\equiv \frac{m\pi}{L}, \quad m = 1, 2, 3, \ldots. \end{aligned}$$

The last part in (11.6) to be solved is:

$$\frac{Z''(z)}{Z(z)} = -c^2, \quad Z(0) = 0, \quad Z(L) = 0$$

where we have written

$$c^2 \equiv \lambda^2 - (a_n^2 + b_m^2). \tag{11.7}$$

The solution is

$$\begin{aligned} Z(z) = Z_\ell(z) &\equiv \sin\frac{\ell\pi z}{L}, \\ c = c_\ell &\equiv \frac{\ell\pi}{L}, \quad \ell = 1, 2, 3, \ldots. \end{aligned}$$

Putting all the eigenvalues into (11.7), we find

$$\begin{aligned} \lambda^2 = \lambda_{nm\ell}^2 \equiv a_n^2 + b_m^2 + c_\ell^2 = (n^2 + m^2 + \ell^2)\pi^2/L^2, \\ n = 1, 2, 3, \ldots, \quad m = 1, 2, 3, \ldots, \quad \ell = 1, 2, 3, \ldots \end{aligned} \tag{11.8}$$

(11.8) is the desired eigenvalue for the Helmoltz equation. The eigenfunction is

$$u(x, y, z) = u_{nm\ell}(x, y, z) \equiv \sin\frac{n\pi x}{L}\sin\frac{m\pi y}{L}\sin\frac{\ell\pi z}{L}.$$

For the original Schrödinger equation, the energy of the electron is found from $\lambda^2 = 2\mu E/\hbar^2$ to be

$$E = E_{nm\ell} \equiv \frac{\hbar^2\pi^2}{2\mu L^2}(n^2 + m^2 + \ell^2), \tag{11.9}$$

which is quantized because n, m and ℓ can only take an integer values.

The general solution is obtained by superposition

$$\psi(x, y, z, t) = \sum_{n=1}^{\infty}\sum_{m=1}^{\infty}\sum_{\ell=1}^{\infty} e^{-i(E_{nm\ell}/\hbar)t}\sin\frac{n\pi x}{L}\sin\frac{m\pi y}{L}\sin\frac{\ell\pi n}{L}. \tag{11.10}$$

Often however, it is the individual eigenfunction and eigenvalues which are discussed and displayed.

11.3 Sound waves in a rectangular cavity

The propagation of sound in a three-dimensional rectangular cavity is governed by

$$\frac{\partial^2}{\partial t^2}\psi = c^2\nabla^2\psi, \tag{11.11}$$

where ψ is the pressure fluctuation in the air caused by the sound wave, and c the speed of sound. Separation of variables:

$$\psi(x, y, z, t) = T(t)u(x, y, z)$$

leads to:

$$\frac{T''(t)}{c^2T(t)} = \frac{\nabla^2 u}{u} = \text{const} \equiv -\lambda^2 \tag{11.12}$$

Again we arrive at the Helmoltz eigenvalue problem for the space dependences:

$$\nabla^2 u = -\lambda^2 u. \tag{11.13}$$

The physical interpretation of the eigenvalue λ can in this case be obtained from solving the time dependence part.

$$T''(t) = -c^2\lambda^2 T(t)$$

The solution is

$$T(t) = A\sin(c\lambda t) + B\cos(c\lambda t), \tag{11.14}$$

and so $\omega \equiv c\lambda$ has the physical interpretation of frequency of oscillation. This frequency is equal to the phase speed c times the "wavenumber" λ. The latter is determined by the geometry of the cavity Equation (11.11) is to be solved subject to the boundary conditions

$$\begin{aligned} u = 0 \text{ at } x &= 0 \text{ and } x = L_1 \\ y &= 0 \text{ and } y = L_2 \\ z &= 0 \text{ and } z = L_3, \end{aligned}$$

if the dimension of the cavity is L_1 by L_2 by L_3. The solution via the method of separation of variables is the same as in the previous section for a cubic box:

$$u(x, y, z) = X(x)Y(y)Z(z).$$

$$\frac{X''(x)}{X(x)} + \frac{Y''(y)}{Y(y)} + \frac{Z''(z)}{Z(z)} = -\lambda^2$$

$$\begin{aligned}
\frac{X''(x)}{X(x)} &= -a^2 : \quad X = X_n(x) \equiv \sin\frac{n\pi X}{L_1}, a = a_n \equiv \frac{n\pi}{L_1}, \quad n = 1, 2, 3, \ldots \\
\frac{Y''(y)}{Y(y)} &= -b^2 : \quad Y = Y_m(y) \equiv \sin\frac{m\pi y}{L_1}, \quad b = b_m = \frac{m\pi}{L_2}, \quad m = 1, 2, 3, \ldots \\
\frac{Z''(z)}{Z(z)} &= -(\lambda^2 - a^2 - b^2) : Z(z) = Z_\ell(z) \equiv \sin\frac{\ell\pi z}{L_3}, \\
&\qquad \sqrt{\lambda^2 - a^2 - b^2} = \frac{\ell\pi}{L_3}, \quad \ell = 1, 2, 3, \ldots
\end{aligned}$$

so the overall eigenvalue is determined:

$$\lambda^2 = \lambda^2_{nm\ell} \equiv \pi^2 \left(\left(\frac{n}{L_1}\right)^2 + \left(\frac{m}{L_2}\right)^2 + \left(\frac{\ell}{L_3}\right)^2 \right) \tag{11.15}$$

The frequency of the oscillation is "quantized":

$$\omega \equiv c\lambda = c\pi \left(\left(\frac{n}{L_1}\right)^2 + \left(\frac{m}{L_2}\right)^2 + \left(\frac{\ell}{L_3}\right)^2 \right)^{1/2} \tag{11.16}$$

The eigenfunction is

$$u_{nm\ell}(x, y, z) = \sin\frac{n\pi x}{L_1} \cdot \sin\frac{m\pi y}{L_2} \cdot \sin\frac{\ell\pi z}{L_3}. \tag{11.17}$$

A one-dimensional oscillator, such as the violin string, has "harmonic" frequencies:

$$\omega_n = n\omega_1, \quad \omega_1 \equiv \frac{c\pi}{L_1}, \quad n = 1, 2, 3, \ldots$$

That is, the higher frequencies are integer multiples of the fundamental frequency ω_1. Our human ear finds the superposition of harmonic frequencies pleasing. On the other hand, sounds from two-dimensional oscillators, such as drums, are not pleasing to the ear because their sounds are a superposition of incommensurable frequencies:

$$\omega_{nm} = c\pi((\frac{n}{L_1})^2 + (\frac{m}{L_2})^2)^{1/2}.$$

[One should have used the circular geometry for the drum head problem, however.]

11.4 Helmoltz eigenvalue problem in a cylinder

$$\nabla^2 u = -\lambda^2 u \tag{11.18}$$

In cylindrical coordinates we let z be measured along the length of the cylinder. $z = 0$ is one end and $z = L$ is the other end. Let r be the radial distance from the center of circular a cross-section of the cylinder and θ is the angle extended by this radius. In such a coordinate system, the Laplacian is given by

$$\nabla^2 u = \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u}{\partial r}) + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}u + \frac{\partial^2}{\partial z^2}u.$$

Separation of variables

$$u(r, \theta, z) = R(r)\Theta(\theta)Z(z)$$

yields

$$\frac{Z''(z)}{Z(z)} + \frac{1}{r^2}\frac{\Theta''(\theta)}{\Theta(\theta)} + \frac{\frac{1}{r}(rR'(r))'}{R} = -\lambda^2 \tag{11.19}$$

We have

$$\frac{Z''(z)}{Z(z)} = -b^2, \quad z(0) = 0,\ z(L) = 0$$

The solution is:

$$Z(z) = Z_\ell(z) \equiv \sin\frac{\ell\pi z}{L}, \quad \ell = 1, 2, 3, \ldots$$
$$b = b_\ell \equiv \frac{\ell\pi}{L}.$$

Equation (11.19) can be rewritten as

$$\frac{\Theta''(\theta)}{\Theta(\theta)} = -\frac{r(rR'(r))'}{R} - (\lambda^2 - b^2)r^2 = \text{const} = -m^2. \tag{11.20}$$

The fact that Θ must be 2π-periodic demands the separation constant m be an integer:

$$\Theta = e^{im\theta}, \quad m = 0, \ \pm 1, \ \pm 2, \ \pm 3, \ldots \tag{11.21}$$

The R equation in (11.19) is:

$$r\frac{d}{dr}(r\frac{d}{dr}R) + [(\lambda^2 - b^2)r^2 - m^2]R = 0, \tag{11.22}$$

and is to be solved subject to the boundary conditions

$$R(0) \text{ bounded, and } R(a) = 0, \text{ where}$$

$r = a$ is the radius of the cylinder.

Equation (11.22) can be put into the form of Bessel's equation by letting

$$x = \sqrt{\lambda^2 - b^2}r, \quad y(x) = R(r)$$

to yield the standard form for Bessel's equation of order m:

$$x^2 \frac{d^2}{dx^2}y + x\frac{d}{dx}y + (x^2 - m^2)y = 0 \tag{11.23}$$

The solution can be obtained by Frobenius series expansion to be

$$y(x) = AJ_m(x) + BY_m(x).$$

$J_m(x)$ is the Bessel's function of the first kind, and has the series expansion of

$$J_m(x) = \sum_{k=0}^{\infty} \frac{(-1)^k}{k!(k+m)!}(\frac{x}{2})^{2k+m}. \tag{11.24}$$

$Y_m(x)$ is the Bessel's function of the second kind. It has a log singularity at $x = 0$ and blows up at $x = 0$. We will not write out the series expansion for $Y_m(x)$ here.

The boundary condition that $R(0)$ be bounded requires that we set $B = 0$. Thus the required solution is:

$$R(r) = AJ_m(\sqrt{\lambda^2 - b^2}r). \tag{11.25}$$

To satisfy the second boundary condition, we require

$$J_m(\sqrt{\lambda^2 - b^2}a) = 0. \tag{11.26}$$

Since the Bessel function is similar to cosine (in fact for large $|z|$, $J_m(z) \cong \sqrt{\frac{2}{\pi z}}\cos(z - \frac{1}{2}m\pi - \frac{1}{4}\pi))$, it has an infinite number of zeros for each m. These zeros are tabulated, and can be denoted by z_{mn}, with

$$0 < z_{m1} < z_{m2} < z_{m3} < \dots$$

The first few zeros are listed in Table 1:

n	1	2	3	4
z_{on}	2.40483	5.52008	8.65373	11.7915
z_{1n}	3.83171	7.01559	10.1735	13.3237
z_{2n}	5.13562	8.41724	11.6198	14.796

Table: 1 The zeros of Bessel's function

Therefore the boundary condition (11.26) is satisfied by setting

$$\sqrt{\lambda^2 - b^2} = \frac{z_{mn}}{a},$$

resulting in the eigenvalue of the Helmoltz's system as:

$$\lambda^2 = \lambda^2_{nm\ell} = \frac{z^2_{mn}}{a^2} + \frac{\ell^2\pi^2}{L^2},\ \ell = 1, 2, 3, \ldots,\ \ n = 1, 2, 3, \ldots,\ \ m = 0, \pm 1, \pm 2, \ldots$$

The eigenfunction is

$$u_{mn\ell}(r, \theta, z) = J_m(z_{mn} r/a) e^{im\theta} \sin \frac{\ell \pi z}{L}.$$

For sound waves in a circular cylinder, the frequency of oscillation is given by (11.14) to be

$$\omega = \omega_{nm\ell} = c\lambda_{nm\ell} = c\{\frac{z^2_{mn}}{a^2} + \frac{\ell^2\pi^2}{L^2}\}^{1/2}.$$

11.5 Helmoltz's eigenvalue problem in a sphere

$$\nabla^2 u = -\lambda^2 u. \tag{11.27}$$

The Laplacian operator in spherical coordinates is givey by:

$$\nabla^2 u = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 \frac{\partial}{\partial r} u) + \frac{1}{r^2 \sin\theta}\frac{\partial}{\partial \theta}(\sin\theta \frac{\partial}{\partial \theta} u) + \frac{1}{r^2 \sin^2 \theta^2 \varphi^2}\frac{\partial^2}{}u,$$

where θ is the latitude (measured from the north poles) and φ is the longitude and r is the radius from the origin. [If you prefer to measure latitude relative to the equator, then all $\sin\theta$ in the above expression is changed to $\cos\theta$.]

We apply the method of separation of variables again:

$$u(r, \theta, \varphi) = R(r) Y(\theta, \varphi)$$

and substitute into (11.27):

$$\frac{\frac{1}{r^2}\frac{d}{dr}(r^2 \frac{d}{dr} R)}{R} + \frac{\frac{1}{r^2 \sin\theta}\frac{\partial}{\partial\theta}(\sin\theta \frac{\partial}{\partial\theta} Y) + \frac{1}{r^2 \sin^2\theta}\frac{\partial^2}{\partial\varphi^2} Y}{Y} = -\lambda^2,$$

to get:

$$\frac{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta \frac{\partial}{\partial\theta} Y) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2} Y}{Y} = -\lambda^2 r^2 - \frac{\frac{d}{dr}(r^2 \frac{d}{dr} R)}{R}.$$

Since the left-hand side is a function of the angles only and the right-hand side is a function of radius only, they can equal to each other only if they each equal to a constant. We set this separation constant to $-\eta$. Thus

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}Y)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}Y+\eta Y=0 \tag{11.28}$$

and

$$R''+\frac{2}{r}R'-(\frac{\eta}{r^2}-\lambda^2)R=0 \tag{11.29}$$

11.5.1 The spherical harmonics

Equation (11.28) is the *spherical harmonic equation.* $Y(\theta,\varphi)$ can further be separated into:

$$Y(\theta,\varphi)=\Theta(\theta)\Phi(\varphi).$$

(11.28) becomes

$$\frac{\sin\theta(\sin\theta\Theta')'+\eta\sin^2\theta\Theta}{\Theta}=-\frac{\Phi''}{\Phi}=\text{const}\equiv\alpha^2. \tag{11.30}$$

Thus

$$\Phi''(\varphi)+\alpha^2\Phi(\varphi)=0,\qquad 0\le\varphi\le 2\pi$$

subject to the periodic boundary condition

$$\Phi(\varphi+2\pi)=\Phi(\varphi).$$

The solution to the equation is:

$$\Phi(\varphi)=Ae^{i\alpha\varphi}+Be^{-i\alpha\varphi}$$

To satisfy the periodic boundary, α must be an integer, $m=0,\ 1,\ 2,\ 3,\ \ldots$:

$$\begin{aligned}\alpha&=m\equiv\alpha_m\\ \Phi(\varphi)&=\Phi_m(\varphi)=A_me^{im\varphi}+B_me^{-im\varphi},\quad m=0,1,2,\ldots\\ &=A_me^{im\varphi},\quad m=0,\quad \pm1,\quad \pm2,\quad \pm3,\ldots,\end{aligned} \tag{11.31}$$

where we have defined A_m for negative m to be $B_{|m|}$.

Equation (11.30) becomes

$$\frac{1}{\sin\theta}\frac{d}{d\theta}(\sin\theta\frac{d}{d\theta}\Theta)+(\eta-\frac{m^2}{\sin^2\theta})\Theta=0,\qquad 0\le\theta\le\pi$$

With a change in varaible:

$$x = \cos\theta, \quad dx = -\sin\theta d\theta, \quad \frac{d}{d\theta} = -\sin\theta\frac{d}{dx}, \quad \sin^2\theta = 1 - \cos^2\theta = 1 - x^2$$

$$\frac{d}{dx}[(1-x^2)\frac{d}{dx}\Theta] + (\eta - \frac{m^2}{1-x^2})\Theta = 0, \quad -1 \leq x \leq 1 \tag{11.32}$$

Equation (11.32) is the associated Legendre equation. It is regular at $x = 0$, but has a regular singular point at $x = \pm 1$. The solutions which are bounded at $x = \pm 1$ are the Associated Legendre functions, $P_n^m(x)$. The eigenvalues are $\eta = \eta_n \equiv n(n+1)$, $n = 0, 1, 2, 3, \ldots$. For η not equal to these discrete values, the solution blows up at $x = \pm 1$, the north and south poles.

$$\Theta = \Theta_n = P_n^m(x), \qquad n = 0, 1, 2, 3, \ldots$$
$$\eta = n(n+1), \qquad m = -n, -n+1, \ldots, n-1, n.$$

The spherical harmonics are defined by

$$Y(\theta,\varphi) = Y_{nm}(\theta,\varphi) = \sqrt{\frac{(2n+1)(n-m)!}{4\pi(n+m)!}} P_n^m(\cos\theta)e^{im\varphi}, \qquad -n \leq m < n \tag{11.33}$$

It is the eigenfunction to equation (11.28) corresponding to the eigenvalue

$$\eta = n(n+1), \qquad n = 0, 1, 2, 3, \ldots$$

satifying 2π-periodic boundary condition in the φ-direction, and boundedness condition at $\theta = 0$ and $\theta = \pi$.

When integrated over the surface of a sphere (at any radius), the spherical harmonic are orthogonal (since $e^{im\varphi}$, and P_n^m are orthogonal):

$$\int_0^{2\pi}\int_0^{\pi} Y_{nm}(\theta,\varphi)Y^*_{n'm'}(\theta,\varphi)\sin\theta d\theta d\varphi = \begin{cases} 0 & \text{if } n \neq n' \text{ or } m \neq m' \\ 1 & \text{if } n = n' \text{ and } m = m' \end{cases} \tag{11.34}$$

11.5.2 The spherical Bessel equation

Equation (11.29) in the radial direction is, with $\eta = n(n+1)$:

$$r^2R''(r) + 2rR'(r) + [\lambda^2r^2 - n(n+1)]R(r) = 0 \tag{11.35}$$

This is to be solved subject to the boundary condition: $R(0)$ bounded, and $R(a) = 0$, where $r = a$ is the radius of the sphere. Equation (11.35) is called the *spherical Bessel equation*. Its relation to the Bessel equation of order p is revealed through the transformation:

$$R(r) = r^{-1/2}y(x), \quad x \equiv \lambda r$$

$$x^2y''(x) + xy'(x) + (x^2 - p^2)y(x) = 0 \tag{11.36}$$

with $p = n + \frac{1}{2}$. The solution to (11.36) is J_p and Y_p (or J_p and J_{-p}).

The solution $R(r)$ which is bounded at $r = 0$ is the spherical Bessel function of the first kind:

$$R(r) = j_n(x) \equiv (\frac{\pi}{2x})^{1/2}J_{n+\frac{1}{2}}(x), \quad n = 0, 1, 2, 3, \ldots \tag{11.37}$$

To satisfy the boundary condition at $r = a$, we require

$$0 = R(a) = j_n(\lambda a) = (\frac{\pi}{2\lambda a})^{1/2}J_{n+\frac{1}{2}}(\lambda a).$$

This determines the eigenvalue λ is

$$\lambda = \lambda_{nk} = \frac{z_{n+\frac{1}{2},k}}{a}, \quad k = 1, 2, 3, \ldots \tag{11.38}$$

where z_{pk} is the kth zero of $J_p(z)$.

It turns out (as we will prove in a minute) that the spherical Bessel functions are related to the trigonometric functions through

$$j_n(x) = x^n(-\frac{1}{x}\frac{d}{dx})^n(\frac{\sin x}{x}). \tag{11.39}$$

So

$$\begin{aligned} j_0(x) &= \frac{\sin x}{x} \\ j_1(x) &= \frac{\sin x}{x^2} - \frac{\cos x}{x} \\ j_2(x) &= (\frac{3}{x^3} - \frac{1}{x})\sin x - \frac{3}{x^2}\cos x, \ldots \end{aligned}$$

The first few zeros, $z_{n+\frac{1}{2},k}$ are listed below

k	1	2	3	4
$z_{1/2,k}$	3.14159	6.283185	9.424778	12.566370
$z_{3/2,k}$	4.493409	7.725252	10.904122	14.066194
$z_{5/21,k}$	5.763459	9.095011	12.322941	15.514603
$z_{7/21,k}$	6.987932	10.417119	13.698023	16.923621

Table 2: Zeros of the spherical Bessel functions

Exercise: For the symmetric case, $n = 0$, find the eigenvalue and eigenfunction of (11.35) satisfying $R(a) = 0$ and $R(0)$ bounded.

Write $x = \lambda r$ and

$$R(r) = x^{-1}w(x)$$

From (11.35) for the case of $n = 0$:

$$x^2 \frac{d^2}{dx^2}R + 2x\frac{d}{dx}R + x^2 R = 0$$

and

$$\begin{aligned} \frac{d}{dx}R &= -x^2 w(x) + x^{-1}w'(x) \\ \frac{d^2}{dx^2}R &= 2x^{-3}w(x) - 2x^{-2}w'(x) + x^{-1}w''(x), \end{aligned}$$

we have:

$$\begin{aligned} 0 &= x^2 \frac{d^2}{dx^2}R + 2x\frac{d}{dx}R + x^2 R \\ &= x\{w''(x) + w(x)\} \end{aligned}$$

The solution for $w(x)$ is

$$w(x) = A\sin x + B\cos x$$

Therefore

$$R(r) = x^{-1}w(x) = A\frac{\sin x}{x} + B\frac{\cos x}{x}.$$

The solution which is bounded at $x = 0$ is constructed by setting $B = 0$:

$$R(r) = A\frac{\sin x}{x} = Aj_0(x).$$

To satisfy the boundary condition $R(a) = 0$, we require

$$0 = R(a) = A\frac{\sin(\lambda a)}{\lambda a},$$

implying

$$\lambda = \lambda_k = k\pi/a, \quad k = 1, 2, 3, \ldots$$

Finally, the eigenfunctions are

$$R(r) = R_k(r) = \frac{\sin(\lambda_k r)}{(\lambda_k r)},$$

corresponding to the eigenvalue:

$$\lambda = \lambda_k = k\pi/a, \quad k = 1, 2, 3, \ldots$$

Exercise: Show that the spherical Bessel functions of zeroth order $j_0(\lambda_k r)$ is orthogonal with respect to weight r^2, specifically:

$$I_{k\ell} \equiv \int_0^a j_0(\lambda_k r) j_0(\lambda_\ell r) r^2 dr = \begin{cases} 0 & \text{if } k \neq \ell \\ \frac{a^3}{2\pi^2 k^2} & \text{if } k = \ell \end{cases}$$

where

$$\lambda_k = k\pi/a, \quad k = 1, 2, 3, \ldots$$

Since

$$j_0(\lambda_k r) = \frac{\sin(\lambda_k r)}{\lambda_k r}$$

$$\begin{aligned} I_{k\ell} &= \int_0^a \frac{\sin(\lambda_k r)\sin(\lambda_\ell r)}{\lambda_k \lambda_\ell} dr \\ &= \int_0^a \frac{\sin(k\pi r/a)\sin(\ell\pi r/a) dr}{\lambda_k \lambda_\ell} \\ &= \frac{a/2}{\lambda_k \lambda_\ell} \delta_{k\ell}, \end{aligned}$$

since

$$\frac{2}{a}\int_0^a \sin(k\pi r/a)\sin(\ell\pi r/a) dr = \delta_{k\ell},$$

from the orthogonality of the sines, previously established.

