Chapter 3

Classical second-order PDEs

In this chapter, we will consider second order partial differential equations. We will derive and analyze the three (so-called) **fundamental equations of mathematical physics**:

$$\frac{\partial u}{\partial t} = \kappa \nabla^2 u \quad \text{— Diffusion (or heat) equation}$$

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u \quad \text{— Wave equation}$$

$$\nabla^2 u = f(\mathbf{r}) \quad \text{— Laplace/Poisson equation}$$

3.1 Classification of second-order linear PDEs

At this point, one may wonder why we should focus on these three particular equations. The underlying reason is that they represent the canonical equations of the main classes of linear second-order PDEs. The most general linear second-order PDE in two variables takes the form

$$a(x,y)\frac{\partial^2 u}{\partial x^2} + b(x,y)\frac{\partial^2 u}{\partial x \partial y} + c(x,y)\frac{\partial^2 u}{\partial y^2} + d(x,y)\frac{\partial u}{\partial x} + e(x,y)\frac{\partial u}{\partial y} + f(x,y)u = g(x,y) \quad (3.1)$$

Here, the coefficients may very well vanish, be constant or be general functions of x and y. Equation (3.1) resembles the equation of conic sections

$$ax^2 + bxy + cy^2 + dx + ey + f = 0 \quad (3.2)$$

In the case of conic sections, we know that we obtain

$$\begin{cases} \text{an } \textbf{ellipse} & \text{if } b^2 - 4ac < 0 \\ \text{a } \textbf{parabola} & \text{if } b^2 - 4ac = 0 \\ \text{a } \textbf{hyperbola} & \text{if } b^2 - 4ac > 0 \end{cases} \quad (3.3)$$

This conic sections classification inspires the following classification for linear second-order PDEs:

- If $b^2 - 4ac < 0$, the PDE (3.1) is called **elliptic**
- If $b^2 - 4ac = 0$, the PDE (3.1) is called **parabolic**
- If $b^2 - 4ac > 0$, the PDE (3.1) is called **hyperbolic**

So the type of the PDE is given by the sign of a kind of ”discriminant” $D = b^2 - 4ac$. This classification can be extended to PDEs in any number of variables using ideas from linear algebra but this is beyond the scope of this module.

A quick look at our usual suspects and we easily realize that Laplace’s and Poisson’s equations are both **elliptic**, while the wave equation is **hyperbolic** and the heat equation is **parabolic**. Our three fundamental equations of mathematical physics are in a sense representatives of the three types of second-order linear PDEs.

Example

- The following equation $u_{xx} + 3u_{xy} + u_{yy} + 2u_x - u_y = 0$ is such that $b^2 - 4ac > 0$ so it is hyperbolic.
- The following equation $u_{xx} + 3u_{xy} + 8u_{yy} + 2u_x - u_y = 0$ is such that $b^2 - 4ac < 0$ so it is elliptic.
- The following equation $u_{xx} - 2u_{xy} + u_{yy} + 2u_x - u_y = 0$ is such that $b^2 - 4ac = 0$ so it is parabolic.

Note that this classification is not only valid for linear second-order PDEs with constant coefficients but as we said coefficients can be general functions of x and y. If the coefficients are variable, the **equation may change type depending on the region of the** (x, y)**-space**.

Example

Consider the equation

$$y\frac{\partial^2 u}{\partial x^2} - 2\frac{\partial^2 u}{\partial x \partial y} + x\frac{\partial^2 u}{\partial y^2} = 0 \tag{3.4}$$

In the (x, y)-plane, we can compute $D = (-2)^2 - 4xy = 4(1 - xy)$. So the sign of D is given by the sign of $1 - xy$ and we find that

- The equation is parabolic on the hyperbola of equation $xy = 1$;
- The equation is elliptic in the two convex regions $xy > 1$;
- The equation is hyperbolic in the connected region $xy < 1$.

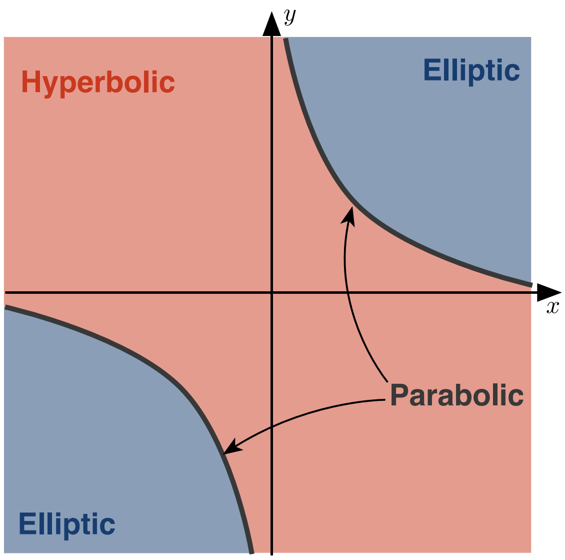

Figure 3.1

3.2 Boundary conditions

One may wonder why it may be a good thing to classify PDEs after all. Are we just giving these equations a label? It is impossible to formulate a general existence theorem that applies to all linear partial differential equations, even if we only consider second-order equations. However, general theorems about each of these classes of equations (elliptic, parabolic and hyperbolic) can be found and are stated and proved in more advanced modules (and graduate-level textbooks for instance). While an interesting subject, this is far beyond the scope of this module (which is less about the theory of PDEs and more about its applications after all!).

Because PDEs typically have so many solutions, we need to impose auxiliary conditions or constraints to be able to single one out. In general, these boundary conditions should be motivated by the underlying problem or the physics. You already know that they come in two flavors: **boundary conditions** and **initial conditions**.

An initial condition specifies the physical state of the system at a particular time t_0 (often, $t = 0$ but not always).

Example

> The initial condition $u(\mathbf{r}, t_0) = u_0(\mathbf{r}) \equiv u_0(x, y, z)$ can represent: the initial concentration/mass density of a substance for the diffusion equation, the initial temperature distribution for the heat equation...
>
> As the wave equation involves a second-order derivative in time, it is quite clear on physical grounds that we need to specify a pair of initial conditions
>
> $$u(\mathbf{r}, t_0) = u_0(\mathbf{r}) \quad \text{and} \quad \frac{\partial u}{\partial t}(\mathbf{r}, t) = v_0(\mathbf{r}) \tag{3.5}$$

In each physical problem, the PDE is defined on a domain Ω. If you consider a vibrating string of length L, then the domain Ω is the interval $0 < x < L$ and the boundary $\partial\Omega$ consists of the two end points in $x = 0$ and $x = L$. If you are concerned with the vibrations of a drumhead, then the domain Ω is the disk formed by the skin of the drumhead and the boundary $\partial\Omega$ is a closed curve (i.e. the circle at the edge of the drumhead). If you consider the diffusion of a chemical substance in water, then Ω is the container holding the water and its boundary $\partial\Omega$ is a surface. Finally, if you consider the Schrödinger's equation governing a free particle, then the domain is all of space and has no boundary.

To single out a solution, it may be necessary to specify some boundary conditions. The three most important kinds of boundary conditions are named as follows:

- A **Dirichlet condition (D)** specifies the value of u;
- A **Neumann condition (N)** specifies the value of the normal derivative $\partial u/\partial n$;
- A **Robin condition (R)** specifies the value of $\partial u/\partial n + au$, where a is a given function of x, y, z and t.

These conditions must hold for all t and for $\mathbf{r} \in \partial\Omega$. For instance, a Neumann boundary condition is written as

$$\frac{\partial u}{\partial n} = f(\mathbf{r}, t), \qquad \mathbf{r} \in \partial\Omega \tag{3.6}$$

where $f(\mathbf{r}, t)$ is a given function and as usual $\mathbf{n} = (n_x, n_y, n_z)$ denotes the outward unit vector normal to $\partial\Omega$ (see Fig. 3.2), while $\partial u/\partial n \equiv \mathbf{n} \cdot \nabla u$ denotes the directional derivative of u in the outward normal direction. If f is equal to zero on any boundary, we call this boundary condition homogeneous, otherwise it is called inhomogeneous.

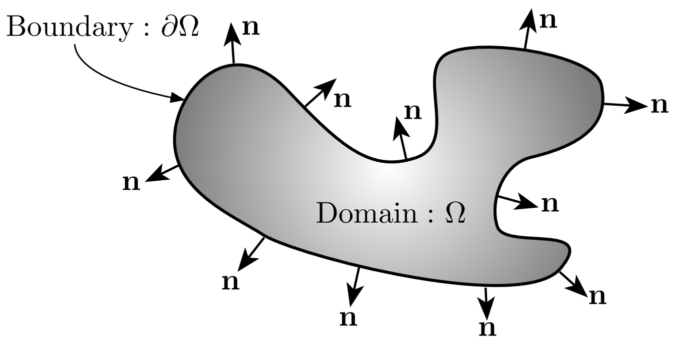

Figure 3.2

The physical problem we are solving should guide our choice of boundary conditions. Depending on the problem, one type of boundary conditions may make sense while another would not. We will try to highlight throughout this chapter the physical meaning of the boundary conditions we use.

Example

Consider the vibrating string problem:

- if the a string is held fixed at both ends (like in a guitar or a violin), we have homogenous Dirichlet conditions;
- if one end of the string is free to move without resistance along a track, then there we are faced with a Neumann condition at that end;
- If now you imagine that the free end is able to move along a track but a Hookean spring or rubber band tends to pull it back to its equilibrium position, then this boundary condition is of Robin type;
- If an end of the string is moved in a simplified way, we have an inhomogeneous Dirichlet condition at that end.

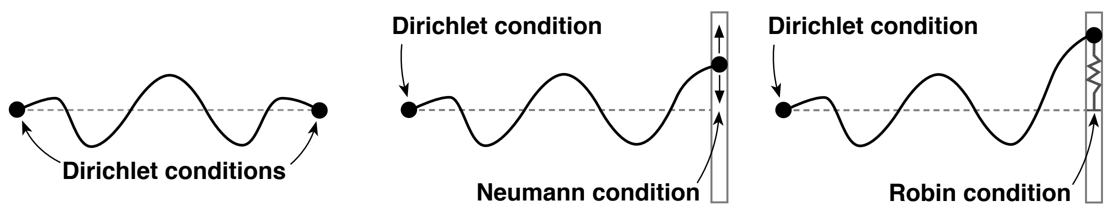

Figure 3.3

The general considerations that are involved in deciding which type of boundary condition are appropriate for a particular problem are complex. In general, whether the various types of boundary conditions are appropriate (in the sense that they help us single out a solution) depends both on the type of second-order equation we are dealing with as well as whether the domain has a closed or open boundary.

There are some natural pairings which can guide your choice. Let us give a couple of illustrative examples. First, if the equation is elliptic, we can solve the **Dirichlet problem**. For instance, if one wants to find the electrostatic potential $u(x, y)$ in the interior of a cylindrical region $x^2 + y^2 < R^2$ when the charge density $\rho(x, y)$ is specified on the boundary and the boundary is required to be an equipotential surface, that person would need to solve the following elliptic boundary-value problem

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = -\rho(x,y), \quad x^2 + y^2 < R^2 \tag{3.7}$$

$$u(x,y) = C, \quad x^2 + y^2 = R^2 \tag{3.8}$$

where C is a constant.