Next we turn to the general case of (11.35):

$$\frac{d}{dx}(x^2 \frac{d}{dx} R) + [x^2 - n(n+1)]R = 0, \tag{11.40}$$

(where we have written $x \equiv \lambda r$) and want to show that (11.39):

$$R = j_n(x) = x^n (-\frac{1}{x}\frac{d}{dx})^n (\frac{\sin x}{x}) \tag{11.41}$$

satisfies it. You may want to do so by substituting (11.41) into (11.40), but the differentiation is tedious. An easier alternative is to use the identity for Bessel functions

$$\frac{d}{dx}[x^{-p} J_p(x)] = -x^{-p} J_{p+1}(x)$$

by making use of the connection

$$j_n(x) \equiv (\frac{\pi}{2x})^{1/2} J_{n+\frac{1}{2}}(x), \quad n = 0, 1, 2, \ldots$$

For $p = n + 1/2$, the identity is

$$\frac{d}{dx}[x^{-n}\frac{1}{x^{1/2}}J_{n+\frac{1}{2}}] = -x^{-n}\frac{1}{x^{1/2}}J_{(n+1)+1/2}(x)$$

and so is

$$\frac{d}{dx}[x^{-n}j_n(x)] = -x^{-n}j_{n+1}(x).$$

Or:

$$j_n(x) = x^n(-\frac{1}{x}\frac{d}{dx})[x^{-n+1}j_{n-1}(x)].$$

For $n = 1$, this is

$$j_1 = x^1(-\frac{1}{x}\frac{d}{dx})j_0(x) = x^1(-\frac{1}{x}\frac{d}{dx})(\frac{\sin x}{x})$$

For $n = 2$ and so on:

$$\begin{aligned}
j_2 &= x^2(-\frac{1}{x}\frac{d}{dx})[x^{-1}j_1(x)] = x^2(-\frac{1}{x}\frac{d}{dx})^2(\frac{\sin x}{x}) \\
j_3 &= x^3(-\frac{1}{x}\frac{d}{dx})^3(\frac{\sin x}{x}) \\
&\vdots \\
j_n &= x^n(-\frac{1}{x}\frac{d}{dx})^n(\frac{\sin x}{x}).
\end{aligned}$$

Chapter 12

Sturm-Liouville Theory

12.1 Introduction

Sturm-Liouville theory provides a general framework for considering eigenvalues and eigenfunctions for equations of the form

$$\frac{d}{dx}[p(x)\frac{d}{dx}y] + [\lambda r(x) - q(x)]y = 0.$$

As seen in the last chapter, this equation arises from separated partial differential equations in various coordinates. All the special functions studied in Chapter 10 are governed by this theory.

12.2 Regular and singular Sturm-Liouville problems

A Liouville differential equation has the general form

$$\frac{d}{dx}[p(x)\frac{d}{dx}y] + [\lambda r(x) - q(x)]y = 0 \qquad (12.1)$$

where λ is a parameter (to be determined), $p(x)$, $r(x)$ and $q(x)$ are specified functions.

In a *regular Sturm-Liouville* problem, the domain should be a closed *finite* interval, $[a, b]$; $p(x)$, $p'(x)$, $q(x)$ and $r(x)$ are continuous in $[a, b]$; $p(x) \neq 0$, $r(x) \neq 0$ in $[a, b]$. (Without loss of generality we assume $p(x) > 0$, and, by changing the sign of λ if necessary, $r(x) > 0$.)

The boundary conditions in a regular Sturm-Liouville problem is of the form:

$$\begin{aligned} c_1 y(a) + c_2 y'(a) &= 0 \\ d_1 y(b) + d_2 y'(b) &= 0. \end{aligned} \tag{12.2}$$

At least one of c_1 and c_2, and at least one of d_1 and d_2, are nonzero.

A singular Sturm-Liouville problem is one consisting of (12.1) either on an infinite interval or on a finite interval but with at least one of the regularity properties not satisfied. Typically one or more of the coefficients in the equation (12.1) either goes to zero or ∞ at an end-point of the interval.

For the singular the problems we will consider here, we still have $p(x)$, $p'(x)$, $q(x)$ and $r(x)$ continuous on the open interval $a < x < b$.

$$p(x) > 0, \quad \text{and} \quad r(x) > 0 \text{ in } a < x < b,$$

but $p(x)$ and/or $r(x)$ may vanish $x = a$ or $x = b$. In this case, the boundary condition (12.2) may not be appropriate; it may be too restrictive. A typical boundary condition at a singular point could be that $y(x)$ be bounded there.

The solution to regular or singular Sturm-Liouville problem is the trivial solution

$$y(x) \equiv 0.$$

Nontrivial solutions exist only for some special values (eigenvalues) of λ.

Examples:

(a) *Fourier:*

$$\begin{gathered} y''(x) + \lambda y(x) = 0, \quad 0 \le y \le L \\ y(0) = 0, \quad y(L) = 0 \end{gathered}$$

This is a regular Sturm-Liouville problem.

(b) *Legendre:*

$$[(1 - x^2)y']' + \mu y = 0, \quad -1 < x < 1$$

$$y(x) \text{ bounded at } x = 1 \text{ and } x = -1.$$

This is a singular Sturm-Liouville system with $p(x) = 1 - x^2$, $r(x) = 1$.

$$p(x) = 0 \text{ at } x = \pm 1, \text{ the boundary end points.}$$

(c) *Bessel:*

$$x^2y'' + xy' + [\lambda x^2 - p^2]y = 0, \quad 0 < x < b$$

This can be put into the Liouville form by dividing the equation by x:

$$(xy')' + [\lambda x - \frac{p^2}{x}]y = 0, \quad 0 < x < b$$

Here $p(x) = x$, $r(x) = x$, $q(x) = p^2/x$. This is a singular system because $p(x) = 0$ at $x = 0$, one of the end points. The appropriate boundary conditions are

$$y(0) \text{ bounded, } d_1y(b) + d_2y'(b) = 0$$

(d) *Spherical Bessel:*

$$x^2y'' + 2xy' + [\lambda x^2 - n(n+1)]y = 0, \quad 0 < x < b$$

$$y(0) \text{ bounded, } d_1y(b) + d_2y'(b) = 0.$$

The differential equation can be put into the Liouville form:

$$(x^2y')' + [\lambda x^2 - n(n+1)]y = 0, \quad 0 < x < a$$

so

$$\begin{aligned} p(x) &= x^2, \quad p(0) = 0 \\ r(x) &= x^2, \quad r(0) = 0 \\ q(x) &= n(n+1). \end{aligned}$$

This is a singular Sturm-Liouville system because $p(0) = 0$, $r(0) = 0$.

(e) *Chebyshev:*

$$(1 - x^2)y'' - xy' + \lambda y = 0, \quad -1 < x < 1.$$

This can be put into the Liouville form by dividing the equation by $(1 - x^2)^{1/2}$

$$(1 - x^2)^{1/2}y'' - \frac{x}{(1 - x^2)^{1/2}}y' + \lambda\frac{1}{(1 - x^2)^{1/2}}y = 0$$

which is,

$$((1-x^2)^{1/2}y')' + \lambda \frac{1}{(1-x^2)^{1/2}} y = 0.$$

Therefore

$$p(x) = (1-x^2)^{1/2}, \quad r(x) = \frac{1}{(1-x^2)^{1/2}}, \; q(x) = 0.$$

The appropriate boundary condition for this singular system is:

$$y(x) \text{ bounded at } x = \pm 1.$$

12.3 Orthogonality Theorem

The eigenfunctions corresponding to different eigenvalues are orthogonal to each other with respect to the weight $r(x)$.

Consider two pairs of eigenfunctions and eigenvalues

$$(\phi_k, \lambda_k), \quad (\phi_j, \lambda_j),$$

where $y(x) = \phi_k(x)$ is the eigenfunction satisfying (12.1) and (12.2) with $\lambda = \lambda_k$; $y(x) = \phi_j(x)$ is the eigenfunction corresponding to $\lambda = \lambda_j$:

$$(p\phi_k')' + [\lambda_k r - q]\phi_k = 0 \tag{12.3}$$

$$(p\phi_j')' + [\lambda_j r - q]\phi_j = 0. \tag{12.4}$$

Multiply (12.3) by ϕ_j and (12.4) by ϕ_k, and subtract:

$$\phi_j(p\phi_k')' - \phi_k(p\phi_j)' = (\lambda_j - \lambda_k) r \phi_j \phi_k. \tag{12.5}$$

The left-hand side can be written as: $\frac{d}{dx}[\phi_j(p\phi_k') - \phi_k(p\phi_j')]$. Integrate both sides of (12.5) from a to b

$$(\lambda_j - \lambda_k) \int_a^b r(x)\phi_j(x)\phi_k(x)dx = [\phi_j(p\phi_k') - \phi_k(p\phi_j')]\Big|_a^b \tag{12.6}$$

The right-hand side of (12.6) vanishes either when the boundary conditions (12.2) are applied, or in the case of boundedness condition in a singular Sturm-Liouville problem when $p(x) = 0$ at the boundary. Thus

$$(\lambda_j - \lambda_k) \int_a^b r(x)\phi_j(x)\phi_k(x)dx = 0.$$

Hence:

$$\int_a^b r(x)\phi_j(x)\phi_k(x)dx = \begin{cases} 0 & \text{if } \lambda_j \neq \lambda_k \\ \int_a^b r(x)\phi_j^2(x)dx & \text{if } \lambda_j = \lambda_k. \end{cases} \tag{12.7}$$

12.4 Uniqueness of eigenfunctions

There is only one eigenfunction corresponding to an eigenvalue.

Let us suppose that this is not true, and that there are two different eigenfunctions $\phi_1(x)$ and $\phi_2(x)$ corresponding to the same eigenvalue λ. Then

$$(p\phi_1') + (\lambda r + q)\phi_1 = 0$$
$$(p\phi_2') + (\lambda r + q)\phi_2 = 0$$

multiply the first equation by ϕ_2 and the second equation by ϕ_1, and then subtract:

$$0 = \phi_2(p\phi_1') - \phi_1(p\phi_2')' = \frac{d}{dx}[p(\phi_2\phi_1' - \phi_1\phi_2')]$$

Integrating:

$$p(\phi_2\phi_1' - \phi_1\phi_2') = \text{ constant.}$$

The constant can be evaluated at one of the boundaries. If the boundary condition is of the regular Sturm-Liouville form of (12.2), then the constant is easily shown to be zero. It is also zero in the singular case where $p(x) = 0$ at the boundary point. It then follows that in the interior of the domain

$$\phi_1\frac{d\phi_2}{dx} - \phi_2\frac{d\phi_1}{dx} = 0,$$

which is

$$\frac{d}{dt}(\phi_2/\phi_1) = 0.$$

Hence

$$\phi_2(x) = c\phi_1(x);$$

they are the same eigenfunction. Note that this result fails for periodic boundary conditions.

12.5 All eigenvalues are real and positive

To show that all eigenvalues are real, we consider (12.1) and its complex conjugate:

$$[py'] + [\lambda r - q]y = 0 \tag{12.8}$$
$$[py^{*\prime}]' + [\lambda^* r - q]y^* = 0. \tag{12.9}$$

Using the same procedure as in section 3, we multiply (12.8) by y^* and (12.9) by y; then subtract and integrate:

$$(\lambda - \lambda^*) \int_a^b r|y|^2 dx = 0. \tag{12.10}$$

Since $\int_a^b r|y|^2 dx \neq 0$, we must have

$$\lambda = \lambda^*. \tag{12.11}$$

Thus λ is real.

All eigenvalues of the Sturm-Liouville system with real coefficients are real.

To show that λ is positive if $q(x) \geq 0$, we multiply (12.11) by y^* and integrate:

$$0 = \int_a^b y^*[py']'dx + \lambda \int_a^b r|y|^2 dx - \int_a^b q|y|^2 dx$$

This gives, after integrating by parts for the first term

$$\lambda = \int_a^b [p|y'|^2 + q|y|^2]dx / \int_a^b r|y|^2 dx \tag{12.12}$$

(12.11) implies that $\lambda \geq 0$ if q is nonnegative in (a, b). [The possibility of $\lambda = 0$ is allowed if $y'(x) \equiv 0$, such as the $n = 0$ case of $\phi_n(x) = \cos \frac{n\pi x}{L}$.]

All eigenvalues of the Sturm-Liouville system with $q(x) \geq 0$ in (a, b) are nonnegative.

12.6 Eigenvalues are infinite in number

The eigenvalues of the Sturm-Liouville system are discrete, and *form an increasing sequence*:

$$\lambda_1 < \lambda_2 < \lambda_3 < \ldots$$

with $\lambda_j \to \infty$ as $j \to \infty$, provided that the domain is finite and $p(x) > 0$ and $r(x) > 0$ in $a < x < b$.

This will be shown in the next section.

12.7 Zeros of eigenfunctions

(Reference: Morse and Feshbach (1953))

Oscillation Theorem

The eigenfunction ϕ_k corresponding to the eigenvalue λ_k (which has been ordered: $\lambda_1 < \lambda_2 < \lambda_3 < \ldots$, has $k-1$ zeros in (a, b).

Consider two solutions $\phi_{(1)}(x)$ and $\phi_{(2)}(x)$, satisfying the Liouville equation (1) with $\lambda = \lambda_{(1)}$ and $\lambda = \lambda_{(2)}$, respectively. $\lambda_{(1)}$ and $\lambda_{(2)}$ are not necessarily the first and second eigenvalues λ_1 and λ_2. As was done previously, we multiply the first equation by $\phi_{(2)}$, the second equation by $\phi_{(1)}$, and subtract:

$$\frac{d}{dx}[p(x)(\phi_{(2)}\frac{d}{dx}\phi_{(1)} - \phi_{(1)}\frac{d}{dx}\phi_{(2)})] = (\lambda_{(2)} - \lambda_{(1)})r(x)\phi_{(1)}\phi_{(2)} \qquad (12.13)$$

We integrate the above equation (12.13) from the left boundary $x = a$ to a point x in the interior

$$[p(x)(\phi_{(2)}(x)\frac{d}{dx}\phi_{(1)}(x) - \phi_{(1)}(x)\frac{d}{dx}\phi_{(2)}(x))] = (\lambda_{(2)} - \lambda_{(1)})\int_a^x r(x)\phi_{(1)}\phi_{(2)}dx \qquad (12.14)$$

since $p(a)\ (\phi_{(2)}(a)\frac{d}{dx}\phi_{(1)}(a) - \phi_{(1)}(a)\frac{d}{dx}\phi_{(2)}(a)) = 0$, either because of the homogeneous boundary condition (12.2), or because $p(a) = 0$ in the singular case.

Choose $x = \xi_1 > a$ to be the smallest value of x for which $\phi_{(1)}(x) = 0$. That is

$$\phi_{(1)}(\xi_1) = 0$$

$$(p\phi_{(2)}\frac{d}{dx}\phi_{(1)})_{x=\xi_1} = (\lambda_{(2)} - \lambda_{(1)})\int_a^{\xi_1} r(x)\phi_{(1)}\phi_{(2)}dx. \qquad (12.15)$$

Since ξ_1 is the smallest zero of $\phi_{(1)}(x)$, $\phi_{(1)}(x)$ does not change sign between $x = a$ and $x = \xi_1$. We therefore can take

$$\phi_{(1)}(x) > 0, \quad a < x < \xi_1,$$

and

$$\frac{d}{dx}\phi_{(1)}(\xi_1) < 0$$

since $\phi_{(1)}(x)$ goes from positive to zero at $x = \xi_1$.

If $\lambda_{(2)} > \lambda_{(1)}$, we want to show that $\phi_{(2)}(x)$ oscillates more rapidly by demonstrating that $\phi_{(2)}(x)$ has an extra zero in $a < x < \xi_1$ (than $\phi_{(1)}(x)$). If $\phi_{(2)}(x)$ did not go to zero in $a < x < \xi_1$, we can take it to be positive in this range. Then since $r(x) > 0$, the right-hand side of (12.15) is positive, while the left-hand side is negative. This contradiction demonstrates that $\phi_{(2)}(x)$ must go through a zero somewhere in $a < x < \xi_1$.

The same argument can be repeated for the range between the first zero ξ_1 of $\phi_{(1)}(x)$ and its second zero ξ_2, and show that $\phi_{(2)}(x)$ must have another zero in $\xi_1 < x < \xi_2$, and so on. Thus:

Sturm's First Comparison Theorem

The number of zeros of $y(x)$ increases as λ is increased.

For a low enough value of λ, there will be no zero of $y(x)$ inside $a < x < b$. Call this smallest λ value λ_1 and the corresponding $y(x)$, $\phi_1(x)$ (if the boundary condition at $x = b$ is satisfied). In other words, λ_1 is the lowest eigenvalue and $\phi_1(x)$ is the eigenfunction with the smallest number of zeros (in fact no zero).

We increase λ from λ_1 using a $y(x)$ which satisfies the boundary condition at $x = a$. At first it will not fit the boundary condition at $x = b$. Then when that boundary condition at $x = b$ is satisfied for higher value of $\lambda = \lambda_2$, the next eigenvalue, the eigenfunction $\phi_2(x)$ must have one more zero than $\phi_1(x)$.

As λ is increased further, the distance between the zeros of $y(x)$ decreases until, at the next eigenvalue λ_3, there is one more zero (than $\phi_2(x)$) inside $a < x < b$.

We order the sequence of eigenfunctions, ϕ_1, ϕ_2, ϕ_3, ..., such that the corresponding eigenvalues are in increasing order:

$$\lambda_1 < \lambda_2 < \lambda_3 < \ldots < \lambda_n < \lambda_{n+1} < \ldots$$

and $\phi_{n+1}(x)$ has one more zero than $\phi_n(x)$. $\phi_n(x)$ has $n-1$ zeros in the interior.

We next want to show that the eigenvalues are *discrete*, i.e. the difference $(\lambda_{n+1} - \lambda_n)$ is finite, if $(b-a)$ is finite.

Take λ to be a value intermediate between λ_n and λ_{n+1}, and $\phi(x)$ to be the corresponding solution of (12.1) satisfying the boundary condition at $x = a$, but not at $x = b$ (otherwise it would have been an eigenfunction). Using the previous result (12.15), we now have:

$$(\lambda - \lambda_n) \int_a^b r(x)\phi_n(x)\phi(x)dx = p(b)(\phi(b)\phi_n'(b) - \phi_n(b)\phi'(b)) \qquad (12.16)$$

Since $\phi(x)$ is not an eigenfunction, the right-hand side is not zero. It remains nonzero even as $n \to \infty$.

Thus unless $\int_a^b r(x)\phi_n(x)\phi(x)dx$ is infinite (which is possible if $b-a$ is infinite), the difference $\lambda - \lambda_n$ is finite. Since $\lambda_{n+1} > \lambda$, we have the result that the difference $(\lambda_{n+1} - \lambda_n)$ cannot be infinitesimal, if $(b-a)$ is not infinite, no matter how large n is.

It follows that the sequence

$$\lambda_1, \lambda_2, \lambda_3, \ldots, \lambda_n, \lambda_{n+1}, \ldots$$

can have no upper bound but must continue to $+\infty$.

Note that the possibility exists for a continuous distribution of λ only if $(b-a)$ is infinite. Nevertheless, if the solution decay sufficiently rapidly as $x \to \infty$ such that $\int_a^b r\phi_n\phi dx$ is finite, the eigenvalues are still discrete even if the domain is infinite.

12.8 Variational Principle

We define the *Rayleigh quotient* for any piecewise continuous function $\psi(x)$ by

$$\Omega(\psi) \equiv \int_a^b (p\psi'^2 + q\psi^2)dx \Big/ \int_a^b r\psi^2 dx \geq 0 \qquad (12.17)$$

The function $\psi(x)$ does not have to satisfy (12.1), but we will assume that it satisfies the same boundary conditions as the eigenfunctions $\phi_k(x)$. Since $\Omega(\psi)$ is nonnegative, it must have a greatest lower bound. That minimum turns out to be λ_1, the lowest eigenvalue, i.e.

$$\lambda_1 = \Omega(\phi_1) = \min \Omega(\psi).$$

To show this, suppose $\Omega(\psi)$ is the minimum for some ψ, then

$$\Omega(\psi(x) + \alpha g(x)) \geq \Omega(\psi(x)) \equiv \mu$$

for any constant α and any continuous differentiable $g(x)$ which vanishes at $x = a$ and $x = b$. Or

$$\left.\frac{\partial \Omega(\psi + \alpha g)}{\partial \alpha}\right|_{\alpha=0} = 0$$

This derivative is

$$0 = \frac{2\int_a^b (p\psi' g' + q\psi g)dx}{\int_a^b r\psi^2 dx} - \frac{2\int_a^b r\psi g dx \int_a^b (p\psi'^2 + q\psi^2)dx}{(\int_a^b r\psi^2 dx)^2},$$

which implies

$$\int_a^b [p\psi' g' + q\psi g - \mu r\psi g]dx = 0.$$

We integrate by parts the above equation to obtain:

$$-\int_a^b g[(p\psi')' + (\mu r - q)\psi]dx = 0.$$

Since this is true for every admisssible function $g(x)$, the expression in the brackets must be zero, i.e.

$$[(p\psi')' + (\mu r - q)\psi] = 0$$

This is the same as the Liouville equation (12.1). So μ must be the eigenvalue λ_1, and ψ must be the eigenfunction $\phi_1(x)$.

By the same procedure we can show that λ_2 is the minimum of $\Omega(\psi)$ under the additional constraint that ψ be orthogonal to the first eigenfunction ϕ_1, i.e.

$$\int_a^b r\psi\phi_1 dx = 0.$$

The minimizing function ψ is ϕ_2. Continuing this way we can show that

$$\lambda_k = \min \Omega(\psi) \tag{12.18}$$

subject to the constraint that ψ be orthogonal to ϕ_1, ϕ_2, ..., ϕ_{k-1}.

12.9 The eigenfunctions are complete

A set of eigenfunctions, $\{\phi_k\}$, is *complete* if a series (a linear superposition of them) can provide an accurate representation of any piecewise continuous function $f(x)$ in the domain where they are defined. By "accurate" representation we mean that the least square-error between $f(x)$ and its representation goes to zero if the number of terms in the series goes to infinity.

Let's expand $f(x)$ in an *eigenfunction expansion* of the form

$$f(x) \sim \sum_{k=1}^{\infty} a_k\phi_k(x) \equiv \tilde{f}(x), \tag{12.19}$$

where

$$a_k = \int_a^b f(x)\phi_k(x)r(x)dx \Big/ \int_a^b \phi_k^2(x)r(x)dx \tag{12.20}$$

is called the *generalized Fourier coefficient*.

(12.20) is obtained from (12.19) by multiplying it by $\phi_j(k)r(x)$, integrating from a to b, and making use of the orthogonality condition $\phi_k(x)$ with respect to weight $r(x)$. The series $\tilde{f}(x)$ is the "representation" of $f(x)$.

Consider a function $\psi(x)$ defined by

$$\psi(x) \equiv f(x) - \sum_{n=1}^{k-1} a_n \phi_n \tag{12.21}$$

$\psi(x)$ is "orthogonal" to the eigenfunctions ϕ_1, ϕ_2, ..., ϕ_{k-1} because, for $j = 1, 2, \ldots, k-1$:

$$\begin{aligned}\int_a^b r\psi\phi_j dx &= \int_a^b r(f - \sum_{n=1}^{k-1} a_n\phi_n)\phi_j dx \\ &= \int_a^b rf\phi_j dx - a_j \int_a^b r\phi_j^2 dx = 0\end{aligned}$$

due to the definition of a_j by (12.20). We further make $\psi(x)$ satisfy the boundary conditions by enforcing the boundary condition on $f(x)$ at the two ends of the domain. $f(x)$ can remain arbitrary in $a < x < b$.

From (12.18), we have

$$\lambda_k \leq \Omega(\psi)$$

From the definition of $\Omega(\psi)$ in (12.17), we have

$$\begin{aligned}\int_a^b r\psi^2 dx &\leq \frac{1}{\lambda_k}\int_a^b [p\psi'^2 + q\psi^2]dx \\ &= \frac{1}{\lambda_k}\{\int_a^b (pf'^2 + qf^2)dx - 2\sum_{n=1}^{k-1} a_n \int_a^b (pf'\phi_n' + qf\phi_n)dx \\ &\quad + \sum_{n=1}^{k-1}\sum_{m=1}^{k-1} a_n a_m \int_a^b (p\phi_n'\phi_m' + q\phi_n\phi_m)dx\}.\end{aligned}$$

Integrating by parts and using (12.1)

$$\begin{aligned}\int_a^b (p\phi_n'\phi_m' + q\phi_n\phi_m)dx &= \lambda_n \int_a^b r\phi_n\phi_m dx \\ &= \begin{cases} 0 & \text{if } m \neq n \\ \lambda_n \int_a^b r\phi_n^2 dx & \text{if } m = n. \end{cases}\end{aligned}$$

$$\int_a^b (pf'\phi_n' + qf\phi_n)dx = \int_a^b f[-(p\phi_n)' + q\phi_n]dx$$
$$= \lambda_n \int_a^b rf\phi_n dx = \lambda_n a_n \int_a^b r\phi_n^2 dx$$

Thus

$$0 \le \int_a^b r\psi^2 dx \le \frac{1}{\lambda_k}\{\int_a^b (pf'^2 + qf^2)dx - \sum_{n=1}^{k-1} \lambda_n a_n^2 \int_a^b r\phi_n^2 dx\}$$
$$\le \frac{1}{\lambda_k}\int_a^b (pf'^2 + qf^2)dx \tag{12.22}$$

Since we have shown in section 12.7 that $\lambda_k \to \infty$ as $k \to \infty$, the right-hand side $\to 0$ as $k \to \infty$.

The least-square mean error for a representation of $f(x)$ by a partial sum of $k-1$ terms is defined by

$$\epsilon_{k-1} \equiv \int_a^b r(f - \sum_{n=1}^{k-1} a_n\phi_n)^2 dx$$
$$= \int_a^b r\psi^2 dx$$

by our definition of ψ in (12.21). The result in (12.22) then implies

$$\lim_{k\to\infty} \epsilon_k \to 0.$$

In other words, the generalized Fourier series representation ($\tilde{f}(x)$) of $f(x)$ converges to $f(x)$ in the mean. The set of eigenfunctions $\{\phi_k\}$ is then said to be *complete*.

12.10 Examples

(a) Fourier sine:

$$y''(x) + \lambda y(x) = 0, \quad 0 < y < L,$$
$$y(0) = 0, \quad y(L) = 0$$

This is a regular Sturm-Liouville system with $p(x) = 1$, $r(x) = 1$ and $q(x) = 0$.

The eigenfunctions are

$$y(x) = \phi_n(x) \equiv \sin \frac{n\pi x}{L},$$

corresponding to the eigenvalues

$$\lambda = \lambda_n \equiv (\frac{n\pi}{L})^2, \quad n = 1, 2, 3, \ldots$$

They are infinite in number, discrete, real and positive. They can be ordered as

$$\lambda_1 < \lambda_2 < \lambda_3 < \ldots$$

with $\lambda_n \to \infty$ as $n \to \infty$.

The orthogonality condition is

$$\frac{2}{L} \int_0^L \sin \frac{m\pi x}{L} \sin \frac{m\pi x}{L} dx = \delta_{mn}.$$

An orbitrary piecewise continuous function $f(x)$ can be represented by a Fourier sine series

$$f(x) = \sum_{n=1}^{\infty} a_n \sin \frac{n\pi x}{L}, \quad 0 < x < L$$

$$a_n = \frac{2}{L} \int_0^L f(x) \sin \frac{n\pi x}{L} dx,$$

and the representation will converge to $f(x)$ in the mean.

Fourier cosine:

$$y''(x) + \lambda y(x) = 0, \quad 0 < y < L$$
$$y'(0) = 0, \quad y'(L) = 0$$

Same as Fourier sine except the eigenfunctions are

$$y(x) = \phi_n(x) \equiv \cos \frac{n\pi x}{L},$$

corresponding to the eigenvalues

$$\lambda = \lambda_n = (\frac{n\pi}{L})^2, \quad n = 0, 1, 2, 3, \ldots$$

The orthogonality condition is

$$\frac{2}{L}\int_0^L \cos\frac{m\pi x}{L}\cos\frac{n\pi x}{L}dx = \begin{cases}\delta_{mn} & \text{if } m \neq 0\\ 2 & \text{if } m = n = 0.\end{cases}$$

An arbitrary piecewise continuous function $f(x)$ can be expanded in a Fourier cosine series

$$f(x) = \sum_{n=0}^{\infty} b_n \cos\frac{n\pi x}{L}, \quad 0 < x < L$$

where

$$\begin{aligned} b_n &= \frac{2}{L}\int_0^L f(x)\cos\frac{n\pi x}{L}dx, \quad n = 1, 2, 3, \ldots \\ b_0 &= \frac{1}{L}\int_0^L f(x)dx. \end{aligned}$$

(b) Legendre:

$$[(1-x^2)y']' + \mu y = 0, \qquad -1 < x < 1$$
$$y \text{ bounded at } x = \pm 1$$

This is a singular Sturm-Liouville system

$$\begin{aligned} &p(x) = 1 - x^2 > 0 \quad \text{in } -1 < x < 1\\ &p(x) = 0 \quad \text{at } x = \pm 1\\ &r(x) = 1\\ &q(x) = 0 \end{aligned}$$

The eigenvalues are

$$\mu = \mu_n \equiv n(n+1), \quad n = 0, 1, 2, 3, \ldots$$

They are infinite in number, real, nonnegative, discrete and tend to infinity as $n \to \infty$.

The eigenfunctions are

$$\begin{aligned} &y(x) = \phi_n(x) \equiv P_n(x)\\ &P_0(x) = 1, \quad P_1(x) = x, \quad P_2(x) = \frac{3}{2}x^2 - \frac{1}{2}\\ &P_3(x) = \frac{5}{2}x^3 - \frac{3}{2}x, \quad \ldots \end{aligned}$$

They are othogonal with respect to weight 1:

$$\int_{-1}^{1} P_m(x)P_n(x)dx = \begin{cases} 0 & \text{if } m \neq n \\ \frac{2}{2n+1} & \text{if } m = n. \end{cases}$$

An arbitrary piecewise continuous function $f(x)$ can be expanded in a Legendre series:

$$f(x) = \sum_{n=0}^{\infty} a_n P_n(x), \quad -1 < x < 1$$

where

$$a_n = \frac{2n+1}{2} \int_{-1}^{1} f(x)P_n(x)dx.$$

The series will converge to $f(x)$ in the mean.

Associated Legendre

$$[(1-x^2)y']' + [\mu - \frac{m^2}{1-x^2}]y = 0, \quad -1 < x < 1$$
$$y \text{ bounded at } x = \pm 1.$$

This is a singular Sturm-Liouville system with

$$\begin{aligned} &p(x) = 1 - x^2 > 0 \text{ in } -1 < x < 1 \\ &p(x) = 0 \text{ at } x = \pm 1 \\ &r(x) = 1 \\ &q(x) = \frac{m^2}{1-x^2}. \end{aligned}$$

The eigenvalues are

$$\mu = \mu_n = n(n+1), \quad n = 0, 1, 2, 3, \ldots.$$

(discrete, real, nonnegative, infinite in number, tending to infinity as $n \to \infty$).

The corresponding eigenfunctions are

$$y(x) = \phi_n(x) \equiv P_n^m(x) = (-1)^m(1-x^2)^{m/2}\frac{d^m}{dx^m}P_n(x).$$

They are orthogonal with respect to weight 1:

$$\int_{-1}^{1} P_n^m(x)P_{n'}^m(x)dx = \frac{2(n+m)!}{(2n+1)(n-m)!}\delta_{nn}.$$

A piecewise continues function $f(x)$ can be expanded in a series of associated Legendre functions:

$$f(x) = \sum_{n=0}^{\infty} a_n P_n^m(x), \qquad -1 < x < 1$$
$$a_n = \frac{(2n+1)(n-m)!}{2(n+m)!} \int_{-1}^{1} f(x) P_n^m(x) dx,$$

and the representation will converge to $f(x)$ in the mean.

(c) Bessel

$$(xy')' + [\lambda x - \frac{m^2}{x}]y = 0, \quad 0 < x < a$$
$$y \text{ bounded at } x = 0, \quad y(a) = 0.$$

This is a singular Sturm-Liouville system with

$$p(x) = x > 0, \;\; 0 < x < a, \text{ but } p(x) = 0 \text{ at } x = 0$$
$$r(x) = x > 0, \;\; 0 < x < a$$
$$q(x) = m^2/x.$$

The eigenfunctions are

$$y(x) = \phi_j(x) \equiv J_m(\sqrt{\lambda_j} x),$$

where the eigenvalues λ_j's are determined implicitly from the zeros of the Bessel function

$$\lambda_j = (z_{mj}/a)^2,$$

where

$$J_m(z_{mj}) = 0, \quad \text{and } z_{mj} \text{ is the } j\text{th root of } J_m(z) = 0.$$

The eigenvalues are discrete, real, positive, infinite in number, and tend to infinity as $j \to \infty$. The eigenfunctions are orthogonal with respect to weight x.

$$\frac{2}{a^2} \int_0^a J_m(\sqrt{\lambda_j} x) J_m(\sqrt{\lambda_k} x) x dx = J_{m+1}^2(z_{mj}) \delta_{jk}.$$

An arbitrary piecewise continuous function $f(x)$ can be expanded in a Bessel series as:

$$f(x) = \sum_{j=1}^{\infty} a_j J_m(z_{mj} x/a), \quad 0 < x < a$$

where

$$a_j = \frac{2}{a^2} \int_0^a f(x) J_m(z_{mj} x/a) x dx / J_{m+1}^2(z_{mj}).$$

and the representation will converge to $f(x)$ in the mean.

(d) Spherical Bessel

$$(x^2 y')' + [\lambda x^2 - n(n+1)]y = 0, \quad 0 < x < a$$

$$y(0) \text{ bounded and } y(a) = 0.$$

This is a singular Sturm-Liouville system with

$$p(x) = x^2 > 0, \quad 0 < x < a, \quad p(x) = 0 \text{ at } x = 0.$$
$$r(x) = r^2 > 0, \quad 0 < x < a$$
$$q(x) = n(n+1)$$

The eigenfunction is

$$y(x) = \phi_j(x) = j_n(\sqrt{\lambda_j} x),$$

where

$$\sqrt{\lambda_j} = z_{nj}/a, \quad j = 1, 2, 3, \ldots.$$

with z_{nj} being the jth positive root to $j_n(z) = 0$

$$0 < \lambda_1 < \lambda_2 < \lambda_3 < \ldots.$$

The eigenfunctions are orthogonal with respect to weight x^2:

$$\frac{2}{a^3} \int_0^a j_n(z_{nj} x/a) j_n(z_{nk} x/a) x^2 dx = j_{n+1}^2(z_{nj}) \delta_{jk}$$

An arbitrary piecewise continuous function $f(x)$ can be expanded in a spherical Bessel series as:

$$f(x) = \sum_{j=1}^{\infty} a_j j_n(z_{nj} x/a), \quad 0 < x < a$$

where

$$a_j = \frac{2}{a^3} \int_0^a f(x) j_p(z_{nj}/a) x^2 dx / j_{n+1}^2(z_{nj}),$$

and the representation will converge to $f(x)$ in the mean.

(e) Chebyshev

$$[(1-x^2)^{1/2}y']' + [\lambda\frac{1}{(1-x^2)^{1/2}}]y = 0, \quad -1 < x < 1$$

$$y \quad \text{bounded at} \quad x = \pm 1.$$

The eigenfunction is

$$y(x) = \phi_n(x) \equiv T_n(x),$$

where the Chebyshev polynomiial of the first kind is defined by

$$T_n(x) = \cos(n\cos^{-1}x).$$

The corresponding eigenvalue is

$$\lambda = \lambda_n \equiv n^2, \quad n = 0, 1, 2, 3, \ldots$$

The eigenfunctions are orthogonal with respect to weight $r(x) = (1-x^2)^{-1/2}$:

$$\frac{2}{\pi}\int_{-1}^{1} T_n(x)T_{n'}(x)(1-x^2)^{-1/2}dx = \begin{cases} \delta_{nn}, & n \neq 0 \\ 2, & n = n' = 0 \end{cases}$$

Any arbitrary piecewise continuous function $f(x)$ can be expanded in a Chebyshov series:

$$f(x) = \sum_{n=0}^{\infty} a_n T_n(x), \quad -1 < x < 1$$

where

$$a_n = \frac{2}{\pi}\int_{-1}^{1} f(x)T_n(x)((1-x^2)^{-1/2}dx, \quad n > 0$$

$$a_0 = \frac{1}{\pi}\int_{-1}^{1} f(x)(1-x^2)^{-1/2}dx.$$

The appretation will converge to $f(x)$ in the mean.

(f) Hermite

$$y'' + (\lambda - x^2)y = 0, \quad -\infty < x < \infty$$

$$y \;\; \text{bounded as } x \to \pm\infty.$$

This is a singular Sturm-Liouville system because the domain is infinite.

The eigenfunctions are

$$y(x) = \phi_n(x) \equiv e^{-x^2/2} H_n(x),$$

where $H_n(x)$ is the Hermite polynomial of order n.

The eigenvalues are discrete:

$$\lambda = \lambda_n \equiv (2n+1), \quad n = 0, 1, 2, \ldots,$$

despite the fact that the domain is infinite. This is because the eigenfunctions decrease so rapidly as $x \to \pm\infty$ that $\int_{-\infty}^{\infty} \phi_n(x)^2 dx$ is finite.

The orthogonality condition is

$$\frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{\infty} e^{-x^2} H_n(x) H_{n'}(x) dx = \delta_{nn}.$$

An arbitrary piecewise continuous function $f(x)$ can be expanded in a Hermite series provided that the integrals are finite (i.e. $f(x)e^{-x^2/2}H_n(x)$ is integrable).

$$f(x) = \sum_{n=0}^{\infty} a_n e^{-x^2/2} H_n(x), \quad -\infty < x < \infty$$

where

$$a_n = \frac{1}{2^n n! \sqrt{\pi}} \int_{-\infty}^{\infty} f(x) e^{-x^2/2} H_n(x) dx.$$

The representation will converge to $f(x)$ in the mean.

12.11 Eigenfunction expansion

The method of eigenfunction expansion is useful in solving non-homogeneous partial differential equations. This will be discussed in a later chapter. Here we demonstrate the concept using ordinary differential equaitons.

The completeness theorem for eigenfunctions for the Sturm-Liouville system allows an arbitrary function $f(x)$ to be represented by an infinite sum of the eigenfunctions. Since any set of Sturm-Liouville eigenfunctions will do, we have the choice of picking a particular set to suit the problem at hand. This will be illustrated in the following examples.

Consider the simple nonhomogeneous boundary value problem

$$y'' + \lambda y = 1, \quad 0 < x < L$$

$$y'(0) = 0, \quad y'(L) = 0.$$

We know that the set of eigenfunctions

$$\phi_n(x) = \cos\frac{n\pi x}{L}, \quad 0 < x < L, \quad n = 0, 1, 2, 3, \ldots$$

is complete, and so an arbitrary function, including the unknown $y(x)$, can be expanded in a cosine series

$$y(x) = \sum_{n=0}^{\infty} b_n \cos\frac{n\pi x}{L}, \quad 0 < x < L$$

The choice of cosines series has the advantage that the boundary conditions at $x = 0$ and $x = L$ are automatically satisfied. Substituting the assumed cosine series into the differential equation, we get:

$$\sum_{n=0}^{\infty}[-(\frac{n\pi}{L})^2 + \lambda]b_n \cos\frac{n\pi x}{L} = \sum_{n=0}^{\infty} f_n \cos\frac{n\pi x}{L}$$

where we have also expanded the forcing term, 1 in this case, in a cosine series. So $f_0 = 1$, $f_n = 0$, $n > 0$.

Equating the coefficients of cosines, we get

$$[\lambda - (\frac{n\pi}{L})^2]b_n = f_n, \quad n = 0, 1, 2, 3, \ldots$$

If $\lambda \neq (\frac{n\pi}{L})^2$, $n = 0, 1, 2, 3, \ldots$, the coefficients b_n can be determined as

$$b_n = f_n/[\lambda - (\frac{n\pi}{L})^2],$$

and so

$$\begin{aligned} &b_n = 0, \quad \text{for } n = 1, 2, 3, \ldots \\ &b_0 = f_1/\lambda = 1/\lambda \end{aligned}$$

The solution is then simply

$$y(x) = 1/\lambda.$$

[One could have guessed this solution by trying $y(x) = \text{constant}$.] If however, λ is equal to one of the nonzero eigenvalues, say $(\frac{\pi}{L})^2$, then b_1 does not need to be zero, and can be arbitrary.

$$y(x) = 1/\lambda + b_1 \cos\frac{\pi x}{L}.$$

[If $\lambda = 0$, then it is easier to go back to the equation:

$$y'' = 1$$

and integrate twice to yield

$$y(x) = \frac{x^2}{2} + Ax + B$$

$A = 0$ to satisfy the boundary condition at $x = 0$. The boundary condition at $x = L$ cannot be satisfied. Therefore there is no solution to this problem. The problem was actually not well posed.]

Now consider the problem:

$$[(1 - x^2)y']' + \lambda y = 1, \qquad -1 < x < 1.$$

We can still use the cosine series to represent the unknown:

$$y(x) = \sum_{n=0}^{\infty} b_n \cos \frac{n\pi x}{L},$$

but because of the nonuniform coefficients $(1 - x^2)$, the first term in the differential equation becomes very complicated when expressed in terms of b_n. A better way is to represent $y(x)$ in terms of Legendre polynomials $P_n(x)$:

$$y(x) = \sum_{n=0}^{\infty} a_n P_n(x), \qquad -1 < x < 1$$

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

since $P_n(x)$ satisfies

$$\frac{d}{dx}[(1 - x^2)\frac{d}{dx}P_n] + n(n+1)P_n = 0.$$

The boundary conditions are also satisfied.

The differential equation implies:

$$\sum_{n=0}^{\infty} [\lambda - n(n+1)] a_n P_n(x) = 1$$

Since $P_0(x) = 1$, we have

$$a_0 = 1/\lambda$$
$$a_n = 0, \quad n = 1, 2, 3, \ldots$$

if $\lambda \neq m(m+1)$, $m = 0, 1, 2, 3, \ldots$.

If $\lambda = m(m+1)$ for some integer $m \neq 0$, the solution becomes

$$y(x) = 1/\lambda + b_m P_m(x),$$

for arbitrary constant b_m.

[If $\lambda = 0$, the equation is

$$[(1 - x^2)y']' = 1$$

Integrate once

$$(1 - x^2)y' = x + A$$
$$y' = \frac{x}{1 - x^2} + \frac{B}{1 - x^2}$$

Integrate again:

$$y(x) = \ell n[(1 - x^2)^{-1/2}] + B\ell n[\frac{(1 + x)^{1/2}}{(1 - x)^{1/2}}] + C$$

$B = -1$ to satisfy one of the boundary conditions. y bounded at $x = 1$.

$$y(x) = \ell n[\frac{1}{1 + x}] + C.$$

The boundary condition at $x = -1$ cannot be satisfied. There is therefore no solution for $\lambda = 0$.]

Chapter 13

Schrödinger's Equation for the Hydrogen Atom

13.1 Introduction

The case of the hydrogen atom is particularly simple, because there is only one electron revolving around a nucleus consisting of only one proton. Because the proton is 1864 times heavier than the electron, the center of mass of the proton-electron system is located at the nucleus, which we will take to be the origin in a spherical coordinate. The wave function ψ for the eletron is described by the Schrödinger's equation.

$$i\hbar\frac{\partial}{\partial t}\psi = -\frac{\hbar^2}{2\mu}\nabla^2\psi + V(r)\psi, \tag{13.1}$$

where $V(x)$ is the force potential. In this case it is the Columb electric potential of the proton on the electron:

$$V(r) = -\frac{e^2}{4\pi\epsilon_0}\frac{1}{r} \equiv -\epsilon^2/r. \tag{13.2}$$

e is the electron charge of the proton (and $-e$ that of the electron). ϵ_0 is the "permittivity of space," and r is the radial distance from the origin (the nucleus). The negative sign implies an attractive force ($F \equiv -\frac{\partial}{\partial r}V = -\epsilon^2/r^2$) towards the nucleus. We now proceed to solve (13.1) with (13.2) as the force potential.

13.2 Separation of Variables

The usual method of sepparation of variables suggests starting with the assumption:

$$\psi = u(\mathbf{x})T(t)$$

and so:

$$i\hbar\frac{T'(t)}{T(t)} = -\frac{\hbar^2}{2\mu}\frac{\nabla^2 u}{u} + V(r) = \text{const} \equiv E \tag{13.3}$$

Becuase the left-hand side is a function of t only and the right-hand side is a function of $\mathbf{x}$ only, they can be equal to each other only if each is equal to a constant. We denote this separation constant by E, so far undetermined. (13.3) splits into two equations of reduced dimension:

$$i\hbar T'(t) = ET(t) \tag{13.4}$$

$$-\frac{\hbar^2}{2\mu}\nabla^2 u = (E - V(r))u \tag{13.5}$$

The time part can be solved simply as

$$T(t) = T(0)e^{-i(E/\hbar)t} \equiv T(0)e^{-i\omega t} \tag{13.6}$$

Since the frequency ω is now $E/\hbar$, and in quantum mechanics, enery = frequency times $\hbar (= \omega\hbar)$, we shall now interprete the separation constant E as the energy of the electron.

The remaining equation (13.5) is a partial differential equation involving space derivatives only. Without the V term, (13.5) is the Helmoltz's equation. The Laplace operator is in spherical coordinates:

$$\nabla^2 u = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}u) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}u) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}u.$$

Separation of variables:

$$u(r,\theta,\varphi) = R(r)Y(\theta,\varphi)$$

yields

$$\begin{aligned}\frac{\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta\frac{\partial}{\partial\theta}Y) + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}Y}{Y} &= -\frac{2\mu}{\hbar^2}(E - V(r))r^2 - \frac{\frac{d}{dr}(r^2\frac{d}{dr}R)}{R} \\ &= \text{constant} \equiv -\eta \end{aligned}\tag{13.7}$$

(13.7) contains two equations:

$$\frac{1}{\sin\theta}\frac{\partial}{\partial\theta}(\sin\frac{\partial}{\partial\theta}Y)+\frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\varphi^2}Y+\eta Y=0, \tag{13.8}$$

and

$$\frac{d}{dr}(r^2\frac{d}{dr}R)+\left[\frac{2\mu}{\hbar^2}(E-V(r))r^2-\eta\right]R=0. \tag{13.9}$$

Equation (13.8) is the spherical harmonic equation for the angular dependences, and is to be solved subject to 2π-periodic boundary condition in φ and boundedness at $\theta=0$ and $\theta=\pi$. The eigenvalues are

$$\eta=\eta_\ell\equiv\ell(\ell+1), \quad \ell=0,1,2,3,\ldots \tag{13.10}$$

with the corresponding eigenfunctions:

$$Y(\theta,\varphi)=Y_{\ell m}(\theta,\varphi)\equiv\sqrt{\frac{(2\ell+1)(\ell-m)!}{4\pi(\ell+m)!}}P_\ell^m(\cos\theta)e^{im\varphi}, \quad -\ell\le m<\ell, \tag{13.11}$$

13.3 Balmer's equation

The radial equation (13.9) is called Balmer's equation in physics. We shall try to put it into the Sturm-Liouville form by defining:

$$b\equiv 2\mu\epsilon^2/\hbar^2, \quad \lambda^2\equiv 2\mu E/\hbar^2, \quad x=r, \quad y(x)=R(r).$$

$$\frac{d}{dx}(x^2\frac{d}{dx}y)+(\lambda^2x^2+bx-\ell(\ell+1))y=0, \quad 0<x<\infty. \tag{13.12}$$

Without the Columb force ($\epsilon=0$), (13.12) is just the spherical Bessel equation, which we have discussed in Chapters 10 and 11. We shall examine the case of $\epsilon\neq 0$ using the Sturm-Liouville theory. (13.12) is a singular Sturm-Liouville system because $p(x)\equiv x^2=0$ at $x=0$, $r(x)\equiv x^2=0$ at $x=0$, and because the domain is infinite. The proper boundary conditions should be

$$y(x) \text{ bounded at } x=0 \quad \text{and as } x\to\infty.$$

An alternate form for (13.12) may be more useful in some cases. This is obtained by letting

$$y(x)=x^{-1}w(x), \quad \frac{d}{dx}(x^2\frac{d}{dx}y)=xw''(x).$$

Thus (13.12) becomes

$$x\{w''(x) + [\lambda^2 + b/x - \ell(\ell+1)/x^2]w(x)\} = 0, \tag{13.13}$$

For large x,

$$[\lambda^2 + b/x - \ell(\ell+1)/x^2] \cong \lambda^2,$$

and so (13.13) becomes

$$w''(x) + \lambda^2 w = 0.$$

For positive λ^2, the solution can be written in the form

$$w(x) \sim Ae^{i\lambda x} + Be^{-i\lambda x}$$

and so

$$y(x) \sim \frac{1}{x}\{Ae^{i\lambda x} + Be^{-i\lambda x}\}, \quad x \gg 1 \tag{13.14}$$

[In Chapter 11 we wrote the solution in the form

$$y(x) = \frac{1}{x}[A\sin(\lambda x) + B\cos(\lambda x)]$$

and discarded the cosine term because it blows up at $x = 0$. Now since the solution is valid only for large x, we cannot apply the boundary condition at $x = 0$. So we need to keep both terms. It is more important to write it in the complex form of (13.14).]