If the equation is now parabolic or hyperbolic, it is more natural to solve the **Cauchy problem** in time-dependent problems, i.e. the problem in which we specify the solution and its time derivative on the line $t = 0$ as well as relevant boundary conditions (D, N or R). For the vibrating string, this corresponds to solving the hyperbolic Cauchy problem

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0, \quad t > 0,\ 0 < x < L \tag{3.9}$$

$$u(x,0) = f_1(x), \quad 0 < x < L \tag{3.10}$$

$$\frac{\partial u}{\partial x}(x,0) = f_2(x), \quad 0 < x < L \tag{3.11}$$

$$u(0,t) = 0, \quad u(L,t) = 0 \tag{3.12}$$

where f_1 and f_2 specify the initial position and velocity of the string and we have used homogeneous Dirichlet boundary conditions (string is fixed at both ends).

3.3 Diffusion (or heat) equation

In the previous chapter, we saw that through the **Cole-Hopf transformation**, we can recast the problem of solving Burgers equation (a non-linear second order PDE) into solving a diffusion equation (an example of a **parabolic PDE**) for an auxiliary function. In this section, we will first provide elementary derivations of the diffusion equation and show its link to the concept of **random walks**. We will then introduce a number of classical techniques to solve the diffusion equation. Some of these resolution techniques will prove useful in solving other second order linear PDEs like the wave equation or Laplace's equation.

Remark. *Note that as far as we are concerned here, the diffusion equation and the heat equation are one and the same. One can consider the diffusion equation to be a more general version (in the sense that it models of variety of systems) of the heat equation which was derived first for the sole problem of heat conduction in a body with uniform density and heat capacity.*

3.3.1 The diffusion equation as a conservation law

To encourage scientific progress, the French Academy used to organize competitions for its prestigious prizes by presenting specific problems in mathematics and physics. In 1811, the Academy chose the problem of heat transfer for its annual prize. The French mathematician Joseph Fourier (1768-1830) – who was not an active scientist, but a politician at the time – was awarded the prize for two important contributions: (1) the development of a partial differential equation (the heat equation) and (2) the development of a method for solving it. The basic idea that Fourier used was that of conservation of energy.

Here, we used the approach used by Fick (1885) to derive the diffusion equation. At the time, Fick noticed than when salt is poured into water the concentration of salt slowly spreads out and eventually becomes uniformly distributed in the water. We want to obtain an evolution equation for the salt concentration. For the sake of simplicity, we will assume that the motion is long the x-axis (i.e. we will consider a one dimension problem). This would model for instance the concentration of salt in a thin and long pipe. Let $u(x,t)$ designate the concentration in salt, which has the dimensions of a number of particles per unit length; this is called the linear density.

Conservation Law

Consider an interval $a \leq x \leq b$, the number of salt particles in this interval can change only for two reasons:

1. They can move along the x-axis and eventually move in or out of the interval. We will denote $J(x,t)$ the net number of salt particles that pass x per unit time. The function J is the **flux of particles**.
2. They can be created or destroyed within the interval. In the case of salt particles, this could happen via chemical reactions or if there are physical sources or sinks of salt particles. We denote $Q(x,t)$ the number of particles created at x per unit time.

Now the rate of change in the total number of salt particles in the interval $[a,b]$ is due to the movement of the particles across the boundaries of the interval $J(a,t) - J(b,t)$ and to the creation of destruction of the particles within the interval. This balance law reads mathematically

$$\frac{d}{dt}\int_a^b u(x,t)dx = J(a,t) - J(b,t) + \int_a^b Q(x,t)dx \tag{3.13}$$

Using the Fundamental Theorem of Calculus, the above integral can be written as

$$\int_a^b \frac{\partial u(x,t)}{\partial t}dx = -\int_a^b \frac{\partial J}{\partial x}dx + \int_a^b Q(x,t)dx \tag{3.14}$$

which leads to

$$\int_a^b \left(\frac{\partial u(x,t)}{\partial t} + \frac{\partial J}{\partial x}dx - Q(x,t)\right)dx = 0 \tag{3.15}$$

As this equation holds for any interval, the integrand must be identically zero and we conclude that

$$\frac{\partial u(x,t)}{\partial t} = -\frac{\partial J}{\partial x} + Q(x,t) \tag{3.16}$$

We have thus obtained an evolution equation for the concentration in salt $u(x,t)$, but this equation is quite general. We still need to specify the functions J and Q for our problem.

Fick's law of diffusion

Fick's assumption (which was based on physical observations) is that particles tend to move from regions of higher concentrations to regions regions of lower concentration. Thus, he assumed that the flux of particles was opposite to the gradient of the particle concentration, i.e.

$$J(x,t) = -D\frac{\partial u}{\partial x} \tag{3.17}$$

where D is a positive constant known as the **diffusion coefficient**. Equation (3.17) is known as **Fick's law of diffusion** (when applied to temperature, it goes by the name of **Fourier law of heat conduction**). This is an example of a **constitutive law**.

In the simplest of cases, it is assumed that particles are neither created nor annihilated which leads to $Q = 0$. In this case, the balance law reduces to

$$\frac{\partial u}{\partial t} = D\frac{\partial^2 u}{\partial x^2} \tag{3.18}$$

This is the **one-dimensional diffusion equation**. This derivation was particularly simple and relied mainly on the prescription for the constitutive law. In more general cases, one could measure the flux J experimentally and then use this information to specify the function J.

Finally, note that the boundary conditions most often used when solving the diffusion equation involve prescribing the value of $u(x, t)$ (i.e. fixing the concentration) or the value of $\partial u/\partial x$ (i.e. fixing the value of the flux at the boundary).

Fourier's derivation of the heat equation

In his derivation of the heat equation, Fourier used the idea of conservation of energy (heat is a form of energy). For the sake of simplicity, consider a solid body which is homogeneous and isotropic, with constant mass density ρ. We also consider that the body can receive energy from an external source (e.g. from an electrical current, a chemical reaction or from external absorption or radiation). We will consider that the external source supplies the body with rate r per unit mass. The dimensions of r are thus

$$[r] = [\text{Energy}] \cdot [\text{Time}]^{-1} \cdot [\text{Mass}]^{-1} = ML^2T^{-2} \cdot T^{-1} \cdot M^{-1} = L^2T^{-3}. \tag{3.19}$$

The conservation of energy can be stated as follows: for an arbitrary control volume V inside the body, the time rate of change of thermal energy in V is equal to the net flux of heat through the boundary S of V due to conduction, plus the time rate at which heat is supplied by the external sources. If we denote $e(\mathbf{r}, t)$ the thermal energy per unit mass, then the total thermal energy inside the volume V is given by

$$\int_V \rho e(\mathbf{r}, t) d\mathbf{r} \tag{3.20}$$

The $\mathbf{q}$ heat flux has dimensions

$$[\mathbf{q}] = [\text{Energy}] \cdot [\text{Surface}]^{-1} \cdot [\text{Time}]^{-1} = ML^2T^{-2} \cdot L^{-2} \cdot T^{-1} = MT^{-3} \tag{3.21}$$

It specifies the direction and magnitude of the rate of flow across a unit area.

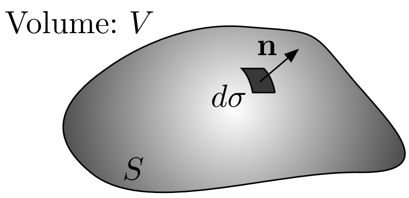

Figure 3.4

If $d\sigma$ is an area element of S with outward facing normal vector $\mathbf{n}$, then $\mathbf{q} \cdot \mathbf{n} d\sigma$ is the energy flow rate through $d\sigma$ and so the total inner heat flux through the surface S is given by

$$-\int_S \mathbf{q} \cdot \mathbf{n} d\sigma = -\int_V \nabla \cdot \mathbf{q} d\mathbf{r} \tag{3.22}$$

where we have used the divergence theorem. Finally, the contribution due to the external source is given by

$$\int_V r\rho d\mathbf{r} \tag{3.23}$$

The conservation of energy can be written mathematically as

$$\frac{d}{dt} \int_V \rho e(\mathbf{r}, t) d\mathbf{r} = -\int_V \nabla \cdot \mathbf{q} d\mathbf{r} + \int_V r\rho d\mathbf{r} \tag{3.24}$$

As V is an arbitrary control volume, we can write that

$$\rho \frac{\partial e}{\partial t} = -\nabla \cdot \mathbf{q} + r\rho \tag{3.25}$$

Just as above, we need to write down a constitutive law for $\mathbf{q}$ to go further. To determine the functional form of the heat flux, Fourier used the experimental observation that "heat flows from hotter places to colder places". Now the direction of maximal growth of a function is given by its gradient, so Fourier postulated

$$\mathbf{q} = -k\nabla u(\mathbf{r}, t) \tag{3.26}$$

where $u(\mathbf{r}, t)$ is the absolute temperature and k is the **thermal conductivity** which depends on the material. In general, k may depend on u, $\mathbf{r}$ or t but in practice, it often varies so little that it is reasonable to consider it to be constant. So we obtain that

$$\nabla \cdot \mathbf{q} = -k\Delta u \tag{3.27}$$

Now, the thermal energy is a linear function of the absolute temperature $e = c_v u(\mathbf{r}, t)$, where c_v is called the **specific heat** (at constant volume) of the material and can be considered constant. We thus finally obtain the following equation

$$\frac{\partial u}{\partial t} = \kappa\Delta u + f \tag{3.28}$$

where we have defined $\kappa = k/(c_v\rho)$ the thermal diffusivity and $f = r/c_v$ represents the varying density of heat sources throughout the material (often, not required in physical applications). Note that κ may depend on position $\mathbf{r}$, in which case the heat equation would become

$$\frac{\partial u}{\partial t} = \nabla \cdot (\kappa\nabla u) \tag{3.29}$$

3.3.2 Solution on a finite domain: the method of separation of variables

Application: Heat conduction in an insulated thin rod

In this first section, we are interested in the evolution of the temperature $u(x, t)$ in a homogeneous one-dimensional heat conducting rod of length L. This can be realized by narrow rods which are laterally insulated. We will consider that the initial temperature of every point on the rod is known (at time $t = 0$) and that both of its ends is kept at a constant temperature (i.e. kept in contact with a temperature bath).

If we assume that there is no internal source that heats of cools the system, the evolution of the local temperature of the rod is mathematically governed by the one-dimensional heat (or diffusion) equation

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} \tag{3.30}$$

where $\kappa > 0$ is the thermal diffusivity (a material property). On this finite domain, our problem is subject to boundary conditions of the form

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

and an initial condition

$$u(x, 0) = f(x), \quad \text{for } 0 \le x \le L. \tag{3.32}$$

Remark. *Note that the problem (3.30)-(3.32) is an initial boundary value problem that is linear and homogeneous and that the boundary condition (3.31) is called a* **Dirichlet condition***. condition.*

The method of separation of variables

We shall introduce a fundamental technique for obtaining solutions of linear partial differential equations: **the method of separation of variables**. Here, we look for particular solutions in the form

$$u(x,t) = X(x)T(t) \tag{3.33}$$

These are called **product solutions** or **separated solutions** and in general, they should satisfy certain additional conditions (which in many cases are homogeneous boundary conditions). The method of separation of variables relies on a few steps:

- **Step 1 —** We derive from the original PDE ordinary differential equations for $X(x)$ and $T(t)$; these equations will contains a parameter called the **separation constant**.
- **Step 2 —** Using a generalization of the superposition principle, we generate out of the separated solutions a more general solution of the PDE, in the form of an infinite series of separated solutions.
- **Step 3 —** We use initial and boundary conditions to compute the coefficient of this series.