The solution (13.14) represents *scattering* solutions. These are possible whenever the energy of the electron, E, is higher than the potential $V(x)$. In that case, the electron is not trapped by the electric Columb attraction and scatters to $r \to \infty$. One of the terms in (13.14), the $e^{i\lambda x}$, represents scattering out towards $r = \infty$, and the other, $e^{-i\lambda x}$, from $r = \infty$ inward. We set $B = 0$ if we know that the electron is initially located near the nucleus.

The solution (13.14) satisfies boundedness condition as $x \to \infty$ *for any real* λ. Therefore the "eigenvalue λ^2", which corresponds to positive energy E, is *continuous*. That is

$$0 < \lambda^2 < \infty \tag{13.15}$$

is a *continuous spectrum*.

The result is anticipated by the singular Strum-Liouville case for an infinite domain, when

$$\int_0^\infty |y(x)|^2 x^2 dx \text{ is unbounded.}$$

[13.14 yield a constant integrand (at least for large x), which does not decay as $x \to \infty$. So the integral is unbounded.]

13.4 The Bound states

Bound states, where the electron is trapped by the Columb potential near the nucleus, is possible only for negative λ^2, i.e. for electron energy less than the far field potential $V(r)$. The possibility of negatige eigenvalues is consistent with Sturm-Liouville theory when $q(x) = \ell(\ell+1) - bx$ is negative. We can still put (13.12) into the Liouville form even for negative λ^2, by defining

$$x = \alpha r, \quad y(x) = R(r), \quad \alpha \equiv (-8\mu E/\hbar^2)^{1/2}.$$

(13.12) becomes the following Sturm-Liouville eigenvalue problem:

$$\frac{d}{dx}(x^2\frac{d}{dx}y) + [\nu x - \ell(\ell+1) - \frac{1}{4}x^2]x = 0, \quad 0 < x < \infty. \tag{13.16}$$

$$y \text{ bounded at } x = 0 \text{ and as } x \to \infty.$$

Here

$$\nu \equiv \frac{2\mu\epsilon^2}{\alpha\hbar^2} = \frac{\epsilon^2}{\hbar}(\frac{\mu}{-2E})^{1/2}$$

is the new eigenvalue parameter.

Sturm-Liouville theory applied to the bound states, with

$$p(x) = x^2 > 0, \quad r(x) = x > 0, \quad \text{in } 0 < x < \infty$$
$$q(x) = \ell(\ell+1) + \frac{1}{4}x^2 > 0, \quad \text{in } 0 < x < \infty,$$

predicts positive and discrete eigenvalues ν provided that

$$\int_0^\infty |y|^2 x dx \text{ is bounded,} \tag{13.17}$$

which it should be for bound states.

Let's investigate the behavior for large x. Again we write

$$y(x) = x^{-1}w(x),$$

and so

$$(x^2y')' = xw''$$

(13.16) becomes (exactly):

$$\frac{d^2}{dx^2}w + [-\frac{1}{4} + \frac{\nu}{x} - \frac{\ell(\ell+1)}{x^2}]w = 0. \tag{13.18}$$

For $x \gg 1$, (13.18) reduces, approximately, to

$$\frac{d^2}{dx^2}w - \frac{1}{4}w = 0, \quad x \gg 1,$$

with the solution

$$w(x) = Ae^{-x/2} + Be^{x/2}.$$

To have a bounded solution as $x \to \infty$, we set $B = 0$. The solution

$$y(x) = \frac{1}{x}w(x) \sim \frac{A}{x}e^{-x/2}$$

decays exponentially to zero as $x \to \infty$. Thus all bound states (with $E < 0$) satisfy (13.17) and the corresponding wave functions ψ are said to be "normalizable":

$$\iiint |\psi|^2 dV = \int_0^\infty r^2 dr \int_0^\pi \sin\theta d\theta \int_0^{2\pi} d\varphi |\psi|^2 = 1,$$

where the integral is performed over an infinite sphere.

Near $x = 0$, the Frobenius solution procedure suggests trying

$$w(x) \sim x^\beta \qquad \text{as } x \to 0$$

to obtain the indicial equation from (13.18):

$$\beta(\beta - 1) - \ell(\ell + 1) = 0.$$

Thus the roots are

$$\beta_1 = -\ell, \quad \beta_2 = \ell + 1.$$

The boundedness boundary condition at $x = 0$ suggests that we should seek the Frobenius series solution corresponding to the index β_2 of the form.

$$w(x) = x^{\ell+1}u(x),$$

where $u(x)$ is a power series. Better yet, we shall try to seek solution of the form:

$$w(x) = x^{\ell+1}e^{-x/2}v(x), \tag{13.19}$$

with

$$v(x) = \sum_{j=0}^{\infty} a_j x^j \tag{13.20}$$

If (13.20) converges and does not grow exponentially, then $y(x)$ satisfies the boundary conditions at both $x = 0$ and $x \to \infty$.

Substituting the assumed form (13.19) into (13.18), we obtain the equation for $v(x)$ to be:

$$x\frac{d^2v}{dx^2} + [2(\ell+1) - x]\frac{dv}{dx} + (\nu - \ell - 1)v = 0 \tag{13.21}$$

This is the generalized Laguerre differential equation. We substitute the power series solution (13.20) into (13.21):

$$\sum_{j=0}^{\infty} j(j+1)a_{j+1}x^j + 2(\ell+1)\sum_{j=0}^{\infty}(j+1)a_{j+1}x^j - \sum_{j=0}^{\infty} j a_j x^j$$
$$+ [\nu - \ell - 1]\sum_{j=0}^{\infty} a_j x^j = 0.$$

Equating the coefficients of like power yields:

$$j(j+1)a_{j+1} + 2(\ell+1)(j+1)a_{j+1} - ja_j + [\nu - \ell - 1]a_j = 0$$

or

$$a_{j+1} = \left\{\frac{(j+\ell+1) - \nu}{(j+1)(j+2\ell+2)}\right\} a_j, \quad j = 0, 1, 2, 3, \ldots. \tag{13.22}$$

Starting from an arbitrary nonzero a_0, the recurrent relationship (13.22) then gives us all the a_j's.

The power series converges, since by ratio test:

$$\lim_{j\to\infty} |a_{j+1}/a_j| = \lim |\frac{(j+\ell+1) - \nu}{(j+1)(j+2\ell+2)}| \to 0.$$

However, the series generally tends to converge to an exponentially growing solution. This can be seen in

$$a_{j+1}/a_j \cong \frac{1}{j+1} \quad \text{for large } j$$

and so

$$a_j \cong \frac{\text{constant}}{j!}$$

Suppose this were exact, then

$$v(x) = \text{const}\sum_{j=0}^{\infty}\frac{1}{j!}x^j = Ae^x.$$

Hence

$$w(x) = x^{\ell+1}e^{-x/2}v(x) = Ax^{\ell+1}e^{x/2}$$

would be unbounded as $x \to \infty$. This is not surprising, because in general $w(x)$ is a superposition of $e^{-x/2}$ and $e^{x/2}$ for large x. This series (13.20) must terminate in order for this not to happen. Therefore, there must be some maximum integer, $j_{\max}$, such that

$$a_{j_{\max}+1} = 0.$$

From (13.22) this occurs when

$$j_{\max} + \ell + 1 - \nu = 0,$$

yielding the eigenvalue:

$$\nu = n \equiv j_{\max} + \ell + 1, \tag{13.23}$$

$n = 1, 2, 3, \ldots$ is called the *principle quantum number.*

The energy is thus determined to be

$$\begin{aligned} E = E_n &= -\frac{\mu\epsilon^4}{2\hbar^2}\frac{1}{\nu^2} = -\frac{\mu\epsilon^4}{2\hbar^2}\frac{1}{n^2} \\ &\equiv \frac{E_1}{n^2}, \quad n = 1, 2, 3, \ldots \end{aligned} \tag{13.24}$$

where

$$E_1 \equiv -\frac{\mu\epsilon^4}{2\hbar^2} = -13.6\text{eV}$$

is the *ground state* energy. The *ground state* is the state of lowest energy and it occurs for $n = 1$. 13.6eV is also the *binding energy* of hydrogen; it is the amount of energy required to ionize the atom, i.e., strip the electron from the nucleus. The energy for $n > 1$ corresponds for *excited states.*

Although a single index, n, characterizes the energy eigenvalue, to characterize completely the eigenfunction (in three dimensions) we need two more indices, ℓ and m. For each n, the possible values of ℓ are, from (13.23):

$$\ell = 0, 1, 2, \ldots, n-1$$

(for varous values of $j_{\max}$; the lower the $j_{\max}$ value, the lower the order of the polynomial for the eigenfunction $v(x)$). For each value of ℓ, there are $(2\ell + 1)$ possible values of m, since

$$-\ell \le m \le \ell.$$

The degree of degeneracy (d) is the number of possible eigenfunctions occupying the same energy level, and so for $E = E_n$ it is

$$d(n) = \sum_{\ell=0}^{n-1}(2\ell + 1) = n^2. \tag{13.25}$$

13.5 The eigenfunctions in the bound states

The eigenfunctions for $v(x)$ are polynomials. These are called the associated Laguerre polynomials:

$$v(x) = v_{n\ell}(x) = L_{n-\ell-1}^{2\ell+1}(x), \tag{13.26}$$

Similar to the associated Legendre functions, it is related to the Laguerre polynomials through differentiation:

$$L_{q-p}^{p}(x) = (-\frac{d}{dx})^2 L_q(x)$$

and the qth Laguerre polynomial of an elementary function:

$$L_q(x) = e^x(\frac{d}{dx})^q(e^{-x}x^q).$$

The hydrogen wave function for each bound state is given by

$$\psi_{n\ell m} = R_{n\ell}(r)Y_{\ell m}(\theta, \varphi).$$

We will derive and work out the details of the first few eigenfuncntions below.

For $n = 1$, the *ground state*, we must have $\ell = 0$ and $m = 0$, and so the eigenfunction is

$$\psi_{100} = R_{10}(r)Y_{00}(\theta, \varphi) = R_{10}(r) \cdot \frac{1}{\sqrt{4\pi}},$$

since $Y_{00}(\theta, \varphi) = 1/\sqrt{4\pi}$. This ground state is spherically symmetric. From (13.23) we have $j_{\max} = 0$ and so the power series for $v(x)$ terminates after one term:

$$\begin{aligned} v(x) &= a_0 \\ R_{10}(r) &= a_0 x^0 e^{-x/2} = a_0 e^{-x/2} = a_0 e^{-r/a}, \end{aligned}$$

where we have written:

$$\alpha = 2/(na), \quad n = 1, 2, 3, \ldots$$
$$a \equiv \hbar^2/(\mu\epsilon^2) = 0.529 \times 10^{-10}m$$

is the so-called *Bohr radius.* The constant a_0 is to be chosen so that the probability density is normalized to 1 when integrated over an infinite sphere.

$$\iiint |\psi_{100}|^2 r^2 dr \sin\theta d\theta d\varphi = \int_0^\infty |R_{10}(r)|^2 r^2 dr = 1.$$

Consequently,

$$\psi_{100}(r, \theta, \varphi) = (\pi a^3)^{-1/2} \cdot e^{-r/a}. \tag{13.27}$$

For $n = 2$, the first excited state, the energy is

$$E_2 = -13.6\text{eV}/4 = -3.4\text{eV}.$$

There are actually four different states which share this same energy level, since for $n = 2$ we can have

$$\ell = 0, \qquad \text{in which case } m \text{ must be } 0,$$

or

$$\ell = 1, \qquad \text{in which case we can have } m = -1,\, 0, \text{ or } 1.$$

For $\ell = 0$, (13.23) imiplies that $j_{\max} = 1$, and so $v(x)$ is a first order polynomial. The recurrence relationship yields $a_1 = -\frac{1}{2}a_0$, and so

$$v(x) = a_0(1 - \frac{1}{2}x)$$
$$R_{20}(r) = a_0(1 - \frac{1}{2}x)e^{-x/2} = a_0(1 - \frac{r}{2a})e^{-r/2a}$$

For $\ell = 1$, $v(x)$ is a constant a_0, and

$$R_{21}(r) = a_0(r/a)e^{-r/2a}$$

[The a_0's are to be determined for each case through normalization.]

For the general n case, the radial eigenfunction is, from (13.6):

$$R_{n\ell}(r) = \text{constant} \cdot e^{-r/(na)}(\frac{2r}{na})^\ell L^{2\ell+1}_{n-\ell-1}(\frac{2}{na}r).$$

Consequently

$$\psi_{n\ell m} = \sqrt{(\frac{2}{na})^3 \frac{(n-\ell-1)!}{2n[(n+\ell)!]^3}} \cdot e^{-r/na} \cdot (\frac{2r}{na})^\ell L^{2\ell+1}_{n-\ell-1}(\frac{2r}{na}) Y_{\ell m}(\theta, \varphi).$$

13.6 The spectrum of Hydrogen

A hydrogen atom in an exited state may transition to a lower energy state by emitting energy in the form of electromagnetic radiation (light). The energy of the emitted radiation is the difference bewteen the initial and final states (before and after the transition)

$$\Delta E = E_{ini} - E_{fin} = -13.6\text{eV}(\frac{1}{n_i^2} - \frac{1}{n_f^2}).$$

According to the Panck formula

$$\text{energy} \;=\; \text{frequency times } \hbar,$$

while the wavelength of light is given by

$$\begin{aligned} \text{wavelength, } \lambda, &= (c/2\pi)/ \text{ frequency,} \\ \lambda &= (ch)/\Delta E \\ \frac{1}{\lambda} &= R(\frac{1}{n_f^2} - \frac{1}{n_i^2}), \end{aligned} \tag{13.28}$$

(13.28) is the *Rydberg formula* for the spectrum of hydrogen discovered in the nineteenth century through empirical experiments. The constant R is known as the Rydberg constant. It is now predicted in terms of fundamental constants of physics:

$$R \equiv \frac{\mu}{4\pi c\hbar^3}(\frac{e^2}{4\pi\epsilon_0})^2 = 1.097 \times 10^7 m^{-1}.$$

Transitions to the ground state ($n_f = 1$) yields ΔE between 10.2 and 13.6eV, and so lie in the ultraviolet. They are known as the Lyman series (for any n_i). Transitions to the first excited state ($n_f = 2$) yields ΔE between 1.9 and 3.4eV, and lie in the visible region; They are known as the Balmer series. Transitions to $n_f = 3$ are in the inferred and are known as the Paschen series, with ΔE between 0.7 and 1.5eV.

Chapter 14

Nonhomogeneous Partial Differential Equations

14.1 Introduction

The method of eigenfunction expansions is used to solve nonhomogeneous partial differential equations.

Consider the following nonhomogeneous heat equation (with a given *heating* term $f(x,t)$) subject to the general boundary condition (which includes Dirichlet and Neumann as special cases):

$$\begin{aligned} &\text{PDE:} && u_t = \alpha^2 u_{xx} + f(x,t), \quad 0 < x < L, \quad t > 0 && (14.1)\\ &\text{BCs:} && \alpha_1 u_x(0,t) + \beta_1 u(0,t) = 0 && (14.2)\\ & && \alpha_2 u_x(L,t) + \beta_2 u(L,t) = 0 &&\\ &\text{IC:} && u(x,0) = \phi(x), \quad 0 < x < L. && (14.3) \end{aligned}$$

14.2 Eigenfunction expansion

Step 1: Find the eigenfunction of the homogeneous problem. That is, first (drop $f(x,t)$ and) solve the following homogeneous problem:

$$\text{PDE:} \quad u_t = \alpha^2 u_{xx}, \quad 0 < x < L, \quad t > 0 \tag{14.4}$$

$$\begin{aligned} \text{BCs}: \quad & \alpha_1 u_x(0,t) + \beta_1 u(0,t) = 0\\ & \alpha_2 u_x(L,t) + \beta_2 u(L,t) = 0. \end{aligned} \tag{14.5}$$

Write its solution in the form

$$u(x,t) = \sum_n T_n(t)X_n(x),$$

where the eigenfunctions, $X = X_n$ are determined by

$$\begin{cases} X''(x) + \lambda^2 x(x) = 0 \\ \alpha_1 X'(0) + \beta_1 X(0) = 0 \\ \alpha_2 X'(L) + \beta_2 X(L) = 0 \end{cases} \tag{14.6}$$

with the eigenvalues, $\lambda = \lambda_n$.

Do not work out $T_n(t)$ yet, since it will turn out that the $T_n(t)$ for the nonhomogeneous problem will be different than the $T_n(t)$ for the homogeneous problem.

Step 2: Expand the forcing term $f(x,t)$:

$$\boxed{f(x,t) = \sum_n f_n(t)X_n(x)}. \tag{14.7}$$

and expand the solution of the nonhomogeneous PDE in terms of these eigenfunction the same way:

$$\boxed{u(x,t) = \sum_n T_n(t)X_n(x)}. \tag{14.8}$$

Step 3: Substitute (10.7) and (10.8) into the PDE (10.1): Note that

$$\begin{aligned} u_t &= \sum_n T_n'(t)X_n(x) \\ u_{xx} &= \sum_n T_n(t)X_n''(x) = -\sum_n \lambda_n^2 T_n(t)X_n(x). \end{aligned}$$

Thus (10.1) becomes

$$\sum_n [T_n'(t) + \alpha^2\lambda_n^2 T_n(t) - f_n(t)]X_n(x) = 0. \tag{14.9}$$

because X_n's are orthogonal, (10.9) implies that

$$T_n'(t) + \alpha^2\lambda_n^2 T_n(t) - f_n(t) = 0. \tag{14.10}$$

Step 4: To satisfy the initial condition, we require

$$\boxed{u(x,0) = \phi(x) = \sum_n T_n(0)X_n(x)}, \tag{14.11}$$

yielding (see (9.22)):

$$T_n(0) = \frac{\int_0^L \phi(x)X_n(x)dx}{\int_0^L X_n^2(x)dx}. \tag{14.12}$$

Step 5: Solve the nonhomogeneous ODE (10.10) to get

$$\boxed{T_n(t) = T_n(0)e^{-\alpha^2\lambda_n^2 t} + \int_0^t e^{-\alpha^2\lambda_n^2(t-\tau)} f_n(\tau)d\tau}. \tag{14.13}$$

14.3 An example

Solve:

$$\begin{array}{ll} \text{PDE:} & u_t = \alpha^2 u_{xx} + \sin(3\pi x), \quad 0 < x < 1, \quad t > 0 \\ \text{BCs:} & u(0,t) = 0, \quad u(1,t) = 0 \\ \text{IC:} & u(x,0) = \sin(\pi x), 0 < x < 1. \end{array} \tag{14.14}$$

The eigenfunctions and eigenvalues of the homogeneous PDE are

$$\begin{aligned} X(x) = X_n(x) &= \sin \lambda_n x \\ \lambda = \lambda_n &= n\pi, \quad n = 1, 2, 3, \ldots \end{aligned}$$

We will therefore use a sine series expansion of the solution:

$$u(x,t) = \sum_{n=1}^{\infty} T_n(t) \sin n\pi x, \quad 0 < x < 1,$$

and the forcing term:

$$f(x,t) = \sin 3\pi x = \sum_{n=1}^{\infty} f_n \sin n\pi x, \quad 0 < x < 1.$$

The latter means simply $f_n = 0$ except $f_3 = 1$. Substituting the expansions into the PDE, we have

$$T_n'(t) - \alpha^2(n\pi)^2 T_n = f_n, \quad n = 1, 2, 3, \ldots.$$

For $n \neq 3$, this is

$$T_n'(t) - \alpha^2(n\pi)^2 T_n(t) = 0,$$

so

$$T_n(t) = T_n(0)e^{-\alpha^2 n^2 \pi^2 t}, \quad n \neq 3.$$

For $n = 3$:

$$T_3'(t) - 9\pi^2\alpha^2 T_3(t) = 1.$$

The solution is:

$$T_3(t) = T_3(0)e^{-9\pi^2\alpha^2 t} + \frac{1}{(3\pi\alpha)^2}[1 - e^{-9\pi^2\alpha^2 t}].$$

To satisfy the initial condition, we require

$$\sin \pi x = \sum_{n=1}^{\infty} T_n(0) \sin n\pi x, \quad 0 < x < 1,$$

so we take $T_n(0) = 0$ except $T_1(0) = 1$. Thus,

$$\begin{aligned} T_1(t) &= e^{-\alpha^2\pi^2 t} \\ T_2(t) &= 0 \\ T_3(t) &= \frac{1}{(3\pi\alpha)^2}[1 - e^{-(3\pi\alpha)^2 t}] \\ T_4(t) &= 0 \\ &\vdots \end{aligned}$$

The final solution is the two-term expansion

$$u(x,t) = e^{-(\alpha\pi)^2 t} \sin \pi x + \frac{1}{(3\pi\alpha)^2}[1 - e^{-(3\pi x)^2 t}] \sin(3\pi x).$$

Comments

For this simple problem where the forcing term $f(x,t)$ is a function of x only, there exists an alternative, perhaps simpler method. We write the solution as the sum of two parts, a steady state solution, $u_{\text{steady}}(x)$, and a transient solution, $u_{\text{transient}}(x,t)$. The steady state solution is to satisfy the steady state PDE, i.e. (10.14) without the time derivative term:

$$0 = \alpha^2 \frac{d^2}{dx^2} u_{\text{steady}} + \sin(3\pi x).$$

This yields

$$u_{\text{steady}}(x) = \frac{1}{(3\pi\alpha)^2}\sin(3\pi x).$$

The transient solution is found by substituting

$$u(x,t) = u_{\text{steady}}(x) + u_{\text{transient}}(x,t)$$

into the original PDE, (10.14). Thus $u_{\text{transient}}$ now satisfies a *homogeneous* PDE:

$$\begin{array}{ll} \text{PDE:} & \dfrac{\partial}{\partial t}u_{\text{transient}} = \alpha^2\dfrac{\partial^2}{\partial x^2}u_{\text{transient}} \\ \text{BC:} & u_{\text{transient}}(0,t) = u_{\text{transient}}(1,t) = 0 \\ \text{IC:} & u_{\text{transient}}(x,0) = \sin(\pi x) - u_{\text{steady}}(x). \end{array}$$

The solution to this system is

$$u_{\text{transient}}(x,t) = e^{-(\alpha\pi)^2 t}\sin(\pi x) - \frac{1}{(3\pi\alpha)^2}e^{-(3\pi\alpha)^2 t}\sin(3\pi x).$$

Chapter 15

Collapsing Bridges

15.1 Introduction

As an application of eigenfunction expansion to nonhomogeneous PDEs, we consider the oscillations of suspension bridges under forcing. The forcing could come from wind, as in the case of the collapse of the Tacoma Narrow's Bridge in 1940, or as a result of a column of soldiers marching in cadence over a bridge, as in the collapse of the Broughton Bridge near Manchester, England in 1831.

These diasters have often been cited in textbooks on ordinary differential equations as examples of *resonance*, which happens when the frequency of forcing matches the natural frequency of oscillation of the bridge, with no discussion given on how the natural frequency is determined, or even where the ordinary differential equation used to model this phenomenon comes from. The modeling of bridge vibration by a partial differential equation, although still simple minded, is a big step forward in connecting to reality.

15.2 Marching soldiers on a bridge, a simple model

When a column of soldiers march in unison over a bridge, a vertical force

$$f(x, t)$$

is exerted on the bridge that is periodic in time t, with a period P determined by the time interval between steps. In this one dimensional problem, with x measured along the length of the bridge, we do not distinguish left-foot steps from right-foot steps. In reality these left-right steps create additional vibrations over the width of the bridge which, in some case, may be more important in causing collapse. This aspect of the problem can be handled by introducing another space dimension into the model, but will be ignored here.

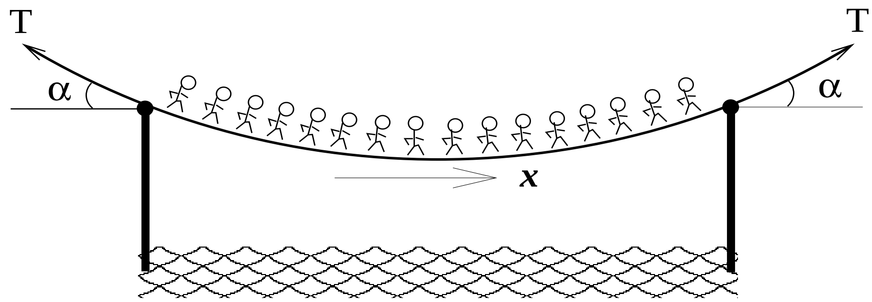


Figure 11.1 A schematic of our simple suspension bridge

Specifically, we will model the bridge as a "guitar string" of length L, suspended at only $x = 0$ and $x = L$. [We know of course that bridges do not behave like elastic strings. Nevertheless this simplification allows us to skip most of the structural mechanics that one needs to know and yet still retain most of the ingredients we need to illustrate the mathematical problem of resonance.] The tension along the bridge, T, is assumed to be uniform and is therefore equal to the force per unit area exerted on the suspension point $x = 0$ or $x = L$. Since the weight of the bridge is borne by these two suspension points, the vertical force exerted on each is half the weight of the bridge, and this should be equal to the projection of T in the vertical direction

$$T \sin\alpha = \frac{1}{2}(\rho L A)g/A = \frac{1}{2}\rho L g,$$

where α is the angle from the horizonal to the tangent of the bridge at the suspension point, $g = 980\text{cm/sec}^2$, ρ is the density of the bridge material and A the cross section of the bridge. Let

$$c^2 \equiv T/\rho = \frac{1}{2}Lg/\sin\alpha. \tag{15.1}$$

The PDE governing the vibration of the "string" has been derived in Chapter 2. The system we need to solve is, with $u(x,t)$ being the vertical displacement of the bridge with respect to its equilibrium position:

$$\text{PDE:} \quad u_{tt} = c^2 u_{xx} + f(x,t), \quad 0 < x < L, \ t > 0, \tag{15.2}$$

$$\text{BCs:} \quad u(0,t) = 0, \quad u(L,t) = 0, \quad t > 0, \tag{15.3}$$

$$\text{IC:} \quad u(x,0) = 0, \quad u_t(x,0) = 0, \quad 0 < x < L. \tag{15.4}$$

The simplest expression for the periodic force exerted by a column of marching soldiers is probably:

$$f(x,t) = a\sin(2\pi t/P)\sin(\pi x/L), \quad 0 < x < L, \tag{15.5}$$

[Actually this is meant to be the force *anomaly*, that is, the difference between the force exerted by the marching soldiers and their static weight. This is why (11.5) can take on positive and negative values. The force due to the static weight of the soldiers, if it is a significant-fraction of the weight of the bridge, can be incorporated in the weight of the bridge in our earlier calculation of the tension T. Nevertheless, the parameter c^2 in (11.1) should not be affected, amazingly!].

15.3 Solution

We use the method of eigenfunction expansions to solve the nonhomogeneous system (11.2)-(11.4). Since the boundary conditions are of the homogeneous Dirichlet type, we use the sine series expansions:

$$u(x,t) = \sum_{n=1}^{\infty} T_n(t)\sin\frac{n\pi x}{L} \tag{15.6}$$

$$f(x,t) = \sum_{n=1}^{\infty} f_n(t)\sin\frac{n\pi x}{L}. \tag{15.7}$$

For the simple model of $f(x,t)$ in (11.5), $f_n = 0$ except

$$f_1(t) = a\sin(2\pi t/P).$$

Substituting (11.6) and (11.7) into (11.2) yields

$$\sum_{n=1}^{\infty}[T_n''(t) + c^2\left(\frac{n\pi}{L}\right)^2 T_n(t)]\sin\frac{n\pi x}{L} = \sum_{n=1}^{\infty} f_n(t)\sin\frac{n\pi x}{L}.$$

Therefore:

$$T_n''(t) + \omega_n^2 T_n(t) = f_n(t), \quad n = 1,2,3,4,5\ldots, \tag{15.8}$$

for $\omega_n \equiv (cn\pi/L)$.

For $n > 1$, (11.8) is

$$T_n''(t) + \omega_n^2 T_n(t) = 0, \tag{15.9}$$

implying that

$$\begin{aligned} T_n(t) &= A_n \sin \omega_n t + B_n \cos \omega_n t \\ &= \frac{T_n'(0)}{\omega_n} \sin \omega_n t + T_n(0) \cos \omega_n t. \end{aligned} \tag{15.10}$$

For $n = 1$, (11.8) is

$$T_1''(t) + \omega_1^2 T_1(t) = a \sin(2\pi t/P). \tag{15.11}$$

The solution to (11.11) consists of particular plus homogeneous solutions. The homogeneous solution is

$$A_1 \sin \omega_1 t + B_1 \cos \omega_1 t,$$

while the particular solution can be obtained by trying

$$D \sin(2\pi t/P)$$

and finding $D = a/(-(2\pi/P)^2 + \omega_1^2)$ upon substituting into (11.11). The solution for $n = 1$ is thus

$$\begin{aligned} T_1(t) &= A_1 \sin \omega_1 t + B_1 \cos \omega_1 t + \frac{a \sin(2\pi t/P)}{\omega_1^2 - (2\pi/p)^2} \\ &= \frac{T_1'(0)}{\omega_1} \sin \omega_1 t + T_1(0) \cos \omega_1 t + \frac{a}{\omega_1^2 - (2\pi/p)^2}[\sin(2\pi t/P) - \frac{(2\pi/P)}{\omega_1} \sin \omega_1 t]. \end{aligned}$$

Setting

$$\begin{aligned} u(x,t) = &\sum_{n=1}^{\infty} [T_n(0) \cos \omega_n t + \frac{T_n'(0)}{\omega_n} \sin \omega_n t] \sin \frac{n\pi x}{L} \\ &+ \frac{a}{\omega_1^2 - (2\pi/p)^2}[\sin(2\pi t/P) - \frac{(2\pi/P)}{\omega_1} \sin \omega_1 t] \sin \frac{\pi x}{L}. \end{aligned} \tag{15.12}$$

Applying the ICs on (11.6), we have

$$\begin{aligned} u(x,0) = 0 &= \sum_{n=1}^{\infty} T_n(0) \sin\left(\frac{n\pi x}{L}\right), \quad 0 < x < L \\ u_t(x,0) = 0 &= \sum_{n=1}^{\infty} T_n'(0) \sin \frac{n\pi x}{L}, \quad 0 < x < L. \end{aligned}$$

These imply, $T_n(0) = 0$, $T_n'(0) = 0$, $n = 1, 2, 3, \ldots$. Finally, the solution (11.12) becomes the two term expression

$$u(x,t) = \frac{a}{\omega_1^2 - (2\pi/p)^2}[\sin(2\pi t/P) - \frac{(2\pi/P)}{\omega_1} \sin \omega_1 t] \sin \frac{\pi x}{L}. \tag{15.13}$$

15.4 Resonance

The solution (11.13) involves the interference of a forced frequency $(2\pi/P)$ with a fundamental frequency ω_1. When the two frequencies get close to each other, the numerator and the denominator of (11.13) both approach zero. Their ratio as $(2\pi/P) \to \omega_1$ is obtained by L'Hospital's rule to be

$$u(x,t) = a\left[\frac{-t\cos\omega_1 t}{2\omega_1} + \frac{\sin\omega_1 t}{2\omega_1^2}\right]\sin\left(\frac{\pi x}{L}\right). \tag{15.14}$$

The oscillation grows in amplitude linearly in time, leading, presumably, to the collapse of the bridge.

The fundamental frequency ω_1 of the bridge is given by

$$\omega_1 = c\pi/L = \pi\sqrt{\frac{1}{2}g/(L\sin\alpha)}.$$

Thus the period P of the forcing which could lead to resonance with this fundamental frequency is given by $2\pi/P = \omega_1$, or

$$P = 2\pi/\omega_1 = \sqrt{8L\sin\alpha/g}, \tag{15.15}$$

which is about 2.8 seconds for a bridge 10 meters long, if the bridge is loosely hung (i.e. $\alpha \sim 90^\circ$). Since the period of forcing P (as measured by the time interval between the marching steps) is usually shorter, we conclude that such a bridge probably would not be resonantly forced by the column of soldiers.

If the bridge is stretched taut, the frequency of the first fundamental mode increases. If the bridge deck is nearly horizontal, say $\alpha \sim 10^\circ$, the period of the first fundamental mode becomes

$$2\pi/\omega_1 = \sqrt{8L\sin\alpha/g} \sim 1.1 \text{ second}.$$

This is closer to the probable forcing frequency and resonance is more likely.

15.5 A different forcing function

Unlike ODE models of resonance, which assume some *given* natural frequency of the system, the PDE model discussed above determines the resonant frequency by the physical parameters of the bridge (via T/ρ) and by the x-shape of the forcing function $f(x,t)$. In the previous model, it was assumed that

$$f(x,t) = a\sin(2\pi t/P)\sin(\pi x/L), \quad 0 < x < L.$$

So the forcing function has the shape of the first fundamental harmonic of the homogeneous system. Consequently, resonance occurs when the forcing frequency $2\pi/P$ equals the frequency ω_1 of this fundamental mode. If we had instead used

$$f(x,t) = a\sin(2\pi t/P)\sin(2\pi x/L), \quad 0 < x < L$$

for our forcing function, resonance would have occurred when the forcing frequency $2\pi/P$ equalled the frequency ω_2 of the second fundamental mode.

This discussion points to the importance of modeling the forcing function realistically. A better model for $f(x,t)$ than (11.5) is probably,

$$f(x,t) = a\sin(2\pi t/P), \quad 0 < x < L, \tag{15.16}$$

which assumes that the force exerted by the soldiers marching in unison is independent of where they are on the bridge. This seemingly simpler forcing function actually has a richer eigenfunction expansion:

$$f(x,t) = \sum_{n=1}^{\infty} f_n(t)\sin\frac{n\pi x}{L}, \quad 0 < x < L, \tag{15.17}$$

where

$$f_n(t) = \begin{cases} 0 & \text{if } n \text{ is even} \\ \frac{4a}{n\pi}\sin(2\pi t/P) & \text{if } n \text{ is odd.} \end{cases} \tag{15.18}$$

The solution to (11.2)-(11.4) now becomes

$$u(x,t) = \sum_{n=1}^{\infty} T_n(t)\sin\frac{n\pi x}{L}, \tag{15.19}$$

where

$$T_n(t) = 0$$

if n is even, and

$$T_n(t) = \frac{4a/\pi}{\omega_n^2 - (2\pi/p)^2}[\sin(2\pi t/P) - \frac{(2\pi/P)}{\omega_n}\sin\omega_n t]/n \tag{15.20}$$

if n is odd.

There are now chances for resonance whenever

$$P = 2\pi/\omega_n \text{ for some } n.$$

However, because the amplitude of $T_n(t)$ decreases with n, probably only the first two modes will have any real impact. To resonate the first harmonic mode, we must have $P \sim 1$ seconds. The next nonzero fundamental mode is the third one. To resonate with this mode, we need

$$P = 2\pi/\omega_3 = (2\pi/\omega_1)/3,$$

which is about 1/3 of a second. A column of soldiers running in unison with 1/3 of a second between steps may be able to induce an oscillation in the third mode. This is not as strong as the first mode if the first mode could be excited. This mode has the distinctive feature that the middle third of the bridge oscillates out of phase with the remaining two thirds of the bridge near the ends, even though the forcing is *independent* of x.

15.6 Tacoma Narrows Bridge

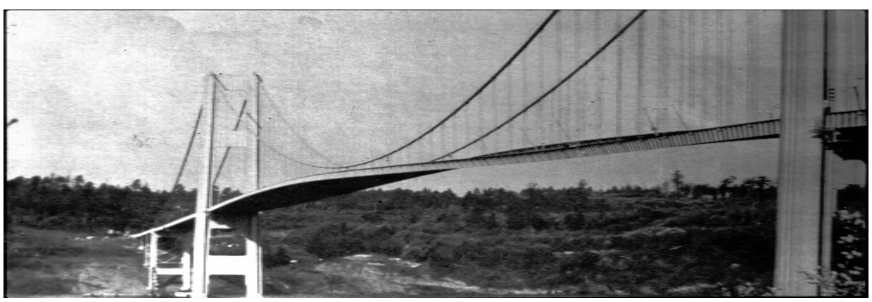


Figure 11.2 Twisting of Tacoma Narrows Bridge just prior to failure.

Even though numerous physics and mathematics textbooks attribute the 1940 collapse of Tacoma Narrows Bridge to "a resonance between the natural frequency of oscillation of the bridge and the frequency of wind-generated vortices that pushed and pulled alternately on the bridge structure" (D. Halliday and R. Resnick, *Fundamentals of Physics*, Wiley, New York, 1988, 3rd ed), that bridge probably did *not* collapse for this reason (see K.Y. Billah and R.H. Scanlan, 1991, *Am. J. Phys.,* **59** (2), 118–124). As observed by Professor Burt Farquharson of University of Washington, the wind speed at the time was 42 mph, giving a fequency of forcing by the vortex shedding mechanism of about 1 Hz. Professor Farquharson also observed that the frequency of the oscillation of the bridge just prior to its destruction was about 0.2 Hz. There was a mismatch of the two frequencies and consequently this simple resonance mechanism probably was not the cause of the bridge's collapse. The bridge collapsed due to a torsional (twisting) vibration as can be seen in old films and in Figure 8.2.

During its brief lifetime late in 1940, the bridge, under low-speed winds, did experience vertical modes of vibration which can probably be modeled by a model similar to the one presented here. However, the bridge endured this excited vibration *safely*. In fact, the bridge's nickname, "Galloping Gertie", was gained from such vertical motions under low wind. And this phenomenon occurred repeatedly since its opening day. Motorists crossing the bridge sometimes experienced "roller-coaster like" sensation as they watched cars ahead disappear from sight, then reappear, and tourists came from afar to experience it without worrying about their safety.

The above discussion points to the fact that although simple linear theories of forced resonance can perhaps explain the initial excitation of certain modes of oscillation, they cannot always be counted on to explain the final collapse of bridges, which is always a very nonlinear phenomenon.

15.7 Exercises

1. Consider the problem of a column of soldiers marching across a suspension bridge of length L. The marching is slightly out of step so the force exerted by the soldiers in the front of the column is opposite that in the rear. A simple model of the forcing term on the bridge is

$$f(x,t) = a\sin(2\pi t/P)\sin(2\pi x/L), \quad 0 < x < L.$$

Solve:

$$\begin{aligned} \text{PDE:} \quad & u_{tt} = c^2 u_{xx} + f(x,t), \quad 0 < x < L, \quad t > 0 \\ \text{BCs:} \quad & u(0,t) = 0, \quad u(L,t) = 0, \quad t > 0 \\ \text{ICs:} \quad & u(x,0) = 0, \quad u_t(x,0) = 0, \quad 0 < x < L. \end{aligned}$$

Discuss the criteria condition for resonance and sketch the shape of the mode excited.

15.8 Solution

1. We wish to solve the nonhomogeneous wave equation with zero boundary and initial conditions where our forcing has the form:

$$f(x,t) = a\sin(2\pi t/P)\sin(2\pi x/L).$$

Our boundary conditions (in x) leads us to the expansion of $u(x,t) = \sum_{n=1}^{\infty} a_n(t)\sin(n\pi x/L)$. Substituting this into our PDE and equating like sine terms we find the equations:

$$a_2(t)'' + \omega_2^2 a_2(t) = a\sin(2\pi t/P) \quad \text{and} \quad a_n(t)'' + \omega_n^2 a_n(t) = 0 \text{ for } n \neq 2$$

where $\omega_n = nc\pi/L$. Solving the a_n equations with our initial conditions gives $a_n(t) = 0$ for $n \neq 2$, and leaves us with a single, second order inhomogeneous equation for $a_2(t)$.

The homogeneous solution is $y_h(x) = A\sin(\omega_2 t) + B\cos(\omega_2 t)$. Thus if $\omega_2 \neq 2\pi/P$, we guess a particular solution of the form:

$$y_p = C\sin(2\pi t/P) + D\cos(2\pi t/P).$$

Substituting into our equation for a_2 we find that $D = 0$ and $C = a/(\omega_2^2 - (2\pi/P)^2)$, which gives the solution:

$$u(x,t) = [A\cos(\omega_2 t) + B\sin(\omega_2 t) + a/(\omega_2^2 - (2\pi/P)^2)\sin(2\pi t/P)]\sin(2\pi x/L).$$

Now we use our initial conditions to find that $A = 0$ and $B = -2\pi a/(P\omega_2(\omega_2^2 - (2\pi/P)^2))$, which gives

$$u(x,t) = [-2\pi a/(P\omega_2(\omega_2^2 - (2\pi/P)^2))\sin(\omega_2 t) + a/(\omega_2^2 - (2\pi/P)^2\sin(2\pi t/P)]\sin(2\pi x/L)$$

Now if $c/L = 1/P$ or $\omega_2 = 2\pi/P$, we have resonance, and our inhomogeneity satisfies homogeneous equation, so we must guess a particular solution of the form:

$$y_p(t) = t(C\sin(\omega_2 t) + D\cos(\omega_2 t)).$$

Solving for the coefficients C and D, we find that $C = 0$ and $D = -a/(2\omega_2)$. Thus, when we have resonance, the solution is:

$$u(x,t) = [A\sin(\omega_2 t) + B\cos(\omega_2 t) - (a/(2\omega_2))t\cos(\omega_2 t)]\sin(2\pi x/L).$$

Now we use our initial conditions to find that $B = 0$ and $A = a/(2\omega_2^2)$, so our final solution is:

$$u(x,t) = [(a/(2\omega_2^2))\sin(\omega_2 t) - (a/(2\omega_2))t\cos(\omega_2 t)]\sin(2\pi x/L).$$

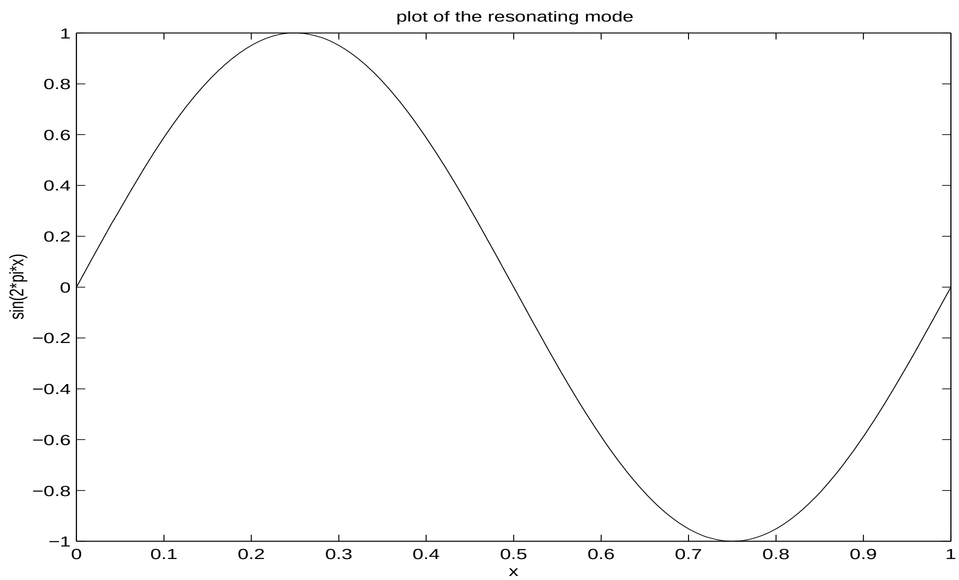


Figure 11.3. Resonating mode.

Chapter 16

Green's Function

16.1 Introduction

The method of Green's functions is an alternative method for solving partial differential equations with general forcing. (Reference: Haberman (2004): *Applied Partial Differential Equations*, 4th ed.)

16.2 Green's functions for ODEs

Let L be the Sturm-Liouville operator:

$$L \equiv \frac{d}{dx}(p(x)\frac{d}{dx}) + q(x).$$

Consider the nonhomogeneous ODE

$$Lu = f(x), \quad a < x < b \tag{16.1}$$

subject to two homogeneous boundary conditions. Instead of solving it with the general forcing $f(x)$, we consider instead the more specific problem

$$LG = \delta(x - \xi), \text{ with the same boundary conditions} \tag{16.2}$$

where $G = G(x, \xi)$ describes the response to a concentrated source located at ξ. $G(x, \xi)$ is called the Green's function for the original problem (16.1), whose solution $u(x)$ is then recovered from

$$u(x) = \int_a^b f(\xi) G(x, \xi) d\xi \tag{16.3}$$

To verify that (16.3) satisfies (16.1), we see that

$$\begin{aligned} Lu &= \int_a^b f(\xi) LG(x,\xi) d\xi \\ &= \int_a^b f(\xi)\delta(x-\xi) d\xi = f(x), \end{aligned}$$

because of a fundamental property of the delta function.

The Green's function is symmetrical with respect to its two arguments, i.e.

$$G(\xi, x) = G(x, \xi) \tag{16.4}$$

The result (16.4) is called Maxwell's reciprocity. Although mathematically it is easily seen from the equation defining $G(x,\xi)$ and the fact that $\delta(x-\xi) = \delta(\xi - x)$, physically Maxwell's reciprocity is not obvious, as it states that the response at x due to a concentrated source at ξ is the same as the response at ξ due to a concentrated source at x.

16.2.1 Jump conditions

Since the Green's function is forced by a delta function, one needs to worry about its continuity. If G is discontinuous, i.e. it has a finite jump at $x = \xi$, then $\frac{d}{dx}G$ has a delta function singularity at the same point and $\frac{d^2}{dx^2}G$ on the left-hand side of (16.2) is more singular than the delta function on the right-hand side. It then follows that G must be continuous at $x = \xi$, but its first derivative must have a jump at $x = \xi$. Its second derivative is then a delta function, consistent with the right-hand side of (16.2).

Integrating (16.2) across $x = \xi$, from $x = \xi^-$ to $x = \xi^+$ ($\xi^- = \xi - \epsilon$, $\xi^+ = \xi + \epsilon$, $\epsilon > 0$ and vanishingly small), we get:

$$p(x)\frac{d}{dx}G \Big|_{x=\xi^-}^{x=\xi^+} = \int_{\xi^-}^{\xi^+} \delta(x-\xi) d\xi = 1, \tag{16.5}$$

This jump condition is supplemented by the matching condition argued earlier:

$$G \big|_{x=\xi^-} = G \big|_{x=\xi^+} \tag{16.6}$$

16.2.2 Green's formula

For any two differentiable functions $u(x)$ and $v(x)$

$$\begin{aligned} uLv - vLu &= u\frac{d}{dx}(p\frac{dv}{dx}) + uqv - v\frac{d}{dx}(p\frac{du}{dx}) - vqu \\ &= u\frac{d}{dx}(p\frac{dv}{dx}) - v\frac{d}{dx}(p\frac{du}{dx}). \end{aligned}$$

so

$$uLv - vLu = \frac{d}{dx}[p(u\frac{dv}{dx} - v\frac{du}{dx})]. \tag{16.7}$$

(16.7) is known as Lagrange's identity. Integrating,

$$\int_a^b [uLu - vLu]dx = p(u\frac{dv}{dx} - v\frac{du}{dx})\ \Big|_a^b\ . \tag{16.8}$$

This is known as Green's formula.

If u and v are any two functions satisfying the same set of homogeneous boundary conditions, or the periodic condition, or $p(x) = 0$ at the boundaries, then the right-hand side of (16.8) vanishes, and therefore

$$\int_a^b [uLv - vLu]dx = 0 \tag{16.9}$$

An operator L satisfying (16.9) is called a self-adjoint operator.