Let us illustrate this technique on the problem defined by (3.30)-(3.32). Again, we are seeking solutions of the form

$$u(x,t) = X(x)T(t) \tag{3.34}$$

A substitution into (3.30) leads to

$$X(x)T(t)' = \kappa X(x)''T(t), \tag{3.35}$$

where the prime denotes for the function $X(x)$ (respectively, $T(t)$) a derivative with respect to x (respectively, to t). Next, we proceed to a simple but decisive step: **the separation of variables step**. We move to one side of the PDE all the functions that depend only on x and to the other side the functions that depend only on t. Here, we thus write

$$\frac{X''(x)}{X(x)} = \frac{T'(t)}{\kappa T(t)} \tag{3.36}$$

Now the LHS above only depends on x, while the RHS is dependent only on t. This expression must hold for all $t > 0$ and $x \in [0, L]$. Since x and t are independent variables, the only way this can be satisfied is if there exists a constant denoted λ (called the **separation constant**) such that

$$\frac{X''(x)}{X(x)} = \frac{T'(t)}{\kappa T(t)} = -\lambda \tag{3.37}$$

We have therefore reduced our PDE to the following system of ordinary differential equations with constant coefficients

$$\begin{cases} X'' = -\lambda X & 0 < x < L, \\ T' = -\lambda T & t > 0, \end{cases} \tag{3.38}$$

which should be easier to solve. The sign of the separation constant λ depends on the type of boundary conditions we impose. In our case, the function u satisfies the boundary conditions (3.31) if and only if

$$u(0,t) = X(0)T(t) = 0 \quad \text{and} \quad u(L,t) = X(L)T(t) = 0. \tag{3.39}$$

Since, u is not the trivial solution $u = 0$, it directly follows that

$$X(0) = X(L) = 0 \tag{3.40}$$

Therefore, the function X is a solution of the boundary value problem

$$\frac{d^2X}{dx^2} + \lambda X = 0, \quad 0 < x < L, \tag{3.41}$$

$$X(0) = X(L) = 0 \tag{3.42}$$

As this problem is not an initial boundary problem for an ODE (for which it is known that there exists a unique solution), it is here not clear a priori that there exists a solution for any value of the separation constant λ. On the other hand, if we write the general solution of the ODE for every λ, then we need to check for which λ there exists a solution that also satisfies the boundary conditions.

Now, remember that (3.41) is a second-order linear ODE with constant coefficients and its general solution depends on λ and has the following form:

- **Case 1 —** If $\lambda < 0$, the general solution can be written $X(x) = \alpha \cosh(\sqrt{-\lambda}x) + \beta \sinh(\sqrt{-\lambda}x)$ with α, β arbitrary real numbers. We know that the hyperbolic cosine is strictly positive, while the hyperbolic sine has a unique root in $x = 0$. Since, $X(x)$ must satisfy $X(0) = 0$, then it follows that $\alpha = 0$. Similarly, the second boundary condition imposes that $\beta = 0$. Thus, $X(x) \equiv 0$ is the trivial solution; thus, our problem does not admit a non-trivial solution when $\lambda < 0$.

- **Case 2 —** If $\lambda = 0$, the general solution can be written as a linear function $X(x) = \alpha + \beta x$ which vanishes at most in one point; thus once again, it cannot satisfy the boundary conditions unless $X(x) \equiv 0$ is the trivial solution.

- **Case 3 —** If $\lambda > 0$, the general solution can be written

$$X(x) = \alpha \cos(\sqrt{\lambda}x) + \beta \sin(\sqrt{\lambda}x) \tag{3.43}$$

Substituting this solution into the boundary condition $X(0) = 0$, we obtain that $\alpha = 0$. The boundary condition $X(L) = 0$ imposes that $\sin(\sqrt{\lambda}L) = 0$ which implies that $\sqrt{\lambda}L = n\pi$, with n a positive integer. Hence, the separation constant must be of the form

$$\lambda_n = \left(\frac{n\pi}{L}\right)^2, \quad n = 1, 2, 3 \cdots \tag{3.44}$$

The solutions for X are thus given by the functions

$$X_n(x) = B_n \sin \frac{n\pi x}{L} \tag{3.45}$$

Let us deal now with the ODE for T. The corresponding solution for T arises from

$$T' = -\lambda\kappa T = -\frac{n^2\pi^2\kappa}{L^2} T \tag{3.46}$$

which has a solution of the form

$$T_n(t) = C_n \exp\left(-\frac{\kappa n^2\pi^2 t}{L^2}\right) \tag{3.47}$$

Remark. *Note that we could have guessed a priori that the problem (3.41)-(3.42) would only admit solutions if $\lambda > 0$. Indeed, from a physical point of view, the solution of (3.46) must decay with time (otherwise, our temperature would be diverging!), hence, we must have $\lambda > 0$.*

Combining the two components of our solution, we found the following sequence of separated solutions

$$u_n(x,t) = X_n(x)T_n(t) = \beta_n \sin\frac{n\pi x}{L}\exp\left(-\frac{\kappa n^2\pi^2 t}{L^2}\right), \quad n = 1,2,3,\cdots \tag{3.48}$$

where we have defined for simplicity $\beta_n = B_nC_n$. Since the heat equation is linear, it follows by superposition principle that any linear combination of the solutions for different n (also called modes) is also a solution. The most general solution of the heat equation that satisfies the Dirichlet boundary conditions is therefore of the form

$$u(x,t) = \sum_{n=1}^{\infty}\beta_n \sin\frac{n\pi x}{L}\exp\left(-\frac{\kappa n^2\pi^2 t}{L^2}\right). \tag{3.49}$$

Finally, the **initial condition** (3.32) imposes that $u(x,0) = f(x)$. Imposing this condition, we see that $f(x)$ is related to the unknown coefficients β_n in the following way

$$f(x) = \sum_{n=1}^{\infty}\beta_n \sin\frac{n\pi x}{L} \tag{3.50}$$

Remark. [Historical note] *we mentioned in Chapter 1 that the problem of heat conduction was first tackled by the French mathematician and physicist Joseph Fourier (1768 - 1830). The brilliant idea that Fourier introduced (but which was not fully justified at the time) was that any arbitrary real function f that satisfies the boundary conditions can be represented as a unique infinite sum over sinusoidal modes. Such a series became known in Fourier theory as a Fourier series (or expansion) of the function f. The β_n are then called the Fourier coefficients of the series.*

We thus recognize (3.50) as a half-range Fourier sine series for $f(x)$ with coefficients

$$\beta_n = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)dx. \tag{3.51}$$

Therefore, the required solution of the heat equation subject to boundary conditions (3.31) and initial condition (3.32) is given by (3.49) and (3.51). This method can be adapted to accomodate boundary conditions on $\partial u/\partial x$, rather than u.

Example

Consider the problem:

$$\frac{\partial u}{\partial t} = \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < \pi, t > 0 \tag{3.52}$$

$$u(0,t) = u(\pi,t) = 0, \quad t \geq 0 \tag{3.53}$$

$$u(x,0) = f(x) = \begin{cases} x & 0 \leq x \leq \pi/2 \\ \pi - x & \pi/2 \leq x \leq \pi \end{cases} \tag{3.54}$$

Applying what we just saw, we can write that the solution to this problem is

$$u(x,t) = \sum_{m=1}^{\infty}\beta_m \sin(mx)e^{-m^2 t} \tag{3.55}$$

with

$$\begin{aligned}\beta_m &= \frac{2}{\pi}\int_0^\pi f(x)\sin(mx)dx \\ &= \frac{2}{\pi}\int_0^{\pi/2} x\sin(mx)dx + \frac{2}{\pi}\int_{\pi/2}^{\pi}(\pi - x)\sin(mx)dx \\ &= \frac{2}{\pi}\left[\frac{-x\cos(mx)}{m} + \frac{\sin(mx)}{m^2}\right]_0^{\pi/2} + \frac{2}{\pi}\left[\frac{-(\pi-x)\cos(mx)}{m} - \frac{\sin(mx)}{m^2}\right]_{\pi/2}^{\pi} \\ &= \frac{4}{\pi m^2}\sin\frac{m\pi}{2} \end{aligned} \tag{3.56}$$

but

$$\sin\frac{m\pi}{2} = \begin{cases} 0 & m = 2n \\ (-1)^{n+1} & m = 2n-1 \end{cases} \tag{3.57}$$

where $n = 1, 2, 3, \cdots$. Therefore, the solution reads

$$u(x,t) = \frac{4}{\pi}\sum_{n=1}^{\infty}\frac{(-1)^{n+1}}{(2n-1)^2}\sin\left[(2n-1)x\right]e^{-(2n-1)^2 t} \tag{3.58}$$

We represent this solution evolving over time in Fig. 3.5.

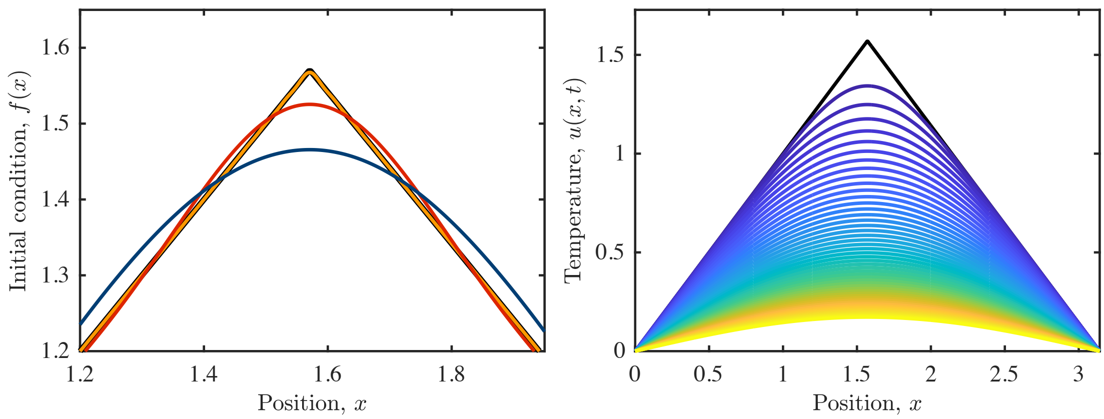

Figure 3.5 (*left*) Initial condition $f(x)$ (black solid line), approximation obtained by summing 3 terms (blue), 7 terms (red) and 100 terms (orange) for the Fourier expansion of $f(x)$. Focusing on the region near the point $x = \pi/2$, we observe as expected that only taking a few terms in the expansion smoothes out the singularity. (*right*) Function $u(x,t)$ of (3.58) for $t \in [0,5]$ increasing linearly (from blue to yellow). Note that the singularity at $t = 0$ is quickly smoothed out. These graphs were generated with 200 terms in the Fourier expansion. Initial profile (at $t = 0$) is drawn as a solid black line.