The multi-dimensional counterparts to these formulae can be easily derived. For $L = \nabla^2$, we note that

$$\begin{aligned} \nabla \cdot (u\nabla v) &= u\nabla^2 v + \nabla u \cdot \nabla v \\ \nabla \cdot (v\nabla u) &= v\nabla^2 u + \nabla v \cdot \nabla u \end{aligned}$$

Subtracting, we get the multidimensional counterpart to (16.7)

$$u\nabla^2 v - v\nabla^2 u = \nabla \cdot (u\nabla v - v\nabla u). \tag{16.10}$$

In three dimensions, the domain is a volume V. The boundary of the volume is denoted by ∂V, which is a closed surface containing V. Integrating (16.10) over V, we get

$$\begin{aligned} &\iiint_V [u\nabla^2 v - v\nabla^2 u]dV \\ &\qquad = \iiint_V \nabla \cdot (u\nabla v - v\nabla u)dV \\ &\qquad = \iint_{\partial V} (u\nabla u - v\nabla u) \cdot \mathbf{n}dS \end{aligned} \tag{16.11}$$

The last step utilizes the divergence theorem, with $\hat{\mathbf{n}}$ being the outward unit normal.

In two dimensions, we have instead

$$\iint_A [u\nabla^2 u - v\nabla^2 u]dA = \int_{\partial A} (u\nabla u - v\nabla u)\cdot \hat{\mathbf{n}} ds$$

where ∂A is the closed curve bounding the area A.

16.2.3 Nonhomogeneous boundary conditions

The Green's function defined for homogeneous boundary conditions is also used to solve problems with nonhomogeneous boundary conditions

$$\begin{aligned} Lu &= f(x), \quad a < x < b \\ u(a) = u_a, &\quad u(b) = u_b. \end{aligned} \tag{16.12}$$

We always define the Green's function to be solution to

$$\begin{aligned} LG &= \delta(x-\xi) \\ G(a,\xi) = 0, &\quad G(b,\xi) = 0 \end{aligned} \tag{16.13}$$

Now we use Green's formula (16.8) with $v(x) = G(x,\xi)$ and $u(x)$ the solution to (16.12)

$$\begin{aligned} &\int_a^b [u(x)LG(x,\xi) - G(x,\xi)Lu]dx \\ &\quad = [u(x)p(x)\frac{d}{dx}G(x,\xi) - G(x,\xi)p(x)\frac{d}{dx}u(x)]_a^b \end{aligned}$$

Using the equation (16.12) for $u(x)$ and (16.13) for $G(x,\xi)$, we have

$$\begin{aligned} &\int_a^b u(x)\delta(x-\xi)dx - \int_a^b G(x,\xi)f(x)dx \\ &\quad = u(b)p(b)\frac{d}{dx}G(x,\xi)\ \Big|_{x=b} - u(a)p(a)\frac{d}{dx}G(x,\xi)\ \Big|_{x=a} \end{aligned}$$

The first term on the left-hand side of the above equation is $u(\xi)$. Therefore if we interchange x and ξ, we will get

$$u(x) = \int_a^b G(x,\xi)f(\xi)d\xi + u_b p(b)\frac{d}{d\xi}G(x,\xi)\ \Big|_{\xi=b} - u_a p(a)\frac{d}{d\xi}G(x,\xi)\ \Big|_{\xi=a} \tag{16.14}$$

16.2.4 Example

$$\frac{d^2}{dx^2}u = f(x), \quad 0 < x < L$$
$$u(0) = 0, \quad u(L) = 0$$

The Green's function satisfies

$$\frac{d^2}{dx^2}G = \delta(x - \xi)$$
$$G(0, \xi) = 0, \quad G(L, \xi) = 0$$

For $x < \xi$:

$$\frac{d^2}{dx^2}G = 0, \quad \text{subject to } G(0, \xi) = 0.$$
$$G(x, \xi) = Ax + B = Ax$$

($B = 0$ because $G(0, \xi) = 0$).

For $x > \xi$:

$$\frac{d^2}{dx^2}G = 0, \quad \text{subject to } G(L, \xi) = 0$$
$$G(x, \xi) = C(x - L).$$

Continuity at $x = \xi$ implies

$$A\xi = C(\xi - L)$$

The jump condition at $x = \xi$ implies

$$C - A = 1.$$

Solving for C and A from these two relationships, we get

$$G(x, \xi) = \begin{cases} -\frac{x}{L}(L - \xi), & x < \xi \\ -\frac{\xi}{L}(L - x), & x > \xi \end{cases}$$

The solution to the original ODE with $f(x)$ as the general forcing term is

$$\begin{aligned} u(x) &= \int_0^L f(\xi) G(x, \xi) d\xi \\ &= \int_0^x -\frac{\xi}{L}(L - x) f(\xi) d\xi + \int_x^L -\frac{x}{L}(L - \xi) f(\xi) d\xi \\ &= \frac{x}{L} \int_0^L \xi f(\xi) d\xi - \int_0^x \xi f(\xi) d\xi - x \int_x^L f(\xi) d\xi. \end{aligned}$$

To verify that this is indeed the solution, we differentiate it twice:

$$\begin{aligned}
\frac{d}{dx}u &= \frac{1}{L}\int_0^L \xi f(\xi)d\xi - xf(x) - \int_x^L f(\xi)d\xi + xf(x) \\
&= \frac{1}{L}\int_0^L \xi f(\xi)d\xi - \int_x^L f(\xi)d\xi \\
\frac{d^2}{dx^2}u &= f(x),
\end{aligned}$$

which is the original OdE. It is easily shown that the boundary conditions are satisfied.

16.2.5 Example: Nonhomogeneous boundary condition

$$\frac{d^2}{dx^2}u = f(x),$$

$$u(0) = a, \quad u(L) = b$$

We always require our Green's function to satisfy the homogeneous boundary conditions. So $G(x, \xi)$ satisfies

$$\frac{d^2}{dx^2}G = \delta(x - \xi)$$

$$G(0, \xi) = 0, \quad G(L, \xi) = 0.$$

Thus $G(x, \xi)$ is the same as found in the previous example.

$$G(x, \xi) = \begin{cases} -\frac{x}{L}(L - \xi), & x < \xi \\ -\frac{\xi}{L}(L - x), & x > \xi \end{cases}$$

$$\frac{d}{d\xi}G(x, \xi) = \begin{cases} x/L, & x < \xi \\ -(L - x)/L, & x > \xi \end{cases}$$

Therefore, the solution from (16.14) is

$$\begin{aligned}
u(x) &= \int_0^L G(x, \xi)f(\xi)d\xi + b(x/L) + a(L - x)/L \\
&= \frac{x}{L}\int_0^L \xi f(\xi)d\xi - \int_0^x \xi f(\xi)d\xi - x\int_x^L f(\xi)d\xi + bx/L + a(L - x)/L.
\end{aligned}$$

16.3 Green's Function for Poisson's Equation

Poisson's equation is Laplace's equation with the addition of a forcing, $f(\mathbf{x})$:

$$\nabla^2 u = f(\mathbf{x}) \tag{16.15}$$

It describes, for example, the electrostatic potential due to a given distributing of electric charges. Or it can describe the gravitational potential due to some given mass distribution.

The Green's function, $G(\mathbf{x}, \boldsymbol{\xi})$, solves the problem for one concentrated source at $\mathbf{x} = \boldsymbol{\xi}$:

$$\nabla^2 G = \delta(\mathbf{x} - \boldsymbol{\xi}). \tag{16.16}$$

subject to *homogeneous* boundary condition. The multidimensional delta function is defined as: in 3-D:

$$\delta(\mathbf{x} - \boldsymbol{\xi}) = \delta(x - \xi)\delta(y - \eta)\delta(z - \xi),$$

and in 2-D:

$$\delta(\mathbf{x} - \boldsymbol{\xi}) = \delta(x - \xi)\delta(y - \eta),$$

where

$$\mathbf{x} = (x, y, z), \quad \boldsymbol{\xi} = (\xi, \eta, \xi) \text{ in 3-D}$$

and

$$\mathbf{x} = (x, y), \quad \boldsymbol{\xi} = (\xi, \eta) \text{ in 2-D.}$$

Using the Green's formula (16.14), and letting $u(\mathbf{x})$ be the solution to (16.15) and $G(\mathbf{x}, \boldsymbol{\xi})$ its Green's function, we have, in 3D:

$$\iiint_V [u\nabla^2 G - G\nabla^2 u] dx\ dy\ dz = \iint_{\partial V} (u\nabla G - G\nabla u) \cdot \hat{\mathbf{n}} dS \tag{16.17}$$

The right-hand side contains the boundary value terms and vanishes if $u(\mathbf{x})$ satisfies homogeneous boundary conditions. For this case, (16.17) becomes

$$\iiint_V [u(x)\delta(\mathbf{x} - \boldsymbol{\xi}) - Gf(\mathbf{x})] dx\ dy\ dz = 0,$$

which is

$$u(\mathbf{x}) = \iiint_V G(\mathbf{x}, \boldsymbol{\xi}) f(\boldsymbol{\xi}) d\xi\ d\eta\ d\xi \tag{16.18}$$

after switching $\mathbf{x}$ with $\boldsymbol{\xi}$. The Green's function formula is a simple extension of the 1-D case. Nonhomogeneous boundary conditions for $u(\mathbf{x})$ can be handled the same way as was done in the 1-D case.

In 2-D, the integral in (16.18) should be replaced by integration over the area.

16.3.1 3D Poisson's equation in infinite domain

$$\nabla^2 G = \delta(\mathbf{x} - \boldsymbol{\xi}) \tag{16.19}$$

$$G(\mathbf{x}, \boldsymbol{\xi}) \text{ bounded as } \mathbf{x} \to \infty.$$

G represent the response at $\mathbf{x}$ to a point source located at $\mathbf{x} = \boldsymbol{\xi}$. Let

$$\mathbf{r} \equiv \mathbf{x} - \boldsymbol{\xi}$$

be the distance measured from the source. In terms of $\mathbf{r}$ there is no preference in the angular direction in the definition of this problem. So we seek a solution which depends on $r = |\mathbf{r}|$ only. We let

$$G(\mathbf{x}, \boldsymbol{\xi}) = G(r).$$

In spherical coordinates,

$$\nabla^2 G(\mathbf{x}, \boldsymbol{\xi}) = \nabla^2 G(r) = \frac{1}{r^2}\frac{d}{dr}(r^2 \frac{d}{dr} G)$$

For $r \neq 0$, the delta function is zero, and we have

$$\frac{d}{dr}(r^2 \frac{d}{dr} G) = 0$$

Integrating

$$r^2 \frac{d}{dr} G = A$$

or

$$\frac{d}{dr} G = A/r^2.$$

Integration again:

$$G(r) = -A/r + B \tag{16.20}$$

We cannot impose the boundedness condition at $r = 0$ because the equation for this G is not valid at $r = 0$. We need to derive the matching condition for $G(r)$ as $r \to 0^+$.

Integrating Eq. (16.19) over a sphere of radius r

$$\iiint \nabla^2 G dV = \iiint \delta(\mathbf{x} - \boldsymbol{\xi}) dV = 1.$$

The left-hand side is, by the divergence theorem

$$\iiint_V \nabla \cdot (\nabla G) dV = \iint_{\partial V} \nabla G \cdot \hat{\mathbf{n}} dS,$$

where $\hat{\mathbf{n}} = \mathbf{r}/r$ is pointing radially, and so

$$\nabla G \cdot \hat{\mathbf{n}} = \frac{\partial}{\partial r} G.$$

$$\begin{aligned} 1 = \iint_{\partial V} \nabla G \cdot \hat{\mathbf{n}} dS &= \int_0^{2\pi} \int_0^{\pi} (\frac{\partial}{\partial r} G) r^2 \sin\theta \; d\theta \; d\varphi \\ &= 4\pi r^2 \frac{\partial}{\partial r} G \end{aligned}$$

From this we obtain the matching condition

$$\lim_{r\to 0^+} r^2 \frac{\partial}{\partial r} G = \frac{1}{4\pi}$$

From (16.20), which is valid for $r > 0$

$$\begin{aligned} \frac{\partial}{\partial r} G(r) &= A/r^2 \\ r^2 \frac{\partial}{\partial r} G &= A = \frac{1}{4\pi} \end{aligned}$$

Finally, we have

$$G(\mathbf{x}, \boldsymbol{\xi}) = G(r) = -\frac{1}{4\pi r} + B$$

This describes, for example, the electrostatic potential at (x, y, z) due to a point electrical charge located at (ξ, η, ζ).

The constant B is arbitrary since a potential is determined only up to an arbitrary constant. We set $B = 0$

$$G(\mathbf{x}, \boldsymbol{\xi}) = -\frac{1}{4\pi} [(x-\xi)^2 + (y-\eta)^2 + (z-\zeta)^2]^{-1/2}.$$

16.3.2 2D Poisson's equation in an infinite domain

Again we let $\mathbf{r} = \mathbf{x} - \boldsymbol{\xi}$, except now

$$\begin{aligned} r &= ((x-\xi)^2 + (y-\eta)^2)^{1/2}, \text{ and} \\ \nabla^2 &= \frac{1}{r}\frac{d}{dr}(r\frac{d}{dr}) + \frac{1}{r^2}\frac{\partial^2}{\partial\theta^2} \end{aligned}$$

in 2D polar coordinates. Since $G(\mathbf{x}, \boldsymbol{\xi})$ depends on r only, we write

$$G(\mathbf{x}, \boldsymbol{\xi}) = G(r)$$

and

$$\nabla^2 G(r) = \frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}G)$$

For $r \neq 0$,

$$\nabla^2 G = 0$$

so

$$\frac{\partial}{\partial r}(r\frac{\partial}{\partial r}G) = 0.$$

Integrating

$$r\frac{\partial}{\partial r}G = A, \quad \frac{\partial}{\partial r}G = A/r$$

$$G(r) = A\ell nr + B.$$

From

$$\iint \nabla^2 G dS = \iint \delta(\mathbf{x} - \boldsymbol{\xi}) dx\ dy = 1$$

and

$$\iint_A \nabla^2 G dS = \iint_A \nabla \cdot (\nabla G) dS = \int_{\partial A} \nabla G \cdot \hat{\mathbf{n}} ds$$

where A is a circular disk of radius r and ∂A a circle of radius r; $ds = rd\theta$.

$$\int_{\partial A} \nabla G \cdot \hat{\mathbf{n}} ds = \int_0^{2\pi} \frac{\partial}{\partial r} G r d\theta = 2\pi r \frac{\partial}{\partial r} G$$

Therefore,

$$2\pi r \frac{\partial}{\partial r} G = 1, \quad r > 0$$

resulting in the matching condition

$$\lim_{r \to 0^+} r\frac{\partial}{\partial r}G = \frac{1}{2\pi}$$

Since

$$G(r) = A\ell nr + B, \quad r > 0$$

$$\frac{\partial}{\partial r}G = A/r$$

$$r\frac{\partial}{\partial r}G = A.$$

Therefore

$$A = \frac{1}{2\pi}.$$

Finally, setting the arbitrary additive constant potential B to zero for convenience, we have

$$\begin{aligned} G(\mathbf{x}, \boldsymbol{\xi}) &= \frac{1}{2\pi} \ell n r, \quad r > 0 \\ &= \frac{1}{2\pi} \ell n [(x-\xi)^2 + (y-\eta)^2]^{1/2}. \end{aligned}$$

16.3.3 Poisson's equation in a finite domain

Green's function in infinite domains, as obtained in the previous section, are actually quite simple. We would like to utilize them to obtain the Green's function for the finite domain problem.

The idea is to treat the solution we obtained for the infinite domain as a particular solution to the problem in the finite domain, and add a homogeneous solution. That is, to solve

$$\nabla^2 G(\mathbf{x}, \boldsymbol{\xi}) = \delta(\mathbf{x} - \boldsymbol{\xi})$$

in a finite domain, we write, in 3D

$$G(\mathbf{x}, \boldsymbol{\xi}) = -\frac{1}{4\pi r} + v(\mathbf{x}, \xi)$$

where $v(\mathbf{x}, \xi)$ satisfies the homogeneous PDE

$$\nabla^2 v(\mathbf{x}, \boldsymbol{\xi}) = 0.$$

We choose the constants in v so that $G(\mathbf{x}, \xi)$ satisfies the boundary condition in the finite domain.

In 2-D, we try

$$G(\mathbf{x}, \xi) = \frac{1}{2\pi} \ell n r + v(\mathbf{x}, \boldsymbol{\xi})$$

where

$$\nabla^2 v(\mathbf{x}, \xi) = 0.$$

We will leave the consideration of these finite domain problems in Exercises.

16.4 Green's Function for the Wave Equation

We are interested in solving the wave equation in the presence of a source $Q(x, t)$:

$$\frac{\partial^2}{\partial t^2} u - c^2 \nabla^2 u = Q(\mathbf{x}, t) \tag{16.21}$$

subject to two initial conditions

$$\begin{aligned} u(\mathbf{x},0) &= f(\mathbf{x}) \\ \frac{\partial}{\partial t}u(\mathbf{x},0) &= g(\mathbf{x}) \end{aligned}$$

We define the Green's function $G(\mathbf{x}, t; \boldsymbol{\xi}, \tau)$ as the solution due to a concentrated source at $\mathbf{x} = \boldsymbol{\xi}$ acting only at $t = \tau$:

$$\frac{\partial^2}{\partial t^2}G - c^2\nabla^2 G = \delta(\mathbf{x} - \boldsymbol{\xi})\delta(t - \tau). \tag{16.22}$$

subject to homogeneous boundary conditions and zero initial conditions. Then it is physically obvious that before the source acts at $t = \tau$, the response would be identically zero, i.e.

$$G(\mathbf{x}, t; \boldsymbol{\xi}, \tau) \equiv 0 \text{ for } t < \tau.$$

This is known as the casuality condition and will be imposed as a mathematical "initial" condition on G.

Because of the delta function in t in (16.22), the forcing term is actually zero for $t > \tau$. Thus the Green's function satisfied the following homogeneous system for $t > \tau$:

$$\frac{\partial^2}{\partial t^2}G - c^2\nabla^2 G = 0, \quad t > \tau. \tag{16.23}$$

subject to homogeneous boundary conditions. The "initial condition" at $t = \tau$ is given by

$$\begin{aligned} G &= 0 \text{ at } t = \tau \\ \frac{\partial}{\partial t}G &= \delta(\mathbf{x} - \boldsymbol{\xi}) \text{ at } t = \tau \end{aligned} \tag{16.24}$$

The second condition is obtained by integrating Eq. (16.22) from $t = \tau^-$ to $t = \tau^+$.

16.4.1 Example: 1-D wave equation in infinite domain

Instead of solving

$$\frac{\partial^2}{\partial t^2}G - c^2\frac{\partial^2}{\partial x^2}G = \delta(x - \xi)\delta(t - \tau), \quad t > 0,$$

we note that the above equation is equivalent to

$$\frac{\partial^2}{\partial t^2}G - c^2\frac{\partial^2}{\partial x^2}G = 0, \quad t > \tau$$

$$G = 0, \quad \text{at } t = \tau$$

$$\frac{\partial}{\partial t} G = \delta(x - \xi) \text{ at } t = \tau$$

The solution to the homogeneous wave equation was discovered by d'Alembert (see Chapter 17) to be of the form

$$G = R(x - c(t - \tau)) + L(x + c(t - \tau))$$

where R and L are arbitrary differentiable functions, to be determined by initial conditions. You can verify that it satisfies the wave equation by differentiation.

Since $G = 0$ at $t = \tau$, we must have

$$R(x) + L(x) = 0.$$

Thus

$$G = R(x - c(t - \tau)) - R(x + c(t - \tau)).$$

Since

$$\begin{aligned} \frac{\partial}{\partial t} G\Big|_{t=\tau} &= -c\, R'(x - c(t - \tau))\big|_{t=\tau} - cR'(x + c(t - \tau))\big|_{t=\tau} \\ &= -2cR'(x) \end{aligned}$$

the second initial condition:

$$\frac{\partial}{\partial t} G \,\big|_{t=\tau} = \delta(x - \xi),$$

becomes

$$-2cR'(x) = \delta(x - \xi)$$

Integrating

$$R(x) = -\frac{1}{2c} \int_{-\infty}^{x} \delta(x' - \xi) dx' + B$$

$$= -\frac{1}{2c} H(x - \xi) = \begin{cases} 0 & \text{if } x < \xi \\ -\frac{1}{2c} & \text{if } x > \xi \end{cases}$$

where $H(x)$ is the Heaviside step function: $H(x) = 0$ for $x < 0$, $H(x) = 1$ for $x > 0$.

The required Green's function is

$$G(x, t; \xi, \tau) = \frac{1}{2c} \left\{ (H(x - \xi) + c(t - \tau)) - H((x - \xi) - c(t - \tau)) \right\}.$$

The constant B cancels out.

The Green's function represents a rectangular pulse expanding from $x = \xi$ to the left and to the right each with speed c. Ahead of the expanding fronts, $G = 0$.

16.4.2 Example: 3-D wave equation in infinite domain

$$\frac{\partial^2}{\partial t^2}G - c^2\nabla^2 G = \delta(\mathbf{r})\delta(t-\tau), \quad \mathbf{r} = \mathbf{x} - \boldsymbol{\xi}$$

$$\nabla^2 G = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}G),$$

since G is independent of the angles.

We solve the following equivalent system for $t > \tau$:

$$\frac{\partial^2}{\partial t^2}G - c^2\nabla^2 G = 0$$

$$G = 0 \text{ at } t = \tau$$
$$\frac{\partial}{\partial t}G = \delta(\mathbf{r}) \text{ at } t = \tau$$

Writing $G \equiv U/r$,

$$\frac{\partial}{\partial r}G = \frac{1}{r}\frac{\partial}{\partial r}U - \frac{1}{r^2}U,$$
$$\frac{\partial}{\partial r}(r^2\frac{\partial}{\partial r}G) = \frac{\partial}{\partial r}(r\frac{\partial}{\partial r}U) - \frac{\partial}{\partial r}U = r\frac{\partial^2}{\partial r^2}U,$$

we obtain a simpler equation for U:

$$\frac{\partial^2}{\partial t^2}U - c^2\frac{\partial^2}{\partial r^2}U = 0, \quad t > \tau$$

Its solution is the d'Alembert's solution discussed for the 1-D wave equation

$$U = R(r - c(t-\tau)) - R(r + c(t-\tau))$$
$$\frac{\partial}{\partial t}G = \frac{\partial}{\partial t}U/r \,\Big|_{t=\tau} = -\frac{2c}{r}R'(r) = \delta(\mathbf{r})$$

For $r \neq 0$, $R'(r) = 0$ and so $R(r) = B$, a constant, which we set to zero. Near $r = 0$, $R(r)$ may have a singularity. To find out, we integrate over a sphere of radius ϵ:

$$\begin{aligned}
1 &= -2c\int_0^\epsilon \frac{1}{r}R'(r)4\pi r^2 dr \\
&= -8\pi c\int_0^\epsilon rR'(r)dr = -8\pi c[rR(r)|_0^\epsilon - \int_0^\epsilon R(r)dr] \\
&= 8\pi c\int_0^\epsilon R(r)dr
\end{aligned}$$

From this we see that $R(r)$ must be a delta function

$$R(r) = \frac{1}{4\pi c}\delta(r),$$

since

$$\int_0^\epsilon \delta(r)dr = \frac{1}{2}\int_{-\epsilon}^\epsilon \delta(r)dr = \frac{1}{2}.$$

Finally,

$$\begin{aligned}
G(\mathbf{x},t;\boldsymbol{\xi},\tau) &= \frac{1}{4\pi c}\frac{[\delta(r-c(t-\tau))-\delta(r+c(t-\tau))]}{r} \\
&= \frac{1}{4\pi c}\frac{\delta(r-c(t-\tau))}{r} \text{ for } r>0, \quad t>\tau,
\end{aligned}$$

where

$$r = [(x-\xi)^2+(y-\eta)^2+(z-\zeta)^2]^{1/2} = |\mathbf{x}-\boldsymbol{\xi}|.$$

This represents a concentrated impulse spreading out from the source in a spherial shell with a radial velocity of c, while its amplitude decays as the distance from the source increases.