Other types of boundary conditions

We finish this section by mentioning boundary conditions that appear frequently in heat conduction problems. We generally distinguish between types of boundary conditions:

- **Separated boundary conditions —** These boundary conditions can be written as

$$B_0[u] = \alpha u(0,t) + \beta\frac{\partial u}{\partial x}(0,t) = 0, \quad B_L[u] = \gamma u(L,t) + \delta\frac{\partial u}{\partial x}(L,t) = 0, \quad t \geq 0 \tag{3.59}$$

where

$$\alpha, \beta, \gamma, \delta \in \mathbb{R}, |\alpha|+|\beta|> 0, |\gamma|+|\delta|> 0. \tag{3.60}$$

Note that by carefully choosing the parameters, we recover the types of boundary conditions introduced in Section 3.2. In particular, $\alpha = \gamma = 1$ and $\beta = \delta = 0$ leads to the **Dirichlet boundary condition**

$$u(0,t) = u(L,t) = 0 \quad t \geq 0 \tag{3.61}$$

which we have seen is also called a **boundary condition of the first kind**. Further, with $\alpha = \gamma = 0$ and $\beta = \delta = 1$, we obtain

$$\frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(L,t) = 0 \quad t \geq 0 \tag{3.62}$$

which is the **Neumann condition** (or **boundary condition of the second kind**).

Each of these type of boundary conditions has a physical interpretation. Indeed, we have seen that imposing Dirichlet boundary conditions to our problem corresponds to fixing the temperature of the ends of the rod, i.e. putting the ends of the rod in contact with a temperature bath. The physical interpretation of a Neumann boundary condition for this heat conduction problem is that there is no heat flow through the boundary; it means that the rod is fully insulated. Imposing a **Robin condition** (or **boundary condition of the third kind**) physically means that the heat flow at the boundary depends linearly on the temperature.

- **Periodic boundary condition —** If instead of rod, we tried to solve the problem of heat evolution along a circular wire of length L, then we would have imposed what is known as a periodic boundary condition. Clearly, in such a geometry, the temperature $u(x,t)$ and all its derivatives are periodic functions of x with a period L. The boundary conditions for this problem are then given by

$$u(0,t) = u(L,t), \quad \frac{\partial u}{\partial x}(0,t) = \frac{\partial u}{\partial x}(L,t) \quad \forall t \geq 0. \tag{3.63}$$

3.3.3 Uniqueness of the solution to the heat equation: Energy method

It is natural to ask whether the solution we obtained above is **unique**. Consider the following problem

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} \tag{3.64}$$

$$u(0,t) = u(L,t) = 0 \quad \text{for } t > 0, \tag{3.65}$$

$$u(x,0) = f(x), \quad \text{for } 0 \leq x \leq L. \tag{3.66}$$

Let u_1 and u_2 be two possible solutions and consider the difference $U = u_1 - u_2$. It is easy to see that then U satisfies the following problem

$$\frac{\partial U}{\partial t} = \kappa \frac{\partial^2 U}{\partial x^2} \tag{3.67}$$

$$U(0,t) = U(L,t) = 0 \quad \text{for } t > 0, \tag{3.68}$$

$$U(x,0) = 0, \quad \text{for } 0 \leq x \leq L. \tag{3.69}$$

We introduce the following quantify

$$E(t) = \frac{1}{2\kappa}\int_0^L [U(x,t)]^2 \, dx \tag{3.70}$$

and note that by definition, $E(0) = 0$. Our solution will be unique provided we can show that $U \equiv 0$. To do so, compute

$$\frac{dE}{dt} = \kappa^{-1} \int_0^L U \frac{\partial U}{\partial t} dx = \int_0^L U \frac{\partial^2 U}{\partial x^2} dx = \left[U \frac{\partial U}{\partial x} \right]_0^L - \int_0^L \left(\frac{\partial U}{\partial x} \right)^2 dx \tag{3.71}$$

after integrating by parts. The integrated term is clearly zero due to boundary conditions. So we conclude that

$$\frac{dE}{dt} \leq 0 \tag{3.72}$$

However, we also have that $E(t) \geq 0$ and $E(0) = 0$. Thus, we conclude that $E(t) = 0$ is identically zero, which implies that $U(x,t) \equiv 0$. The solution to the heat equation is thus unique.

3.3.4 Solution on an infinite or semi-infinite domain: Fourier transforms

Consider now that $L \to \infty$, we are now faced with a PDE problem on a semi-infinite domain. The method of separation of variable relied on Fourier series expansion and so is not adapted to our problem anymore. Instead, on infinite or semi-infinite domains, we can make use of Fourier transforms to obtain solutions.

Here, we then consider the following problem

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2}, \quad 0 < x < \infty, \ t > 0, \tag{3.73}$$

$$u(0,t) = 0, \quad t \geq 0 \tag{3.74}$$

$$u(x,0) = f(x), \quad 0 < x < \infty \tag{3.75}$$

and u bounded as $x \to \infty$ for all t.

The **Fourier transform method** consists in taking a Fourier transform in x of the PDE to convert it into an ordinary differential equation (which is usually simpler to solve). Since the problem is posed over a semi-infinite domain, we could take either a Fourier cosine or sine transform. Recall that if we take a cosine transform of a second derivative of u, we require the knowledge of $\partial u/\partial x$ at $x = 0$, while if we take a sine transform we need to know u itself at $x = 0$. So whether one should take a cosine or a sine transform will be dictated by the boundary conditions. In view of the boundary condition (3.74) we are imposing, we will take a Fourier sine transform of equation (3.73) and obtain

$$\frac{\partial \widehat{u}_s}{\partial t} = -\omega^2 \kappa \widehat{u}_s + \omega \kappa u(0,t) \tag{3.76}$$

where $\widehat{u}_s(\omega,t)$ is the Fourier sine transform of $u(x,t)$ with respect to x. Substituting $u(0,t)$ from (3.74), we obtain a first order linear ODE which we can integrate to obtain

$$\widehat{u}_s(\omega,t) = B(\omega) e^{-\omega^2 \kappa t} \tag{3.77}$$

To determine the integration constant, we need to take the Fourier sine transform of the initial condition (3.75) and we obtain $\widehat{u}_s = \widehat{f}_s(\omega)$ at $t = 0$, allowing us to determine $B(\omega) = \widehat{f}_s(\omega)$, and hence

$$\widehat{u}_s = \widehat{f}_s(\omega) e^{-\omega^2 \kappa t} \tag{3.78}$$

At this point, we can apply the inversion formula for the Fourier sine transform to write the solution to the original PDE in the form

$$u(x,t) = \frac{2}{\pi} \int_0^\infty \widehat{f}_s(\omega) e^{-\omega^2 \kappa t} \sin(\omega x) d\omega, \tag{3.79}$$

where

$$\widehat{f}_s(\omega) = \int_0^\infty f(x)\sin(\omega x)dx. \tag{3.80}$$

There is an example of this procedure in Problem Sheet # 4.

3.3.5 Fundamental solution to the diffusion equation

For linear partial differential equations, we have already seen various techniques of resolution, which often boil down to reducing the PDE to an ODE (or a system of ODEs). However, these approaches are not very useful when it comes to nonlinear partial differential equations. Here, we introduce an approach which identifies equations for which the solution depends on certain groupings of the independent variables. While this is a technique that is very useful for a certain class of nonlinear PDEs, we illustrate it here first on the diffusion (a homogeneous linear PDE) for the sake of simplicity.

Invariance under space and time transformation

Consider the homogeneous diffusion equation give by

$$\frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2} = 0 \tag{3.81}$$

where D is called the diffusion coefficient and $u(x,t)$ represents the mass density of a substance of interest. Equation (3.81) has important properties.

- **Time reversal —** The function

$$v(x,t) = u(x,-t) \tag{3.82}$$

  obtained by the change of variable $t \mapsto -t$, is a solution of the **backward** equation

$$\frac{\partial v}{\partial t} + D\frac{\partial^2 v}{\partial x^2} = 0 \tag{3.83}$$

  Note that to be consistent, Equation (3.81) is also called the **forward** equation.

  Remark. *The fact that (3.81) is not invariant with respect to time reversal (i.e. a change of sign in time) points to the irreversibility of the diffusion process. Think about adding a drop of milk to your coffee, over time the milk will diffuse and at long times, the milk concentration will become homogeneous in your cup; the reverse process which would correspond to the drop of pure milk reforming at the center of your cup from a homogeneous concentration in milk will never be observed. This is ensured by the second law of thermodynamics.*

- **Space and time translation invariance —** For fixed $(y,s) \in \mathbb{R}\times\mathbb{R}_+$, the function

$$v(x,t) = u(x-y,t-s) \tag{3.84}$$

  is still of solution of (3.81) and clearly for fixed (x,t), $u(x-y,t-s)$ is solution of the backward equation (3.83).

- **Space and time dilations —** Consider the following transformation

$$x \mapsto ax, \quad t \mapsto bt, \quad u \mapsto cu, \quad (a,b,c) > 0. \tag{3.85}$$

This transformation represents a dilation or a contraction of the graph of u. Naturally, we want to check for which values of a, b, c the function

$$u^*(x,t) = cu(ax, bt) \tag{3.86}$$

is also solution of 3.81. We reinject u^* in the forward equation and obtain

$$\frac{\partial u^*}{\partial t} - D\frac{\partial^2 u^*}{\partial x^2} = cb\frac{\partial u}{\partial t}(ax, bt) - Dca^2\frac{\partial^2 u}{\partial x^2}(ax, bt) \tag{3.87}$$

and so u^* is a solution of 3.81 if

$$b = a^2. \tag{3.88}$$

The transformation under which the diffusion equation is left invariant is thus called a **parabolic dilation** and is given by

$$x \mapsto ax, \quad t \mapsto a^2 t \quad a > 0. \tag{3.89}$$

Under this transformation the following groupings of variables

$$\frac{x^2}{Dt} \quad \text{or} \quad \frac{x}{\sqrt{Dt}} \tag{3.90}$$

are left unchanged. They are thus invariant with respect to a parabolic dilation. Notice that moreover, these are **dimensionless groups** for the problem at hand as $[D] = L^2T^{-1}$. It is then not surprising that these combinations of independent variables occur frequently in the study of diffusion phenomena.

- **Dilations and conservation of mass (or energy) —** Maintaining invariance of the equation under space and time dilation (or contraction) provided a constraint on the transformation itself (i.e. a relation between a and b). Can we obtain a further constraint and help determine c? Let $u(x,t)$ be a solution of (3.81). Suppose that u satisfies the following condition

$$\int_{\mathbb{R}} u(x,t)dx = m, \quad \forall t > 0. \tag{3.91}$$

If u represents the concentration of a substance (i.e. the mass density), equation (3.91) states that the total mass m is constant over time. If now u is a temperature (equation (3.81) is then seen as the heat equation), equation (3.91) states that the total internal energy of the system is constant. Here, we ask for which a, c the solution u^* still satisfies mass (or energy) conservation. We have

$$\int_{\mathbb{R}} u^*(x,t)dx = c\int_{\mathbb{R}} u(ax, a^2t)dx \tag{3.92}$$

Letting $y = ax$, $dy = adx$, we find

$$\int_{\mathbb{R}} u^*(x,t)dx = ca^{-1}\int_{\mathbb{R}} u(y, a^2t)dy = ca^{-1}m \tag{3.93}$$

and so for (3.91) to be satisfied, we must have

$$c = a \tag{3.94}$$

In conclusion, if $u(x,t)$ is a solution of the forward equation (3.81) in the half-space $\mathbb{R} \times \mathbb{R}_+$ satisfying (3.91), then so is

$$u^*(x,t) = au(ax, a^2t) \tag{3.95}$$

Remark. *All these properties can easily be generalized to the case of a n-dimensional diffusion equation.*

Fundamental solution of the diffusion equation ($n = 1$)

To help with intuition, keep in mind that the problem we are dealing with here is the diffusion of a substance (for instance, milk in your coffee or a pollutant in air) of total mass m and suppose we want to keep the total mass constant (and equal to m) over time. We have seen above that the grouping of independent variables $x/\sqrt{Dt}$ is (1) invariant with respect to parabolic dilations and (2) dimensionless. It is then quite natural to check if there exist solutions of (3.81) which involve this dimensionless group.