16.4.3 Example: 2-D wave equation in infinite domain

The 2-D problem turns out to be more difficult than even the 3-D problem. This problem becomes simpler if we treat the 2-D case as a 3-D problem but with no z-dependence of the source function.

$$\text{3-D} : (\frac{\partial^2}{\partial t^2} - c^2\nabla^2)G_{3D} = \delta(x-\xi)\delta(y-\eta)\delta(z-\zeta)\delta(t-\tau)$$

$$\text{2-D} : (\frac{\partial}{\partial t^2} - c^2\nabla^2)G_{2D} = \delta(x-\xi)\delta(y-\eta)\delta(t-\tau)$$

The 2-D forcing can be obtained by integrating the 3-D forcing from $\zeta = -\infty$ to $\zeta = +\infty$. It then follows that the 2-D Green's function can be obtained from 3-D Green function, integrated from $\zeta = -\infty$ to $\zeta = \infty$.

The 3-D Green's function was found to be:

$$\begin{aligned} G_{3D}(\mathbf{x}, t; \boldsymbol{\xi}, \tau) &= \frac{\delta(r - c(t-\tau))}{4\pi c\, r} \\ G_{2D}(\mathbf{x}, t; \boldsymbol{\xi}, \tau) &= \int_{-\infty}^{\infty} \frac{\delta(r - c(t-\tau))}{4\pi c\, r} d\zeta, \end{aligned}$$

where $r = [(x-\xi)^2 + (y-\eta)^2 + (z-\zeta)^2]^{1/2}$.

Let

$$\begin{aligned} z' &= \zeta - z, \quad d\zeta = dz' \\ \rho &= [(x-\xi)^2 + (y-\eta)^2]^{1/2}, \\ r^2 &= \rho^2 + z'^2, \quad 2z'dz' = 2r dr \end{aligned}$$

$$\begin{aligned} G_{2D}(\mathbf{x}, t; \boldsymbol{\xi}, \tau) &= \int_{-\infty}^{\infty} \frac{\delta(r - c(t-\tau))dr}{4\pi c z'} \\ &= \frac{2}{4\pi c} \int_0^{\infty} \frac{\delta(r - c(t-\tau))dr}{\sqrt{r^2 - \rho^2}} = \frac{2}{\sqrt{c^2(t-\tau)^2 - \rho^2}} \int_0^{\infty} \delta(r - c(t-\tau))dr \\ &= \begin{cases} \frac{(1/2\pi c)}{\sqrt{c^2(t-\tau)^2 - \rho^2}}, & \rho < c(t-\tau) \\ 0, & \rho > c(t-\tau) \end{cases} \end{aligned}$$

Unlike the 3-D case, the effect at $t - \tau$ due to an impulsive source is spread over the entire regions $\rho < c(t-\tau)$, instead of concentrated at $\rho = c(t-\tau)$.

16.4.4 The solution to the nonhomogeneous wave equation

After finding the Green's function, we now return to finding the solution u to the original problem (16.21), which is rewritten as

$$\mathcal{L}u = Q(\mathbf{x}, t), \tag{16.25}$$

$$\mathcal{L} \equiv \frac{\partial^2}{\partial t^2} - c^2 \nabla^2,$$

subject to homogeneous boundary conditions and initial conditions.

The solution is

$$u(\mathbf{x},t) = \int_0^\infty \iiint_V G(\mathbf{x},t;\boldsymbol{\xi},\tau)Q(\boldsymbol{\xi},\tau)d\xi d\eta d\zeta d\tau, \tag{16.26}$$

where the Green's function satisfies (16.22) and homogeneous boundary and zero initial conditions.

$$\begin{aligned}\mathcal{L}u(\mathbf{x},t) &= \int_0^\infty \iiint_V \mathcal{L}G(\mathbf{x},t;\boldsymbol{\xi},\tau)Q(\boldsymbol{\xi},\tau)d\xi d\eta d\zeta d\tau \\ &= \int_0^\infty \iiint_V \delta(\mathbf{x}-\boldsymbol{\xi})\delta(t-\tau)Q(\boldsymbol{\xi},\tau)d\xi d\eta d\zeta d\tau \\ &= Q(\mathbf{x},t),\end{aligned}$$

which is (16.25).

If instead of the above, $u(\mathbf{x},t)$ satisfies nonzero initial conditions:

$$\begin{aligned} u(\mathbf{x},0) &= f(\mathbf{x}) \\ \frac{\partial}{\partial t}u(\mathbf{x},0) &= g(\mathbf{x}),\end{aligned}$$

(16.26) should then be viewed only as a particular solution, and a homogeneous solution, $v(\mathbf{x},t)$ satisfying

$$Lv = 0$$

subject to homogeneous boundary conditions, but

$$\begin{aligned} v(\mathbf{x},0) &= f(\mathbf{x}) \\ \frac{\partial}{\partial t}v(\mathbf{x},0) &= g(\mathbf{x}), \end{aligned} \tag{16.27}$$

should be added to (16.26).

Alternatively, the same Green's function (satisfying zero initial conditions) can also be used to construct the solution for nonzero initial conditions. This is because of the Green's formula, which for the operator $\mathcal{L}$ involving space and time derivatives, is, with t_i and t_f being any "initial" and "final" times:

$$\begin{aligned}&\int_{t_i}^{t_f} \iiint_V [u\mathcal{L}v - v\mathcal{L}u]dV dt \\ &\quad = \iint_V (u\frac{\partial v}{\partial t} - v\frac{\partial u}{\partial t})\Big|_{t_i}^{t_f} dV - c^2 \int_{t_i}^{t_f} \iint_{\partial V} (u\nabla v - v\nabla u)\cdot \hat{\mathbf{n}} dS\end{aligned}$$

We let $v = G$ be the Green's function satisfying (16.22) with homogeneous boundary conditions and zero initial conditions and u the required solution satisfying nonzero initial conditions and (16.25). The left-hand side of above formula becomes

$$\begin{aligned}
&\int_{t_i}^{t_f} \iiint_V [u\mathcal{L}G - G\mathcal{L}u] dV\, dt \\
=&\int_{t_i}^{t_f} \iiint_V [u\delta(\mathbf{x}-\boldsymbol{\xi})\delta(t-\tau) - G\cdot Q(\mathbf{x},t)] dV\, dt \\
=&u(\boldsymbol{\xi},\tau) - \int_{t_i}^{t_f} G(\mathbf{x},t;\boldsymbol{\xi},\tau) Q(\mathbf{x},t) dV\, dt
\end{aligned}$$

The first term on the right-hand side of the above Green's formula is

$$\begin{aligned}
&\iiint_V (u\frac{\partial G}{\partial t} - G\frac{\partial u}{\partial t})\Big|_{t_i}^{t_f} dV \\
=-&\iiint_V [f(\mathbf{x})\frac{\partial}{\partial t}G\Big|_{t=0} - g(\mathbf{x})G\Big|_{t=0}] dV
\end{aligned}$$

after we evaluate at $t_i = 0$ and $t_f = \infty$.

After switching $\boldsymbol{\xi}$ with $\mathbf{x}$, and τ with t, we obtain the general formula for finding $u(\mathbf{x}, t)$:

$$\begin{aligned}
u(\mathbf{x},t) =& \int_0^\infty \iiint_V Q(\boldsymbol{\xi},\tau) G(\mathbf{x},t;\boldsymbol{\xi},\tau) d\xi\ d\eta\ d\zeta\ d\tau \\
&- \iiint_V [f(\boldsymbol{\xi})\frac{\partial}{\partial \tau}G\Big|_{\tau=0} - g(\boldsymbol{\xi})G\Big|_{\tau=0}] d\xi\ d\eta\ d\zeta \\
&- c^2 \int_0^\infty \iint_{\partial V} [u\nabla G - G\nabla u]\cdot \hat{\mathbf{n}} dS
\end{aligned}$$

The first term on the right-hand side deals with the effect of the forcing Q on the solution, the second term the effect of the initial conditions and the third term that of the nonhomogeneous boundary conditions. (The integral is on the boundary of V and the variable of integration and gradient is with respect to $\boldsymbol{\xi}$. It vanishes for homogeneous boundary conditions on u.) It is amazing that the same Green's function, which satisfies zero initial conditions and homogeneous boundary conditions, is all that is needed to construct the general solution.

Example

Solve
$$\left(\frac{\partial^2}{\partial t^2} - c^2\frac{\partial^2}{\partial x^2}\right)u = Q(x,t), \quad -\infty < x < \infty, \quad t > 0$$
subject to initial conditions
$$u(x,0) = f(x)$$
$$\frac{\partial u}{\partial t}(x,0) = g(x), \quad -\infty < x < \infty.$$

Method 1

We first find the solution to the homogeneous PDE satisfying the correct initial condition, i.e. find $v(x,t)$ satisfying
$$\left(\frac{\partial^2}{\partial t^2} - c^2\frac{\partial^2}{\partial x^2}\right)v = 0$$
$$v(x,0) = f(x), \quad \frac{\partial u}{\partial t}(x,0) = g(x).$$
d'Alembert's solution is of the form
$$v(x,t) = R(x-ct) + L(x+ct).$$
To satisfy initial conditions:
$$v(x,0) = f(x) = R(x) + L(x)$$
$$\frac{\partial}{\partial t}v = -cR'(x-ct) + cL'(x+ct)$$
$$g(x) = \frac{\partial}{\partial t}v(x,0) = -cR'(x) + cL'(x)$$
Integrating:
$$L(x) - R(x) = \frac{1}{c}\int_0^x g(\bar{x})d\bar{x} + K,$$
where K is an arbitrary constant of integration. Adding it to
$$L(x) + R(x) = f(x)$$
we get
$$L(x) = \frac{1}{2}f(x) + \frac{1}{2c}\int_0^x g(\bar{x})d\bar{x} + \frac{K}{2}.$$

Subtracting, we get

$$R(x) = \frac{1}{2}f(x) - \frac{1}{2c}\int_0^x g(\bar{x})d\bar{x} - \frac{K}{2}$$

Finally,

$$\begin{aligned} v(x,t) &= R(x-ct) + L(x+ct) \\ &= \frac{1}{2}f(x-ct) + \frac{1}{2}f(x+ct) + \frac{1}{2c}\int_{x-ct}^{x+ct} g(\bar{x})d\bar{x}. \end{aligned}$$

The constant K cancels out.

The particular solution is, from (16.26) and an earlier section (16.4.1):

$$\begin{aligned} u_p(x,t) &= \int_0^\infty \int_{-\infty}^\infty G(x,t;\xi,\tau)Q(\xi,\tau)d\xi d\tau \\ &= \frac{1}{2c}\int_0^\infty \int_{-\infty}^\infty \{H((x-\xi)+c(t-\tau)) - H((x-\xi)-c(t-\tau))\}Q(\xi,\tau)d\xi d\tau \\ &= \frac{1}{2c}\int_0^\infty \int_{x-c(t-\tau)}^{x+c(t-\tau)} Q(\xi,\tau)d\xi \; d\tau \end{aligned}$$

The full solution is

$$u(x,t) = v(x,t) + u_p(x,t).$$

Method 2

Using the Green's function exclusively, the solution is

$$\begin{aligned} u(x,t) = &\int_0^\infty \int_{-\infty}^\infty G(x,t;\xi,\tau)Q(\xi,\tau)d\xi d\tau \\ &- \int_{-\infty}^\infty [f(\xi)\frac{\partial}{\partial\tau}G\Big|_{\tau=0} - g(\xi)G\Big|_{\tau=0}]d\xi \end{aligned}$$

Since

$$\begin{aligned} G(x,t;\xi,\tau) &= \frac{1}{2c}\{H((x-\xi)+c(t-\tau)) - H((x-\xi)-c(t-\tau))\} \\ G|_{\tau=0} &= \frac{1}{2c}\{H((x-\xi)+ct) - H((x-\xi)-ct)\} \\ \frac{\partial}{\partial\tau}G\Big|_{\tau=0} &= -\frac{1}{2}\{\delta((x-\xi)+ct) + \delta((x-\xi)-ct)\} \end{aligned}$$

The last integral for $u(x,t)$ is

$$
\begin{aligned}
&-\int_{-\infty}^{\infty} -\frac{1}{2}[f(\xi)\{\delta((x-\xi)+ct)+\delta((x-\xi)-ct)\} \\
&- g(\xi)\frac{1}{2c}\{H((x-\xi)+ct)-H((x-\xi)-ct)\}]d\xi \\
&= \frac{1}{2}f(x-ct)+\frac{1}{2}f(x+ct)+\frac{1}{2c}\int_{x-ct}^{x+ct} g(\xi)d\xi.
\end{aligned}
$$

This is the same as the homogeneous solution found in Method 1, showing that the two methods yield the same solution.

16.4.5 Example: In 3-D infinite space

$$
\frac{\partial^2}{\partial t^2}u - c^2\nabla^2 u = Q(\mathbf{x},t)
$$

subject to zero initial conditions, the solutiono is,

$$
\begin{aligned}
u(\mathbf{x},t) &= \int_0^{\infty} d\tau \iiint_V G(\mathbf{x},t;\boldsymbol{\xi},\tau)Q(\boldsymbol{\xi},\tau)d\xi d\eta d\zeta \\
&= \int_0^{t} d\tau \iiint_V G(\mathbf{x},t;\boldsymbol{\xi},\tau)Q(\boldsymbol{\xi},\tau)d\xi d\eta d\zeta
\end{aligned}
$$

since $G(\mathbf{x},t;\boldsymbol{\xi},\tau)\equiv 0$ for $\tau > t$.

Using the Green's function derived in the previous section, we have

$$
u(\mathbf{x},t) = \frac{1}{4\pi c}\int_0^{t} d\tau \iiint_V \frac{1}{r}\delta(r-c(t-\tau))Q(\boldsymbol{\xi},\tau)d\xi d\eta d\zeta
$$

where

$$
r = [(x-\xi)^2+(y-\eta)^2+(z-\zeta)^2]^{1/2}
$$

Because of the presence of the delta function in the integrand, the response, $u(\mathbf{x},t)$, at $\mathbf{x}$ is a superposition of the sources which satisfy

$$
|\mathbf{x}-\boldsymbol{\xi}| = c(t-\tau)
$$

divided by the distance between $\boldsymbol{\xi}$, the source location, and $\mathbf{x}$, where the response is measured.

16.5 Green's Function for the Heat Equation

We are interested in solving for the temperature $u(\mathbf{x},t)$ in the presence of a heat source distribution $Q(\mathbf{x},t)$. u satisfies the following nonhomogeneous PDE:

$$\frac{\partial}{\partial t}u = \alpha^2\nabla^2 u + Q(\mathbf{x},t) \tag{16.28}$$

We first consider the case where u satisfies homogeneous boundary conditions and zero initial condition. The Green's function is defined by

$$\frac{\partial}{\partial t}G = \alpha^2\nabla^2 G + \delta(\mathbf{x}-\boldsymbol{\xi})\delta(t-\tau), \tag{16.29}$$

subject to the same homogeneous initial and boundary conditions. The original solution is then constructed using

$$u(\mathbf{x},t) = \int_0^\infty d\tau \iiint_V G(\mathbf{x},t;\boldsymbol{\xi},\tau)Q(\boldsymbol{\xi},\tau)d\xi d\eta d\zeta \tag{16.30}$$

This can be verified by substituting (16.30) into (16.28)

$$\begin{aligned}
(\frac{\partial}{\partial t}u - \alpha^2\nabla^2 u) &= \int_0^\infty d\tau \iiint_V (\frac{\partial}{\partial t} - \alpha^2\nabla^2)G(\mathbf{x},t;\boldsymbol{\xi},\tau)Q(\boldsymbol{\xi},\tau)d\xi d\eta d\zeta \\
&= \int_0^\infty d\tau \iiint_V \delta(\mathbf{x}-\boldsymbol{\xi})\delta(t-\tau)Q(\xi,\tau)d\xi d\eta e\zeta \\
&= Q(\mathbf{x},t).
\end{aligned}$$

Next we consider the case of $u(\mathbf{x},t)$ satisfying (16.28) and homogeneous boundary conditions, but nonzero initial condition

$$u(\mathbf{x},0) = f(\mathbf{x}).$$

We still use the same Green's function defined in (16.29) satisfying zero initial condition, but add an extra term in the formula (16.30):

$$\begin{aligned}
u(\mathbf{x},t) = &\int_0^\infty d\tau \iiint_V G(\mathbf{x},t;\boldsymbol{\xi},\tau)Q(\boldsymbol{\xi},\tau)d\xi d\eta d\zeta \\
&+ \iiint_V G(\mathbf{x},t;\boldsymbol{\xi},0)f(\boldsymbol{\xi})d\xi d\eta d\zeta.
\end{aligned} \tag{16.31}$$

Since $\left(\frac{\partial}{\partial t} - \alpha^2\nabla^2\right)G(\mathbf{x},t;\boldsymbol{\xi},0) = 0$ for $t > 0$, the last term added in (16.31) satisfies the homogeneous heat equation.

Since the Green's function should be zero before the source is tunred on at $t = \tau$, we have

$$G(\mathbf{x}, t; \boldsymbol{\xi}, \tau) \equiv 0, \quad \text{for } t < \tau,$$

and so the upper limit in the τ-integration in (16.31) can be replaced by t, i.e.

$$\begin{aligned} u(\mathbf{x}, t) = &\int_0^t d\tau \iiint_V G(\mathbf{x}, t; \boldsymbol{\xi}, \tau) Q(\boldsymbol{\xi}, \tau) d\xi d\eta d\zeta \\ &+ \iiint_V G(\mathbf{x}, t; \boldsymbol{\xi}, 0) f(\xi) d\xi d\eta d\zeta \end{aligned} \tag{16.32}$$

Therefore,

$$\begin{aligned} \lim_{t \to 0^+} u(\mathbf{x}, t) &= 0 + \lim_{t \to 0^+} \iiint_V G(\mathbf{x}, t; \xi, 0) f(\xi) d\xi d\eta d\zeta \\ &= f(\mathbf{x}). \end{aligned}$$

This is because integrating (16.29) in t:

$$\begin{aligned} G(\mathbf{x}, t; \boldsymbol{\xi}, 0) = \alpha^2 &\int_0^t \nabla^2 G(\mathbf{x}, t; \boldsymbol{\xi}, 0) dt \\ &+ \delta(\mathbf{x} - \boldsymbol{\xi}) \int_0^t \delta(t) dt \\ = &\ \delta(\mathbf{x} - \boldsymbol{\xi}) \text{ as } t \to 0^+. \end{aligned}$$

Solution in infinite space

Taking advantage of the fact that

$$G(\mathbf{x}, t; \boldsymbol{\xi}, \tau) = 0 \text{ for } t < \tau$$

and

$$G(\mathbf{x}, t; \xi, \tau) = \delta(\mathbf{x} - \boldsymbol{\xi}) \text{ for } t = \tau$$

we can obtain the Green's function without the forcing term on the right-hand side of (16.29) by solving the following "initial value" problem

$$\begin{aligned} \frac{\partial}{\partial t} G = \alpha^2 \nabla^2 G, &\quad t > \tau \\ G = \delta(\mathbf{x} - \boldsymbol{\xi}) &\quad \text{at } t = \tau \end{aligned} \tag{16.33}$$

In one-dimension, this problem in the infinite domain is the same as the Drunken Sailor problem solved previously using Fourier transforms. The solution is

$$G(x,t;\xi,\tau) = \frac{1}{\sqrt{4\pi\alpha^2(t-\tau)}} \exp\left\{-\frac{(x-\xi)^2}{4\alpha^2(t-\tau)}\right\} \tag{16.34}$$

In n-dimensions, the infinite space Green's function for the heat equation is

$$G(\mathbf{x},t;\boldsymbol{\xi},\tau) = [\frac{1}{4\pi\alpha^2(t-\tau)}]^{\frac{n}{2}} \exp\{-\frac{|\mathbf{x}-\boldsymbol{\xi}|^2}{4\alpha^2(t-\tau)}\}.$$

This is because, in Fourier transform solution, each dimension involves its own Fourier integral and the n-dimensional problem is simply n one-dimensional problem.

Chapter 17

Wave Equations in Infinite Domains

17.1 Introduction

For disturbances ("waves") which propagate at finite speed starting from an initially localized shape ("of compact support"), the effect of the boundaries is not felt until much later, when the waves reach the boundaries. Although we can still use in this case the eigenfunction expansion method discussed earlier, that method is not *efficient*: Each eigenmode is a result of solving a boundary value problem and is therefore heavily influenced by the presence of boundaries. It represents the normal mode achieved after the wave bounces back and forth from the boundaries a few times. A localized disturbance which has not yet seen the effect of boundary can still be represented by superposition of these normal modes by virtue of the completeness theorem discussed in Chapter 12. However it needs many of these modes to render an accurate representation, because none of these modes look like the localized disturbance.

An alternate method is to ignore the boundaries (for the duration before the disturbance reaches one of them). We then have a problem in an infinite domain. Integral transform methods can be used, or the *method of characteristics* can be applied. These methods will be discussed in this chapter.

17.2 1-D wave equation

Consider the simple wave equation in one dimension:

$$\frac{\partial^2}{\partial t^2}u = c^2\frac{\partial^2}{\partial x^2}u, \quad -\infty < x < \infty, \quad 0 < t < \infty. \tag{17.1}$$

subject to the initial condition that

$$\begin{aligned} u(x,0) &= f(x), \quad && -\infty < x < \infty \\ u_t(0,0) &= g(x), \quad && -\infty < x < \infty, \end{aligned} \tag{17.2}$$

where $f(x)$ and $g(x)$ are given functions. We shall assume that they are of compact support, i.e., $f(x) \to 0$, $g(x) \to 0$ as $x \to \pm\infty$. The boundary conditions are that

$$u(x,t) \to 0 \quad \text{as } x \to \pm\infty$$

or that

$$u(x,t) \text{ bounded as } x \to \pm\infty,$$

but if t is finite, the disturbance will not have seen the boundaries and there may not be an opportunity to apply the boundary conditions.

This problem, being in an infinite domain, can be solved using Fourier transforms. This was done in Chapter 8. d'Alembert (1746), however, had a simpler method, but it works only on the wave equation.

17.3 d'Alembert's approach

d'Alembert recognized that any function of either $x+ct$ or $x-ct$ will satisfy the wave equation. We can simply verify that any trial solution

$$\boxed{u(x,t) = L(x+ct) + R(x-ct)} \tag{17.3}$$

satisfies the PDE (14.1) for any functions L and R (which have second derivatives, of course).

To show this, let us write

$$\begin{aligned} \xi &\equiv x + ct \\ \eta &\equiv x - ct, \end{aligned}$$

and

$$u(x,t) = L(\xi) + R(\eta).$$

We use a prime to denote ordinary differentiation with respect to the argument of the function, e.g.

$$L'(\xi) \equiv \frac{d}{d\xi}L(\xi), \quad R'(\eta) \equiv \frac{d}{d\eta}R(\eta).$$

The partial derivatives are calculated in the following way:

$$\begin{aligned}
\frac{\partial}{\partial t}L(\xi) &= L'(\xi)\frac{\partial \xi}{\partial t} = cL'(\xi) \\
\frac{\partial}{\partial x}L(\xi) &= L'(\xi)\frac{\partial \xi}{\partial x} = L'(\xi) \\
\frac{\partial^2}{\partial t^2}L(\xi) &= \frac{\partial}{\partial t}(cL'(\xi)) = \frac{d}{\partial \xi}(cL'(\xi))\frac{\partial \xi}{\partial t} = c^2 L''(\xi) \\
&= \frac{\partial}{\partial x}(L'(\xi)) = \frac{d}{d\xi}(L'(\xi))\frac{\partial \xi}{\partial x} = L''(\xi).
\end{aligned}$$

Similarly,

$$\begin{aligned}
\frac{\partial}{\partial t}R(\eta) &= R'(\eta)\frac{\partial \eta}{\partial t} = -cR'(\eta) \\
\frac{\partial}{\partial x}R(\eta) &= R'(\eta)\frac{\partial \eta}{\partial x} = R'(\eta) \\
\frac{\partial^2}{\partial t^2}R(\eta) &= \frac{\partial \eta}{\partial t}\frac{d}{d\eta}(-cR'(\eta)) = c^2 R''(\eta) \\
\frac{\partial^2}{\partial x^2}R(\eta) &= \frac{\partial \eta}{\partial x}\frac{d}{d\eta}(R'(\eta)) = R''(\eta).
\end{aligned}$$

It is seen that both $L(\xi)$ and $R(\eta)$ satisfy the wave equations, i.e.

$$\left(\frac{\partial^2}{\partial t^2} - c^2\frac{\partial}{\partial x^2}\right)L(\xi) = 0,$$

and

$$\left(\frac{\partial^2}{\partial t^2} - c^2\frac{\partial^2}{\partial x^2}\right)R(\eta) = 0.$$

Therefore the combination, (14.3), also satisfies the wave equation.