Now since $\sqrt{Dt}$ has the dimension of a length, the quantity $m/\sqrt{Dt}$ is a density (in this 1D problem), it is the typical order of magnitude for the concentration. Thus, it makes sense to look for solutions of the form

$$u^*(x,t) = \frac{m}{\sqrt{Dt}} U\left(x/\sqrt{Dt}\right) \tag{3.96}$$

where U is a dimensionless function of a single variable. We have reduced our problem to finding a function $U(\eta)$ such that u^* is solution to (3.81). Solutions of the form (3.96) are then called **similarity solutions**.

A solution of a particular evolution problem is a **similarity** or **self-similar** solution if its graph (or spatial structure) remains similar to itself at all times during the evolution. In one dimension, self-similar solutions have the general form

$$u(x,t) = a(t)F(x/b(t)) \tag{3.97}$$

where u/a and x/b are dimensionless quantities.

The fact that u^* is a concentration imposes that $U \geq 0$. The conservation of total mass imposes

$$1 = \frac{1}{\sqrt{Dt}} \int_{\mathbb{R}} U\left(\frac{x}{\sqrt{Dt}}\right) dx \underset{\eta \to x/\sqrt{Dt}}{=} \int_{\mathbb{R}} U(\eta) d\eta \tag{3.98}$$

We thus require that

$$\int_{\mathbb{R}} U(\eta) d\eta = 1 \tag{3.99}$$

Further, we have

$$\begin{aligned}
\frac{\partial u^*}{\partial t} &= \frac{m}{\sqrt{D}} \left[-\frac{1}{2} t^{-3/2} U(\eta) - \frac{1}{2\sqrt{D}} x t^{-2} U'(\eta) \right] \\
&= -\frac{m}{2t\sqrt{Dt}} \left[U(\eta) + \eta U'(\eta) \right] && (3.100) \\
\frac{\partial^2 u^*}{\partial x^2} &= \frac{m}{(Dt)^{3/2}} U''(\eta) && (3.101)
\end{aligned}$$

leading to

$$\frac{\partial u^*}{\partial t} - D \frac{\partial^2 u^*}{\partial x^2} = -\frac{m}{t\sqrt{Dt}} \left[U''(\eta) + \frac{1}{2}\eta U'(\eta) + \frac{1}{2} U(\eta) \right] \tag{3.102}$$

We see that u^* is a solution of (3.81) if U is a solution in $\mathbb{R}$ of the following ordinary differential equation

$$U''(\eta) + \frac{1}{2}\eta U'(\eta) + \frac{1}{2} U(\eta) = 0 \tag{3.103}$$

We have thus reduced the difficulty of our problem to finding solution to a second order ODE. Since $U \geq 0$, (3.99) implies that

$$U(-\infty) = U(+\infty) = 0 \tag{3.104}$$

As (3.103) is invariant with respect to the change of variables $\eta \mapsto -\eta$, we look for even solutions, i.e. solution such that $\forall \eta, U(-\eta) = U(\eta)$. Then, we can restrict ourselves to $\eta \geq 0$, asking

$$U'(0) = 0 \quad \text{and} \quad U(+\infty) = 0. \tag{3.105}$$

We observe that (3.103) can be written in the form

$$\frac{d}{d\eta}\left[U'(\eta) + \frac{1}{2}\eta U(\eta)\right] = 0 \tag{3.106}$$

which we can integrate in

$$U'(\eta) + \frac{1}{2}\eta U(\eta) = C, \quad C \in \mathbb{R} \tag{3.107}$$

We can determine the constant C by using the conditions (3.105) and we deduce that $C = 0$ leading to

$$U'(\eta) + \frac{1}{2}\eta U(\eta) = 0 \tag{3.108}$$

The general solution to equation (3.108) is

$$U(\eta) = c_0 e^{-\eta^2/4}, \tag{3.109}$$

a function which is even, positive, integrable and vanishes at infinity. The condition (3.99) imposes

$$c_0 \int_{\mathbb{R}} e^{-\eta^2/4} d\eta \underset{\eta \mapsto 2z}{=} 2 \int_{\mathbb{R}} e^{-z^2} dz = 2c_0\sqrt{\pi} = 1 \tag{3.110}$$

and so $c_0 = (4\pi)^{-1/2}$.

Finally, going back to our original variable, we have found the following of (3.81)

$$u^*(x,t) = \frac{m}{\sqrt{4\pi D t}} e^{-x^2/(4Dt)}, \quad x \in \mathbb{R}, t > 0. \tag{3.111}$$

which is such that

$$\int_{\mathbb{R}} u^*(x,t)dx = m, \quad \forall t > 0. \tag{3.112}$$

If one chooses $m = 1$, then the solution we obtained above is the well-known Gaussian function. It is thus natural to then think of a **normal probability density**. In particular, we will see in the next section the link between diffusion and random walks.

Definition 3.3.1: Fundamental solution ($n = 1$)

The function

$$f_D(x,t) = \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}}, \quad x \in \mathbb{R}, t > 0 \tag{3.113}$$

is called the **fundamental solution** of the one-dimensional diffusion equation

$$\frac{\partial u}{\partial t} - D\frac{\partial^2 u}{\partial x^2} = 0 \tag{3.114}$$

As can be intuitively observed on Fig. 3.6, for every $x \neq 0$

$$\lim_{t \to 0^+} f_D(x,t) = \lim_{t \to 0^+} \frac{1}{\sqrt{4\pi D t}} e^{-\frac{x^2}{4Dt}} = 0 \tag{3.115}$$

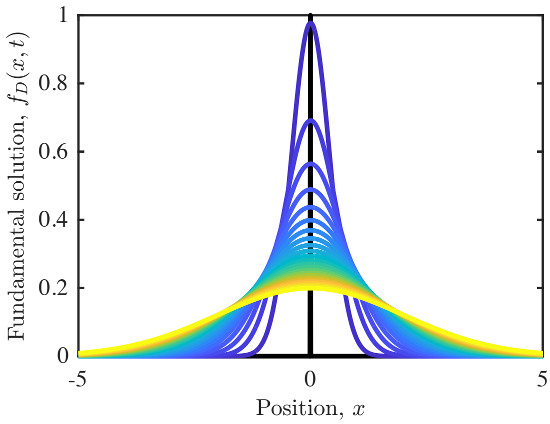

Figure 3.6 Fundamental solution $f_1(x,t)$, for $0 < t < 1$ with time increasing from blue to yellow.

while

$$\lim_{t \to 0^+} f_D(0,t) = \lim_{t \to 0^+} \frac{1}{\sqrt{4\pi D t}} = +\infty \tag{3.116}$$

So if we interpret f_D as a probability density, then the previous limits points to the fact that when $t \to 0^+$ the fundamental solution tends to concentrate mass around the origin; eventually, the whole probability mass is concentrated at $x = 0$. The limiting density distribution is the so-called **Dirac distribution** at the origin. So we say that the fundamental solution satisfies the initial condition

$$f_D(x,0) = \delta(x) \tag{3.117}$$

If at $t = 0$ the unit mass is concentrated at a point $y \neq 0$, by translational invariance, the fundamental solution $f_D(x-y,t)$ is a solution of the diffusion equation, and it satisfies the initial condition

$$f_D(x-y,0) = \delta(x-y) \tag{3.118}$$

where $\delta(x-y)$ is the Dirac measure at y defined via the formula

$$\int \delta(x-y)\varphi(x)dx = \varphi(y) \tag{3.119}$$

The fundamental solution is the solution of the diffusion equation with a unit source at $t = 0$. Indeed, $f_D(x,t)$ gives the concentration at point x and time t generated by the diffusion of a unit mass initially concentrated at the origin. If you imagine this unit mass as being composed of a large number N of particles, then $f_D(x,t)dx$ gives the probability of finding a particle between x and $x+dx$ at time t or said differently, the percentage of particles inside the interval $[x, x+dx]$ at time t.

Remark. *Note that as initially f_D is zero outside of the origin. As soon at $t > 0$, f_D becomes positive everywhere; this implies that the unit mass diffuses instantaneously all over the x-axis. In our particle picture, this means that a particle has a non-zero chance of moving infinitely far from the origin in an infinitesimal time and so travel at* **infinite speed***, which is prohibited. This is a well-known limitation of the diffusion equation in modelling real systems.*

Finally, note that the fundamental solution of the heat equation is also called a **heat kernel**. This heat kernel can be used to find a general solution of the heat equation over some domains. In particular, in the case of the one-dimensional heat equation on an infinite domain, one can obtain the general solution of the initial value problem with initial conditions $u(x, 0) = u_0(x)$ for $x \in \mathbb{R}$ and $t > 0$ by applying a convolution

$$u(x,t) = \int f_D(x-y,t)u_0(y)dy \tag{3.120}$$

of the heat kernel with the initial condition. We will see later in this Chapter that this is related to the more general concept of Green's functions (namely, the heat kernel is the Green's function of the heat equation).

3.3.6 Higher dimensions

In the previous sections, we mainly considered the problem of heat conduction in a finite thin, laterally insulated rod. Now consider the following problem: at $t = 0$, we add a small drop of dye in the center of a large container of water. If the container is large enough, we can even consider it to be infinite. The question is then to determine the evolution of the concentration of dye at any point in the container over time. Solving this problem requires being able to solve the diffusion equation in higher dimensions.

One can easily generalize the argument used in the derivation of the fundamental solution to $n > 1$.

Definition 3.3.2: Fundamental solution ($n > 1$)

The function

$$f_D(\mathbf{r},t) = \frac{1}{(4\pi Dt)^{n/2}} \exp\left[-\frac{|\mathbf{r}|^2}{4Dt}\right], \quad \mathbf{r} \in \mathbb{R}^n, t > 0 \tag{3.121}$$

is called the **fundamental solution** of the diffusion equation

$$\frac{\partial u}{\partial t} - D\Delta u = 0 \tag{3.122}$$

where Δ is the Laplacian.

Figure 3.7

The methods of separation of variables and Fourier transforms can also be used on the heat equation in two and three dimensions. However the variables in the boundary conditions need to be separated for this technique to work, and so the methods are of limited use for problems with complicated geometries. We may see some examples of this in Problem Sheets.

3.3.7 Random walks and diffusion

In the previous section, we have shown that the fundamental solution of the 1D diffusion equation takes the form of a gaussian function. You may remember having encountered the Gaussian function in your statistics modules before! In this section, we will explore the connection between probabilistic and deterministic models; in particular, we will explore the link between random walks (a *stochastic model discrete in space and time*) and diffusion (a *deterministic model continuous in space and time*). In doing so, we will try to clarify the nature of the diffusion coefficient.

Consider a unit mass particle that moves randomly along the x-axis. Assume that the particle starts from $x = 0$ and that in an interval of time τ, it takes one step of size h, where τ (a time) and h (a length) are constant. Here, we will consider that our random walks is symmetric and thus at each step, the particle moves to the left or to the right with probability $p = 1/2$, independently of the previous step (see Fig. 3.8).