The functional forms of L and R should be determined from initial conditions.

Since

$$u(x,t) = L(x+ct) + R(x-ct), \quad u_t(x,t) = cL'(x+ct) - cR'(x-ct),$$

it follows from the initial conditions that,

$$u(x,0) = L(x) + R(x) = f(x), \quad -\infty < x < \infty \tag{17.4}$$
$$u_t(x,0) = cL'(x) - cR'(x) = g(x), \quad -\infty < x < \infty. \tag{17.5}$$

The second equation, (14.5), can be integrated with respect to x to yield

$$L(x) - R(x) = \frac{1}{c}\int_0^x g(\overline{x})d\overline{x} + K, \tag{17.6}$$

where K is an arbitrary constant. Adding (14.6) to (14.4) yields

$$\boxed{L(x) = \frac{1}{2}f(x) + \frac{1}{2c}\int_0^x g(\overline{x})d\overline{x} + \frac{K}{2}}, \tag{17.7}$$

and subtracting (14.6) from (14.4) yields

$$\boxed{R(x) = \frac{1}{2}f(x) - \frac{1}{2c}\int_0^x g(\overline{x})d\overline{x} - \frac{K}{2}}. \tag{17.8}$$

We change x to ξ in (14.7) and x to η in (14.8), and then add:

$$u(x,t) = L(\xi) + R(\eta).$$

Thus

$$\boxed{u(x,t) = \frac{1}{2}f(x+ct) + \frac{1}{2}f(x-ct) + \frac{1}{2c}\int_{x-ct}^{x+ct} g(\overline{x})d\overline{x}}. \tag{17.9}$$

This is the full solution to the wave equation in an infinite spatial domain.

17.4 Example

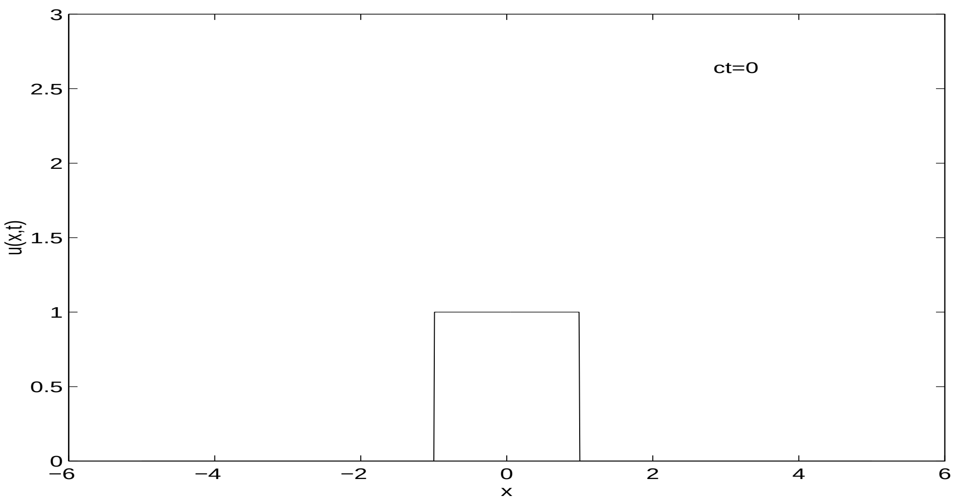
Solve:

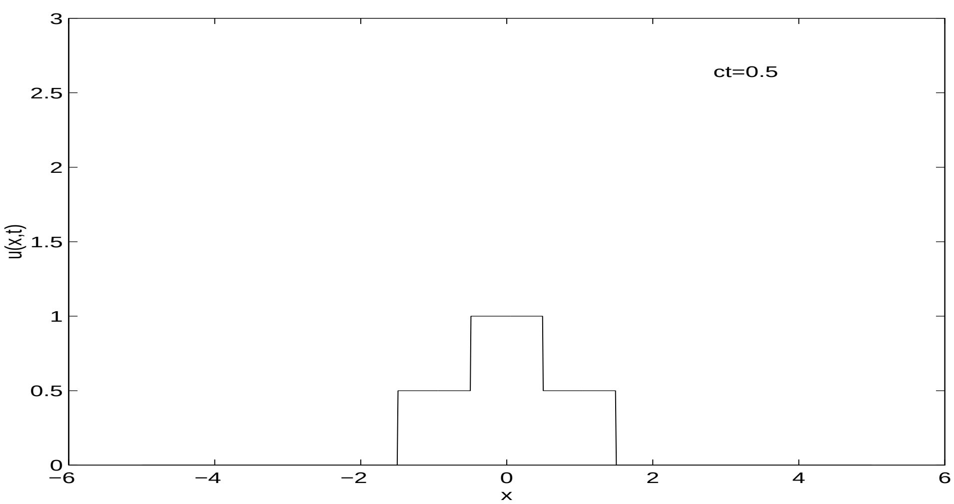
$$\begin{aligned}
&\text{PDE:} \quad u_{tt} = c^2 u_{xx}, \quad -\infty < x < \infty, \quad t > 0 \\
&\text{ICs:} \quad u(x,0) = f(x) = \begin{cases} 1, & -1 < x < 1 \\ 0, & \text{elsewhere} \end{cases} \\
&\qquad\quad u_t(x,0) = 0, \quad -\infty < x < \infty.
\end{aligned}$$

Since $g \equiv 0$, d'Alembert's solution is

$$u(x,t) = \frac{1}{2}[f(x+ct) + f(x-ct)].$$

We simply divide the initial shape in two halves. Let one half move to the left with speed c and the other half to the right with speed c. In the interval where the two halves overlap we add their amplitudes.





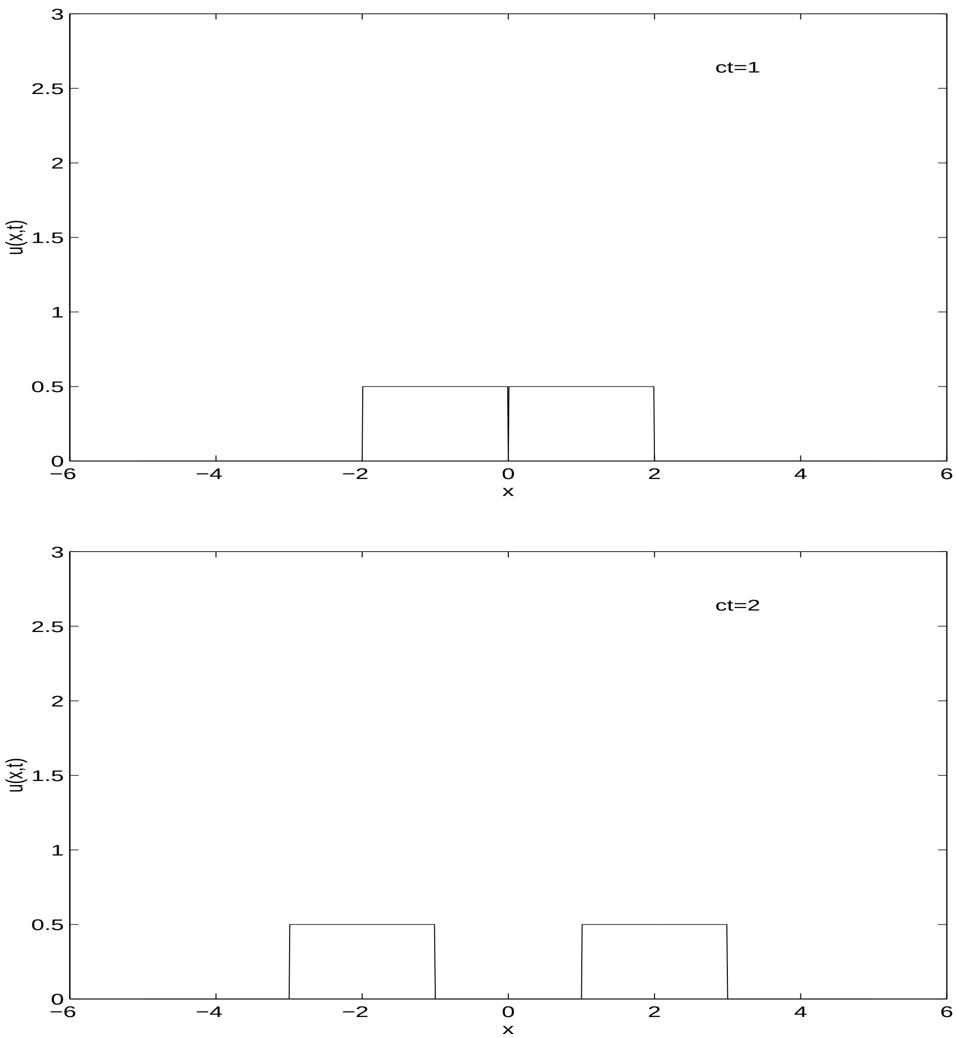


Figure 14.1. Wave propagation in an infinite domain.

17.5 Method of characteristics

The lesson learned from d'Alembert can be generalized. What we learned was that the wave equation, (14.1), can be rewritten as

$$(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x})(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x})u = 0. \tag{17.10}$$

And so if we define a new coordinate system

$$\begin{aligned} \xi &= x + ct \\ \eta &= x - ct, \end{aligned} \tag{17.11}$$

(14.10) will take the simpler "canonical" form:

$$-4c^2 \frac{\partial^2}{\partial\eta\partial\xi} u = 0. \tag{17.12}$$

This is because

$$\begin{aligned} \frac{\partial}{\partial x} &= \frac{\partial\xi}{\partial x}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial x}\frac{\partial}{\partial\eta} = \frac{\partial}{\partial\xi} + \frac{\partial}{\partial\eta} \\ \frac{\partial}{\partial t} &= \frac{\partial\xi}{\partial t}\frac{\partial}{\partial\xi} + \frac{\partial\eta}{\partial t}\frac{\partial}{\partial\eta} = c\frac{\partial}{\partial\xi} - c\frac{\partial}{\partial\eta}, \end{aligned}$$

and so

$$\begin{aligned} (\frac{\partial}{\partial t} - c\frac{\partial}{\partial x}) &= -2c\frac{\partial}{\partial\eta} \\ (\frac{\partial}{\partial t} + c\frac{\partial}{\partial x}) &= 2c\frac{\partial}{\partial\xi}. \end{aligned}$$

(14.12) can be solved simply by integration:

$$\frac{\partial}{\partial\xi} u = \text{ function of } \xi.$$

Upon another integration:

$$\begin{aligned} u &= \text{ function of } \xi + \text{ function of } \eta \\ &= L(\xi) + R(\eta). \end{aligned}$$

This is the same as (14.3), assumed by d'Alembert. It says that part of $u(x,t)$ is invariant when viewed by an observer moving with wave speed c and the other part of it is invariant when the observer moves with speed $-c$.

$$\begin{aligned} u(x,t) &= u_1(x,t) + u_2(x,t) \\ u_1(x,t) &= L(\xi), \quad u_2(x,t) = R(\eta) \end{aligned}$$

$$\frac{du_1}{dt} = 0 \cdot \text{ (i.e. } u_1(x,t) = \text{constant)}$$

when

$$\frac{dx}{dt} = -c \cdot \text{ (i.e. along } x + ct = \xi = \text{const).} \tag{17.13}$$

$$\frac{du_2}{dt} = 0 \cdot \text{ (i.e. } u_2(x,t) = \text{constant)}$$

when

$$\frac{dx}{dt} = c \cdot \text{ (i.e. along } x - ct = \eta = \text{const)} \tag{17.14}$$

(14.13) defines the "left characteristics":

$$\xi = x + ct = \text{constant} = x_0.$$

(14.14) defines the "right characteristics":

$$\eta = x - ct = \text{const} = x_0$$

17.6 Inviscid Burgers equation

Burgers equation is a prototype equation for one-dimensional fluid flow. It is, for velocity $u(x,t)$ of the fluid:

$$\frac{\partial}{\partial t}u + u\frac{\partial}{\partial x}u = \nu\frac{\partial^2}{\partial x^2}u, \quad -\infty < x < \infty. \tag{17.15}$$

[The real equation for fluids is the Navier-Stokes equation, which has an extra term $-\frac{1}{\rho}\frac{\partial}{\partial x}p$ on the right-hand side of (14.15), representing the pressure force (p is the pressure, ρ is the density of the fluid). The presence of two additional unknowns, p and ρ, require additional equations. Burgers equation does not include the pressure force and consequently is simply a *prototype*.]

Burgers equation incorporates the effectt of *viscosity*, the term on the right-hand side of (14.15), where ν is a coefficient of viscosity. Viscosity acts to smooth out gradients. Burgers equation also includes a *nonlinear* advection term, the second term on the left-land side. In the absence of the nonlinear term, Burgers equation reduces to the diffusion (or heat) equation:

$$\frac{\partial}{\partial t}u = \nu\frac{\partial^2}{\partial x^2}u, \quad -\infty < x < \infty,$$

which we have solved using the transform methods in Chapter 8.

Now we consider the nonlinear version of Burgers equation in the limit as $\nu \to 0$. Therefore:

$$(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x})u = 0. \tag{17.16}$$

17.6.1 Linear advection

Befpre we solve (14.15), let's apply the method of characteristics to a linear version of (14.15):

$$(\frac{\partial}{\partial t} + \overline{u}\frac{\partial}{\partial x})u = 0, \tag{17.17}$$

with $\overline{u}$ beging a constant. We shall solve (14.17) subject to the initial condition:

$$u(x, 0) = f(x). \tag{17.18}$$

(14.17) implies that if we more with an observer whose location $x(t)$ is determined by

$$\frac{d}{dt}x = \overline{u},$$

then the solution u will appear to be invariant:

$$\frac{d}{dt}u = 0.$$

That is, instead of the observer sitting in a fixed location x, we let him move, and so $x = x(t)$. For $u = u(x(t), t)$, $\frac{d}{dt}u$ will involve two partial derivatives, first with respect to the first argugment, $x(t)$, and the second with respect to the second argument, t.

$$\begin{aligned} \frac{d}{dt}u(x(t), t) &= \frac{d}{dt}x\frac{\partial}{\partial x}u + \frac{\partial}{\partial t}u \\ &= (\frac{\partial}{\partial t} + \frac{dx}{dt}\frac{\partial}{\partial x})u. \end{aligned}$$

We still have the option to choose the velocity of the observer. We choose it to be:

$$\frac{dx}{dt} = \overline{u}. \tag{17.19}$$

Then

$$\frac{d}{dt}u = (\frac{\partial}{\partial t} + \overline{u}\frac{\partial}{\partial x})u = 0, \tag{17.20}$$

from the equation (14.17).

(14.19) can be solved:

$$x(t) = x_0 + \overline{u}t, \tag{17.21}$$

where x_0 is the initial position. Rearranging, (14.21) becomes:

$$x_0 = x(t) - \overline{u}t. \tag{17.22}$$

(14.20) implies that u will appear to be unchanging if we move with $x(t)$. That is,

$$\begin{aligned} u(x(t),t) &= \text{constant} = u(x_0,0) \\ &= f(x_0) = f(x(t) - \overline{u}t). \end{aligned} \tag{17.23}$$

Now we revert back to our stationary coordinate system ($x(t) \to x$):

$$u(x,t) = f(x - \overline{u}t). \tag{17.24}$$

(14.24) is the final solution of (14.17) satisfying the initial condition (14.18), as can be verified by differentiation. As seen in Figure 14.1(a), the initial shape is simply advected by the velocity $\overline{u}$ for $t > 0$.

17.6.2 Nonlinear advection

Now we apply the same method of characteristics to the nonlinear advection equation (14.16), which can be written as

$$\frac{d}{dt}u = (\frac{\partial}{\partial t} + \frac{dx}{dt}\frac{\partial}{\partial x})u = (\frac{\partial}{\partial t} + u\frac{\partial}{\partial x})u = 0, \tag{17.25}$$

if the observer moves with velocity

$$\frac{dx}{dt} = u. \tag{17.26}$$

The solution to (14.26) is more difficult because the observer moves with the fluid velocity u, which is what we want to solve. Nevertheless, since (14.25) says that u is an invariant, i.e.

$$u(x(t),t) = u(x_0,0) = f(x_0), \tag{17.27}$$

the right-hand side of (14.26) can be taken as a constant. We then have

$$x(t) = x_0 + ut,$$

or

$$x_0 = x(t) - ut. \tag{17.28}$$

Substituting (14.28) into (14.27), we get

$$u(x(t),t) = f(x(t) - ut).$$

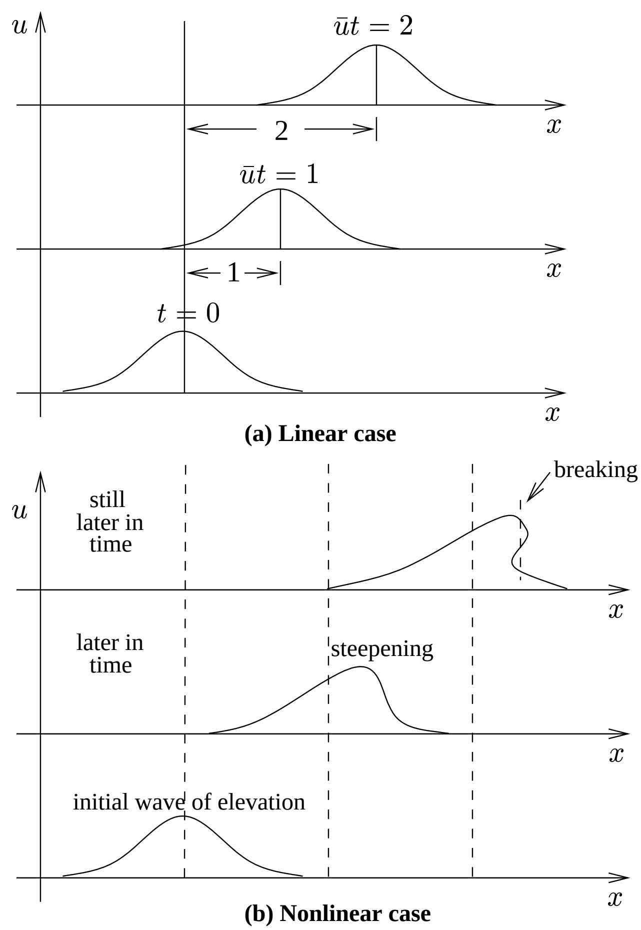


Figure 17.1: Linear and nonlinear advections.

Finally, we change $x(t)$ to x:

$$u(x,t) = f(x - ut) \tag{17.29}$$

This is now our solution albeit in an implicit form.

We can verify that (14.29) satisfies the equation (14.16) in the original coordinate system (x, t):

$$\begin{aligned} \frac{\partial}{\partial t}u &= f'(x-ut)\cdot(-u - \frac{\partial}{\partial t}u\cdot t) \\ \frac{\partial}{\partial x}u &= f'(x-ut)\cdot(1 - \frac{\partial}{\partial x}u\cdot t) \end{aligned}$$

So:

$$\frac{\partial}{\partial t}u = \frac{-uf'(x-ut)}{1+tf'(x-ut)} \tag{17.30}$$

$$\frac{\partial}{\partial x}u = \frac{f'(x-ut)}{1+tf'(x-ut)}. \tag{17.31}$$

Thus

$$\frac{\partial}{\partial t}u + u\frac{\partial}{\partial x}u = 0.$$

The evolution of an initial shape is shown in Figure 14.1(b). The slopes of the characteristics are given by the initial shape of u. The characteristics orginating from the location where the initial shape $f(x)$ is larger have larger shapes in the $t-x$ plane (actually shallower slopes in the $x-t$ plane plotted), than those from the smaller part of the initial shape. As a consequence the peak of the wave travels faster than other parts of the wave, eventually tilts over and "breaks". We consider breaking to have occurred when the solution becomes multivalued, i.e., there are more than one value of u for the same value of x. In reality, our inviscid solution ceases to be valid in the part of the solution where the wave shape becomes vertical, i.e.

$$|\frac{\partial u}{\partial x}| \to \infty.$$

From (14.31), the first time this occurs is

$$t = t_c \equiv \min_{\text{over } x_0}\{-1/f'(x_0)\} \tag{17.32}$$

The critical time t_c is also the time when the characteristics first intersect each other.

17.6.3 Shocks

Just before the wave breaks, its leading edge form a *shock*. A shock is a high gradient region. It is a region where u becomes discontinuous in the inviscid solution. Discontinuities can never form in the presence of viscosity, which tends to smooth out high gradient regions. The viscous term on the right-hand side of Burgers equation, (14.16), is not negligible no matter how small the coefficient ν. The smaller the ν, the thinner is the shock.

Burgers equation, including the viscous term, can be written as

$$\frac{\partial}{\partial t}u + \frac{\partial}{\partial x}(\frac{1}{2}u^2) = \frac{\partial}{\partial x}(\nu\frac{\partial}{\partial x}u)$$

We shall consider the case $\nu \to 0^+$.

Integrate this equation across the shock from $x = A$ on the left-side of the shock to $x = B$ on the right-side of the shock. Inside the shock the viscous term is important. Outside the shock it can be ignored. A and B are outside the shock.

$$\frac{\partial}{\partial t}\int_A^B udx + \frac{1}{2}u^2(B) - \frac{1}{2}u^2(A) = \nu\frac{\partial}{\partial x}u\bigg|_A^B \to 0 \tag{17.33}$$

The right hand side approaches zero as $\nu \to 0^+$ because the points A and B are outside the shock and so the gradients, $\frac{\partial}{\partial x}u$, there are finite.

Let the shock be located at

$$x = X(t), \quad A < X(t) < B$$

$$\int_A^B udx = \int_A^{X(t)} udx + \int_{X(t)}^B udx.$$

We shall ignore the variations of u with respect to x between A and $X(t)$, and between $X(t)$ and B, since the rapid variations are concentrated across the shock at $X(t)$.

$$\int_A^B udx = u(A)[X(t) - A] + u(B)[B - X(t)]$$

$$\frac{\partial}{\partial t}\int_A^B udx = [u(A) - u(B)]\frac{d}{dt}X$$

(14.6.33) becomes

$$[u(A) - u(B)]\frac{d}{dt}X + \frac{1}{2}[u^2(B) - u^2(A)] = 0,$$

yielding:

$$\frac{d}{dt}X = \frac{1}{2}[u(A) + u(B)]. \tag{17.34}$$

That is, the shock moves with a velocity which is the average of the fluid velocities on the left and right sides of the shock.

17.6.4 Fans

Consider the following simple example

$$(\frac{\partial}{\partial t} + u\frac{\partial}{\partial x})u = 0, \qquad -\infty < x < \infty$$
$$u(x,0) = f(x) = \begin{cases} 1 & \text{for } x < 0 \\ 2 & \text{for } x > 0. \end{cases}$$

No shock will form in this case because the smaller amplitude wave is behind the larger amplitude one and so will never catch up. Instead a "fan" will form. Applying the method of characteristics, we have

$$\frac{du}{dt} = 0$$

along

$$\frac{dx}{dt} = u.$$

The second equation is integrated, using the fact that u is an invariant, deduced from the first equation.

$$x(t) = ut + x_0$$

or

$$x_0 = x(t) - ut.$$

The solution is

$$u(x(t), t) = \text{constant} = u(x_0, 0) = f(x_0).$$

So

$$u(x,t) = \begin{cases} 1 & \text{for } x_0 < 0, \text{ which means } x < t, \\ 2 & \text{for } x_0 > 0, \text{ which means } x > 2t. \end{cases}$$

Between $t < x < 2t$, the characteristics orignate from $x_0 = 0$, and so are described by

$$x = ut.$$

This is

$$u(x,t) = x/t, \quad t < x < 2t$$

and so varies from $u = 1$ to $u = 2$ smoothly.

The characteristics

$$x = ut, \quad 1 < u < 2$$

"fan" out from the origin in the x-t plane.