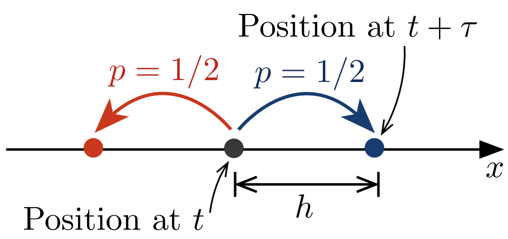

Figure 3.8

Question: can we compute the probability $\mathcal{P}(x,t)$ of finding the particle at position x at time t?

At some time $t = N\tau$, i.e. after N steps, the particle will be at a point $x = mh$, such that $-N \le m \le N$. To reach x, the particles takes some number of steps to the right, say k and $N-k$ steps to the left. In this case, we can write

$$m = k - (N-k) = 2k - N \tag{3.123}$$

We can conclude that N and m are then necessary both even or both odd and we can write

$$k = \frac{1}{2}(N+m) \tag{3.124}$$

The probability that the particle is in x at time t is then given by $\mathcal{P}(x,t) = \mathcal{P}_k$ where

$$\mathcal{P}_k = \frac{\text{number of walks with } k \text{ steps to the right after } N \text{ steps}}{\text{number of possible walks of } N \text{ steps}} \tag{3.125}$$

The total number of possible walks is clearly 2^N, while the number of walks with k steps to the right and $N-k$ steps to the left is given by the binomial coefficient

$$\binom{N}{k} = \frac{N!}{k!\,(N-k)!} \tag{3.126}$$

so we conclude the probability to be in $x = mh$ after N steps (i.e. at $t = N\tau$) is the probability of a walk with k steps to the right and $N-k$ steps to the left with $k = (N+m)/2$. This probability then reads

$$\mathcal{P}_k = \frac{1}{2^N}\binom{N}{k} \tag{3.127}$$

Provided this probability, one can easily ask questions such as what is the **mean displacement** of the particle or what is the **average distance from the origin** after N steps. While the mean displacement is given by $\langle x\rangle = \langle m\rangle\, h$, the average distance from the origin is given by the square root of the second moment $\langle x^2\rangle = \langle m^2\rangle h^2$. Given that $m = 2k - N$, we would need to calculate $\langle k\rangle$ and $\langle k^2\rangle$.

One can easily do this by using the probability generating function. While this is something you may do in a statistics module, it is beyond the scope of this module so I shall just give the result. Using the definition of $\mathcal{P}_k$, one would obtain that

$$\langle k\rangle = \frac{N}{2} \quad \text{and} \quad \langle k^2\rangle = \frac{N(N+1)}{4} \tag{3.128}$$

which leads to

$$\langle m\rangle = 0 \quad \text{and} \quad \langle m^2\rangle = N \tag{3.129}$$

So we can conclude that the average displacement is $\langle x\rangle = 0$, which is not surprising given the symmetry of the random walk. However, we see that $\sqrt{\langle x^2\rangle} = \sqrt{N}h$ (which is the standard deviation of x as $\langle x\rangle = 0$). This is an important result which tells us that at time $N\tau$, the distance from the origin is of order $\sqrt{N}h$. Said differently, the order of the time scale is the square of the space scale. So if we want to leave the standard deviation unchanged, we must rescale the time as the square of the space, i.e. use a space-time parabolic dilation which should sound familiar!

Now as the motion of the particle has no memory (each step is independent from the previous one), if a particle is located at x at time $t+\tau$, it means that it was located at time t in $x-h$ or $x+h$ with equal probability. Mathematically, this statement is written

$$\mathcal{P}(x, t+\tau) = \frac{1}{2}\mathcal{P}(x-h, t) + \frac{1}{2}\mathcal{P}(x+h, t) \tag{3.130}$$

while our initial conditions gave us

$$\mathcal{P}(0,0) = 1 \quad \text{and} \quad \mathcal{P}(x,0) = 0, \quad \text{if } x \neq 0 \tag{3.131}$$

Keeping x and t fixed, let us examine what happens as we take $\tau \to 0$ and $h \to 0$. Here, it is most convenient to think of $\mathcal{P}$ as a **probability density**, a smooth function defined in the whole half space $\mathbb{R} \times (0, +\infty)$. Using Taylor's expansion, we can write

$$\mathcal{P}(x, t+\tau) = \mathcal{P}(x,t) + \frac{\partial \mathcal{P}}{\partial t}(x,t)\tau + o(\tau) \tag{3.132}$$

$$\mathcal{P}(x \pm h, t) = \mathcal{P}(x,t) \pm \frac{\partial \mathcal{P}}{\partial x}(x,t)h + \frac{1}{2}\frac{\partial^2 \mathcal{P}}{\partial x^2}(x,t)h^2 + o(h^2) \tag{3.133}$$

Substituting this into (3.130), we find that

$$\frac{\partial \mathcal{P}}{\partial t}(x,t)\tau + o(\tau) = \frac{1}{2}\frac{\partial^2 \mathcal{P}}{\partial x^2}(x,t)h^2 + o(h^2) \tag{3.134}$$

which after dividing by τ yields

$$\frac{\partial \mathcal{P}}{\partial t}(x,t) + o(1) = \frac{h^2}{2\tau}\frac{\partial^2 \mathcal{P}}{\partial x^2}(x,t) + o(h^2/\tau) \tag{3.135}$$

Now, if we want to obtain something non trivial when $h, \tau \to 0$, we must require that h^2/τ has a finite and positive limit. So we write that

$$\frac{h^2}{\tau} = 2D \tag{3.136}$$

for some constant $D > 0$. Then, when passing to the limit $h, \tau \to 0$, we obtain

$$\frac{\partial \mathcal{P}}{\partial t} = D \frac{\partial^2 \mathcal{P}}{\partial x^2} \tag{3.137}$$

with the initial condition given by

$$\lim_{t \to 0^+} \mathcal{P}(x,t) = \delta(x) \tag{3.138}$$

We conclude that the probability of finding the random walker in position x at time t obeys the linear diffusion equation.

In the previous section, we have shown that the solution of this problem was given by the heat kernel

$$p(x,t) = f_D(x,t) \tag{3.139}$$

and we conclude that the constant that we just defined D is precisely the **diffusion coefficient** appearing in the diffusion equation. Going back to the random walk, we had

$$h^2 = \frac{\langle x^2 \rangle}{N} \quad \text{and} \quad \tau = \frac{t}{N} \tag{3.140}$$

giving

$$\frac{h^2}{\tau} = \frac{\langle x^2 \rangle}{t} = 2D \tag{3.141}$$

which means that **in unit time, the particle diffuses an average distance of** $\sqrt{2D}$. The dimensions of the diffusion coefficient are given by

$$[D] = L^2 T^{-1} \tag{3.142}$$

which means that the combination x^2/Dt is dimensionless (which is what we used to obtain the similarity solution). Finally, we also deduce from (3.136) that

$$\frac{h}{\tau} = \frac{2D}{h} \to \infty \tag{3.143}$$

which shows that the average speed h/τ of the particle at each step diverges. This is consistent with the earlier observation that the particle diffuses in unit time to a finite average distance.

3.3.8 Nonlinear diffusion: porous medium equation

In this section so far, we have examined linear diffusion processes. However, in nature, most real problems are in fact nonlinear. As we have seen in Chapter 2, the presence of nonlinearity in a mathematical model gives rise to interesting new phenomena which cannot occur in the linear case. Here, we will explore how nonlinear diffusion differs from the physical picture we developed for the linear diffusion equation. In this section, we will consider the so-called porous medium equation:

$$\frac{\partial u}{\partial t} = \Delta(u^m) \tag{3.144}$$

for some $m > 1$ (we can see that if $m = 1$, we recover the linear diffusion equation). **Where does this equation arise?** The porous medium equation has been used in various contexts including in models of animal and insects dispersal in biology and in plasma physics. But originally, it was derived to describe the flow of fluids in porous media. A porous medium is a solid material containing pores (voids) which can be filled with liquid or gas (e.g. sponges, wood, soil, rocks, sand etc.). A porous material is often characterized by (1) its **porosity** $\kappa \in [0, 1]$ which measures the amount of void (it is the ratio of the volume of the voids to the total volume of material) and (2) its **permeability** k which measure the ability of a fluid to pass through the porous medium. While related these two quantities are both important and distinct; indeed, a material can have a high porosity (i.e. have lots of void), if these voids are not connected in some way, fluids will not be able to flow through and so the permeability will be very low.

Flows in porous media are ubiquitous. They may describe how water flows through soil after irrigation or rainfall. It is also relevant to engineering applications like filtration in porous media (e.g. filtration of water in sand). One more example can be in the environmental sciences. Indeed, attempts to mitigate or reverse global warming has led to the development of carbon dioxide removal processes. These processes usually involve the capture and sequestration of industrially produced carbon dioxide in subsurface aquifers, reservoirs or old oil fields. If the main point is to store this gas to remove it from the atmosphere, studying the long-time dynamics of carbon dioxide in the ground and the possibility that it may resurface when flowing through porous rocks is of prime importance.

Derivation of the porous medium equation

Consider a gas of density $\rho = \rho(\mathbf{r}, t)$ flowing through a porous medium of porosity κ. We will denote the velocity of the gas $\mathbf{v} = \mathbf{v}(\mathbf{r}, t)$. The derivation of the porous medium equation relies on three key ingredients:

- **Conservation of mass** which reads in this three-dimensional case

$$\kappa \frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{v}) = 0 \tag{3.145}$$

  (this is a generalization to 3D of the mass conservation arguments we have used many times in both Chapters 2 and 3).

- **Darcy's law** which relates the fluid velocity and the pressure in the fluid

$$\mathbf{v} = -\frac{k}{\mu} \nabla p \tag{3.146}$$

  with $p = p(\mathbf{r}, t)$ the pressure, k the permeability of the medium and μ the dynamic viscosity of the gas. We assume that k and μ are positive constants. Darcy's law states that the gas moves from high pressure to low pressure regions.

- Finally, an **equation of state** specify how the pressure in the gas depends on the gas density, namely

$$p = p_0 \rho^{\gamma}, \quad p_0 > 0, \ \gamma > 0. \tag{3.147}$$

  Physically, we can understand this as the statement that pressure in the gas increases with its density, i.e. pressure increases if one tries to pack a quantity of gas in a smaller volume for instance.

The last two ingredients are constitutive (empirical) laws stemming from physical experimentations. Armed with these three equations, we may hope to derive a closed-form equation for the gas density alone.

Combining (3.146) and (3.147), we can write that

$$\nabla \cdot (\rho \mathbf{v}) = \nabla \cdot \left[\left(\frac{p}{p_0} \right)^{1/\gamma} \left(-\frac{k}{\mu} \nabla p \right) \right] \tag{3.148}$$

$$= -\frac{k}{\mu p_0^{1/\gamma}} \nabla \cdot \left[p^{1/\gamma} \nabla p \right] \tag{3.149}$$

Now, we can simplify this expression further remembering that

$$\nabla \left(p^{1+1/\gamma} \right) = (1 + 1/\gamma)\, p^{1/\gamma} \nabla p \Rightarrow \nabla \cdot \left[p^{1/\gamma} \nabla p \right] = \frac{1}{1 + 1/\gamma} \Delta \left(p^{1+1/\gamma} \right) \tag{3.150}$$

which leads to

$$\nabla \cdot (\rho \mathbf{v}) = -\frac{\mu}{(1 + 1/\gamma)\nu p_0^{1/\gamma}} \Delta \left(p^{1+1/\gamma} \right) \tag{3.151}$$

Denoting $m = 1 + \gamma > 1$, we get

$$\nabla \cdot (\rho \mathbf{v}) = -\frac{(m-1) k p_0}{m \mu} \Delta \left[\rho^m \right] \tag{3.152}$$

which to the following closed equation for ρ:

$$\frac{\partial \rho}{\partial t} = \frac{(m-1) k p_0}{\kappa m \mu} \Delta \left[\rho^m \right] \tag{3.153}$$

If for instance, we rescale the time such that

$$t \mapsto \frac{(m-1) k p_0}{\kappa m \mu} t \tag{3.154}$$

then we obtain the **porous medium equation**

$$\frac{\partial \rho}{\partial t} = \Delta \left[\rho^m \right] \tag{3.155}$$

Since, we have

$$\Delta(\rho^m) = \nabla \cdot (m \rho^{m-1} \nabla \rho) \tag{3.156}$$

We can see this equation as a diffusion equation

$$\frac{\partial \rho}{\partial t} = \nabla \cdot \left[D(\rho) \nabla \rho \right] \tag{3.157}$$

which a diffusion coefficient $D(\rho) = m\rho^{m-1}$, which varies as a power of the diffused quantity itself. We see that the diffusion coefficient increases as the density increases and goes to zero as $\rho \to 0$. This is fundamental difference with the linear diffusion equation we studied in the previous sections.

Similarity solutions for the porous medium equation

As in the case of the linear diffusion equation, one can look for point source solutions. The question is then how the gas expands in the porous medium and whether there is a well-defined free boundary between the region invaded by the gas and the empty regions.

Let us see how we can approach this problem in 1D. While the porous medium equation is a strongly nonlinear equation, we may be able to approach the problem using similarity solutions. Here, we assume that we start with a unit mass of gas located in $x = 0$ ($\rho(x, 0) = \delta(x)$) and look for nonnegative self-similar solutions of the form

$$\rho(x,t) = t^{-\alpha} U(xt^{-\beta}) \tag{3.158}$$

which satisfy the following conservation of mass condition

$$\int_{-\infty}^{+\infty} \rho(x,t)dx = 1 \tag{3.159}$$

and the following condition

$$\lim_{x\to+\infty} \rho(x,t) = \lim_{x\to-\infty} \rho(x,t) = 0 \tag{3.160}$$

Here, U is called the self-similar profile and the constants (α, β) are called similarity exponents; one can understand α as a density contraction rate (it controls how the graph of the solution shrinks vertically) and β as a space dilation rate (it controls how the graph of the solution expands horizontally).

What values of (α, β) are allowed? The conservation of mass condition requires

$$1 = \int_{-\infty}^{+\infty} t^{-\alpha} U(xt^{-\beta})dx = t^{\beta-\alpha} \int_{-\infty}^{+\infty} U(\xi)d\xi \tag{3.161}$$

where we have defined $\xi = xt^{-\beta}$. So we conclude that we must have $\alpha = \beta$ **and**

$$1 = \int_{-\infty}^{+\infty} U(\xi)d\xi \tag{3.162}$$

If we substitute this in (3.155), we find that by the chain rule that

$$\frac{\partial \rho}{\partial t} = -\alpha t^{-\alpha-1} U(\xi) - \alpha t^{-\alpha} U'(\xi) x t^{-\alpha-1} = -\alpha t^{-\alpha-1}(U + \xi U') \tag{3.163}$$

$$\frac{\partial^2 \rho^m}{\partial x^2} = t^{-\alpha m} t^{-2\alpha} \left(U^m\right)'' \tag{3.164}$$

i.e.

$$-\alpha t^{-\alpha-1}(U + \xi U') = t^{-\alpha m - 2\alpha} \left(U^m\right)'' \tag{3.165}$$

If we pick the exponent $\alpha = 1/(m+1)$, we obtain the following differential equation for U

$$(m+1)\left(U^m\right)'' + \xi U' + U = 0 \tag{3.166}$$

which we can write in the form

$$\frac{d}{d\xi}\left[(m+1)\left(U^m\right)' + \xi U\right] = 0 \tag{3.167}$$

This can be integrated in

$$(m+1)\left(U^m\right)' + \xi U = C \tag{3.168}$$

but the condition $\lim_{x\to+\infty}\rho(x,t)=0$ requires the integration constant C to be equal to zero; thus, we get

$$(m+1)\left(U^m\right)' = -\xi U \tag{3.169}$$

but as we have

$$(m+1)\left(U^m\right)' = (m+1)mU^{m-1}U' \tag{3.170}$$

we conclude that

$$(m+1)mU^{m-1}U' = -\xi U \Rightarrow (m+1)mU^{m-2}U' = -\xi \tag{3.171}$$

which is equivalent to

$$\frac{(m+1)m}{m-1}\left(U^{m-1}\right)' = -\xi \tag{3.172}$$

This last ODE has for solution

$$U(\xi) = \left[A - B_m\xi^2\right]^{1/(m-1)} \tag{3.173}$$

where A is an arbitrary constant and $B_m = (m-1)/2m(m+1)$. To make sure that the solution is physically admissible, we must have $A > 0$ and $A - B_m\xi^2 > 0$. In conclusion, we have found solution of the porous medium equation of the form

$$\rho(x,t) = \begin{cases} t^{-\alpha}\left[A - B_m x^2/t^{2\alpha}\right]^{1/(m-1)} & \text{if } x^2 \leq At^{2\alpha}/B_m \\ 0 & \text{if } x^2 > At^{2\alpha}/B_m \end{cases} \tag{3.174}$$

These solutions are known as the **Barenblatt solutions** (or ZKB solutions). We can see that the solution goes to zero at a finite value of x; the points

$$x = \pm\sqrt{A/B_m}t^{\alpha} \equiv \pm r(t) \tag{3.175}$$

represent the gas interface, i.e. the interface between the part of the porous medium filled with the gas and the empty part. The speed of propagation of this interface is given by

$$\dot{r}(t) = \alpha\sqrt{A/B_m}t^{\alpha-1} \tag{3.176}$$

So we conclude that the effect of the nonlinearity in this case is to lead to solutions with compact support and a finite diffusion speed, which is in contrast with the infinite diffusion speed which we exhibited in the previous section in the linear case! We represent various Barenblatt solutions on Fig. 3.9.

Remark. *Note that the free parameter A is not really free, it is determined by the mass conservation condition; however, it is not as simple as it sounds and is not needed for our argument here.*

3.3.9 Back to Burgers equation

At the end of Chapter 2, we saw that we could recast the problem of solving Burgers equation (a non-linear second order PDE) into solving a diffusion equation (a linear second order PDE) for an auxiliary function via the Cole-Hopf transformation. This will be done in more details in Problem Sheet #4.

3.4 Wave equation

In this second section, we will study the canonical **hyperbolic equation**: the wave equation.

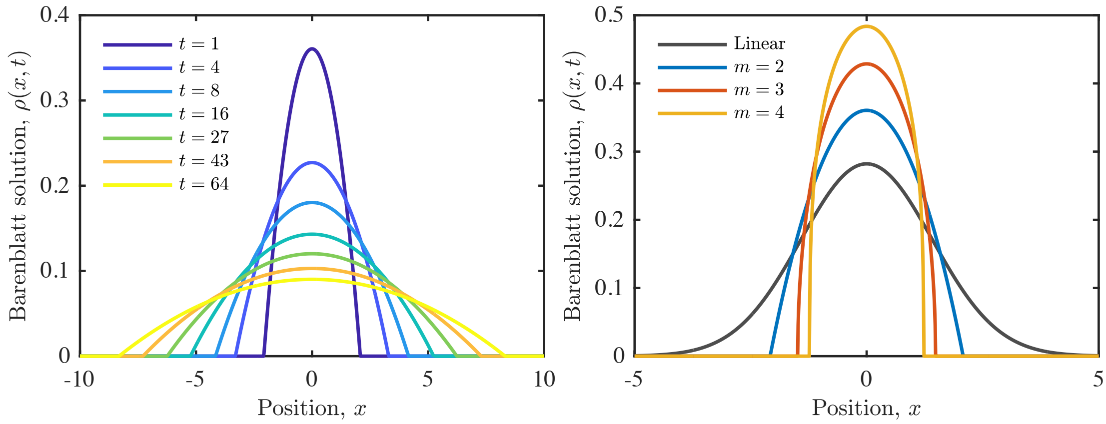

Figure 3.9 *(Left)* Barenblatt solution for various times for $m = 2$ and *(Right)* Comparison of the fundamental solution of the heat equation (with $D = 1$) and Barenblatt solutions for $m = 2, 3, 4$ at $t = 1$.

3.4.1 Physical derivation of the wave equation

Imagine an elastic string, which at rest is stretched in between two fixed anchor points (e.g. a guitar string). In this section, we derive a model for the small transverse vibrations of the string.

Modelling assumptions

We make the following assumptions:

1. *Vibrations of the string have small amplitudes*, i.e. that the change in slope of the string from the horizontal equilibrium position are very small.
2. *Each point on the string undergoes vertical displacement only*, i.e. horizontal displacements can be neglected.
3. *Vertical displacement of a point on the string depends on time and its position on the string*. i.e. we will denote the displacement $u(x,t)$ of a point located at x when the string is at rest. We have $|u_x(x,t)| \ll 1$.
4. *The string is perfectly flexible*, i.e. there is no resistance to bending. Any point on the string is only subject to tangential forces called *tension*.
5. *There is no friction.*

Transverse vibrations of a string

Using the assumptions above, we can derive the equation of motion for the string using **mass conservation** and **Newton's laws of motion.** We work in Cartesian coordinates and consider that the anchor points are at $x = 0$ and $x = L$. We consider that this elastic string has a linear density (i.e. a mass per unit length) $\rho_0(x)$ at rest and let $\rho(x,t)$ be its linear density at time t. If you consider an arbitrary part of the string between x and $x + \Delta x$, mass conservation imposes that the length of the element of string Δs at time t be given by

$$\rho_0(x)\Delta x = \rho(x,t)\Delta s \tag{3.177}$$

We want to find an evolution equation for the small **transverse** displacements $u(x,t)$ of the string (see Fig. 3.10). For that, we need to write Newton's law of motion which requires from us to determine the forces acting on our element of string.

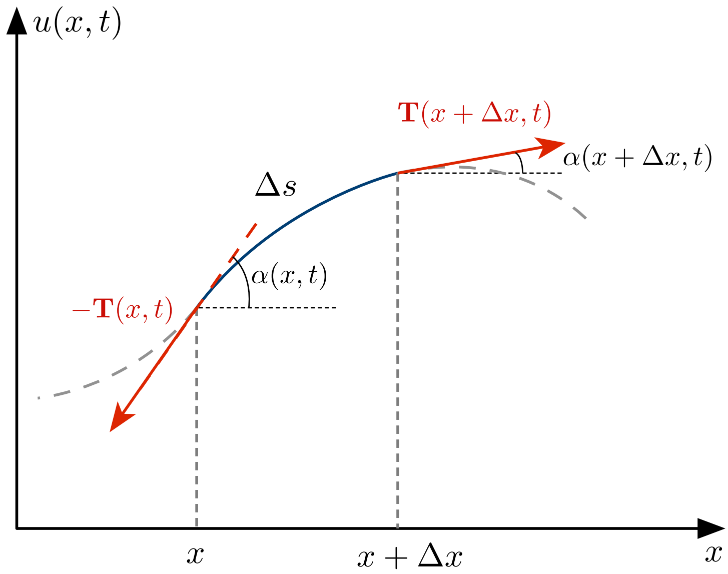

Figure 3.10 Forces acting on an element of a string.

By Assumption 2, the motion of the string is vertical and so the horizontal forces have to balance. By Assumption 4, we know that the only forces acting on our element of string come from tension in the string. Denoting $\tau(x,t)$ the magnitude of the tension at x and time t, force balance gives us (see Fig. 3.10)

$$\tau(x+\Delta x,t)\cos\alpha(x+\Delta x,t)-\tau(x,t)\cos\alpha(x,t)=0 \tag{3.178}$$

Dividing by Δx and taking the limit $\Delta x\to 0$, we obtain

$$\frac{\partial}{\partial x}[\tau(x,t)\cos\alpha(x,t)]=0 \tag{3.179}$$

so, we can define a positive function $\tau_0(t)$ (measuring the magnitude of the tension in the string) given by

$$\tau_0(t)=\tau(x,t)\cos\alpha(x,t) \tag{3.180}$$

Now, the vertical forces can be coming from: (1) the vertical component of the tension in the string and (2) body forces like gravity or other external loads. The scalar vertical component of the tension at position x and time t is given by

$$\tau_v(x,t)=\tau(x,t)\sin\alpha(x,t)=\tau_0(t)\tan\alpha(x,t) \tag{3.181}$$

The assumption of small transverse displacements imply that the angles $\alpha(x,t)$ are small. By definition, at any point on the string, the slope is $\tan\alpha=\partial u/\partial x$. So we obtain

$$\tau_v(x,t)=\tau_0(t)\frac{\partial u}{\partial x} \tag{3.182}$$

We can conclude that the vertical component of the net force acting on our small piece of string **due to tension** is

$$\tau_v(x+\Delta x,t)-\tau_v(x,t)=\tau_0(t)\left[\frac{\partial u}{\partial x}(x+\Delta x,t)-\frac{\partial u}{\partial x}(x,t)\right] \tag{3.183}$$

In all generality, we denote $f(x,t)$ the magnitude of the vertical body forces per unit mass. The magnitude of the body forces acting on our small piece of string is then given by

$$\int_x^{x+\Delta x} \rho(y,t) f(y,t) dy = \int_x^{x+\Delta x} \rho_0(y) f(y,t) dy \tag{3.184}$$

where we have used the conservation of mass (3.177) and small amplitudes displacements.

Finally, the vertical acceleration of the string at any point x and time t is given by u_{tt}. We conclude that Newton's second law allows us to write

$$\int_x^{x+\Delta x} \rho_0(y) \frac{\partial^2 u}{\partial t^2}(y,t) dy = \tau_0(t) \left[\frac{\partial u}{\partial x}(x+\Delta x, t) - \frac{\partial u}{\partial x}(x,t) \right] + \int_x^{x+\Delta x} \rho_0(y) f(y,t) dy \tag{3.185}$$

If we divide by Δx and let $\Delta x \to 0$, we obtain the 1D wave equation

$$\frac{\partial^2 u}{\partial t^2} - c^2(x,t) \frac{\partial^2 u}{\partial x^2} = f(x,t) \tag{3.186}$$

where we have defined the wave speed $c(x,t) = \sqrt{\tau_0(t)/\rho_0(x)}$. Note that if the **string is homogeneous** then ρ_0 is a constant and if it is **perfectly elastic** then τ_0 is a constant. In this case, the wave speed itself is a constant.

Example

> For instance, guitar and violin strings are nearly homogeneous, perfectly flexible and perfectly elastic.

Longitudinal vibration of an elastic rod

It can be shown that the **longitudinal** vibrations of an elastic rod obey a very similar equation, namely

$$\frac{\partial^2 u(x,t)}{\partial x^2} = \frac{\rho}{E} \frac{\partial^2 u(x,t)}{\partial t^2} \tag{3.187}$$

where here ρ is the density (i.e. mass per unit volume) and E is called the Young's modulus (a material property measuring its stiffness). One can also define a longitudinal wave speed $c = \sqrt{E/\rho}$.

Transverse vibrations of a stretched membrane

Finally, note that one can also show that the transverse vibrations of a stretched membrane subject to an external vertical force density $f(x,y,t)$ is given by the generalized wave equation

$$\tau(t) \left(\frac{\partial^2 u(x,t)}{\partial x^2} + \frac{\partial^2 u(x,t)}{\partial y^2} \right) + f(x,y,t) = \rho(x,y) \frac{\partial^2 u(x,t)}{\partial t^2} \tag{3.188}$$

where ρ is the mass per unit area of the membrane and τ is the magnitude of the tension in the membrane.

3.4.2 Energy of a vibrating string

Suppose that a perfectly flexible and elastic string has length L at rest (in the horizontal position). Since, $u_t(x,t)$ is the vertical velocity of the point at x, the expression

$$E_k(t) = \frac{1}{2} \int_0^L \rho_0 \left(\frac{\partial u}{\partial t} \right)^2 dx \tag{3.189}$$

represents the total **kinetic energy during the vibration**. As it is stretched, the string also stores **potential energy**, due to the work of elastic forces. The elastic forces stretch an element of length Δx at rest by

$$\Delta s - \Delta x = \int_x^{x+\Delta x} \sqrt{1 + \left(\frac{\partial u}{\partial x}\right)^2} dx - \Delta x = \int_x^{x+\Delta x} \left(\sqrt{1 + \left(\frac{\partial u}{\partial x}\right)^2} - 1\right) dx \quad (3.190)$$

Recall that to linear order, if $\varepsilon \ll 1$, then $\sqrt{1+\varepsilon} - 1 \approx \varepsilon/2$. So we obtain that

$$\Delta s - \Delta x \approx \frac{1}{2}\left(\frac{\partial u}{\partial x}\right)^2 \Delta x \quad (3.191)$$

since $|\partial u/\partial x| \ll 1$. The work done by the elastic forces on this string element is by definition equal to the elastic force multiplied by the stretch

$$dW = \frac{1}{2}\tau_0 \left(\frac{\partial u}{\partial x}\right)^2 \Delta x \quad (3.192)$$

Integrating over the whole string to sum all the contributions to the work, we obtain that the **potential energy** of the stretched string is given by

$$E_p(t) = \frac{1}{2}\int_0^L \tau_0 \left(\frac{\partial u}{\partial x}\right)^2 dx \quad (3.193)$$

Summing kinetic and potential energy, we find that

$$E(t) = \frac{1}{2}\int_0^L \left[\rho_0 \left(\frac{\partial u}{\partial t}\right)^2 + \tau_0 \left(\frac{\partial u}{\partial x}\right)^2\right] dx \quad (3.194)$$

Taking the time derivative of the total energy, we find

$$\frac{dE}{dt} = \int_0^L \left[\rho_0 \frac{\partial u}{\partial t}\frac{\partial^2 u}{\partial t^2} + \tau_0 \frac{\partial u}{\partial x}\frac{\partial^2 u}{\partial x \partial t}\right] dx \quad (3.195)$$

(remember that $\rho = \rho(x)$ and that τ_0 is a constant as we assume a perfectly elastic string). By an integration by parts, we get

$$\int_0^L \tau_0 \frac{\partial u}{\partial x}\frac{\partial^2 u}{\partial x \partial t} dx = \tau_0 \left[\frac{\partial u}{\partial x}(L,t)\frac{\partial u}{\partial t}(L,t) - \frac{\partial u}{\partial x}(0,t)\frac{\partial u}{\partial t}(0,t)\right] - \int_0^L \tau_0 \frac{\partial u}{\partial t}\frac{\partial^2 u}{\partial x^2} dx \quad (3.196)$$

Thus, we finally obtain

$$\frac{dE}{dt} = \int_0^L \left[\rho_0 \frac{\partial^2 u}{\partial t^2} - \tau_0 \frac{\partial^2 u}{\partial x^2}\right] \frac{\partial u}{\partial t} dx + \tau_0 \left[\frac{\partial u}{\partial x}(L,t)\frac{\partial u}{\partial t}(L,t) - \frac{\partial u}{\partial x}(0,t)\frac{\partial u}{\partial t}(0,t)\right] \quad (3.197)$$

and as u is assumed to be solution the wave equation (3.186), we find that

$$\frac{dE}{dt} = \int_0^L \rho_0 f(x,t) \frac{\partial u}{\partial t} dx + \tau_0 \left[\frac{\partial u}{\partial x}(L,t)\frac{\partial u}{\partial t}(L,t) - \frac{\partial u}{\partial x}(0,t)\frac{\partial u}{\partial t}(0,t)\right] \quad (3.198)$$

We conclude that if $f = 0$ and u is constant at the end points $x = 0$ and $x = L$, we have $dE/dt = 0$ which implies that

$$E(t) = E(0) \quad (3.199)$$

and so we have **conservation of energy**.

3.4.3 Solution on a finite domain

Method of separation of variable

Similarly to what we have done in Section 3.3.2, we will see here that one can use the method of separation of variables to obtain a solution to the wave equation. We consider here the one-dimensional wave equation on a finite domain of size L. Consider the following problem: we want to solve the following PDE for $u(x,t)$

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial u^2}{\partial x^2} \tag{3.200}$$

with boundary conditions

$$u(0,t) = u(L,t) = 0 \quad t \geq 0 \tag{3.201}$$

and the initial conditions

$$u(x,0) = f(x) \quad \text{and} \quad \frac{\partial u}{\partial t}(x,0) = 0 \quad (0 \leq x \leq L). \tag{3.202}$$

We seek here a solution to (3.200) of the 'separated-variables' form

$$u(x,t) = X(x)T(t) \tag{3.203}$$

Substituting this expression in (3.200), we obtain

$$X(x)T''(t) = c^2 X''(x)T(t) \tag{3.204}$$

by dividing both sides by c^2XT, we can write this as

$$\frac{T''(t)}{c^2T(t)} = \frac{X''(x)}{X(x)}. \tag{3.205}$$

Observing that the LHS of this expression only depends on t, while the RHS only depends on x, we conclude that the only way for this expression to hold for all $t > 0$ and $x \in [0, L]$ is for the LHS and RHS to be equal to a constant. In other words, we must have

$$\frac{X''}{X} = K = \frac{T''}{c^2T} \tag{3.206}$$

We have here reduced our PDE to two second order ODEs with constant coefficients which are easier to solve. The boundary conditions in (3.201) imply that

$$X(0) = X(L) = 0 \tag{3.207}$$

with the function $X(x)$ satisfying

$$X'' - KX = 0. \tag{3.208}$$

The form of the general solution for this ODE depends on whether K is positive, negative or zero. We consider each of these cases independently:

- **Case 1 —** If $K > 0$, the general solution of (3.208) is given by

  $$X(x) = A\cosh(\sqrt{K}x) + B\sinh(\sqrt{K}x) \tag{3.209}$$

  The boundary conditions impose

  $$X(0) = 0 \Rightarrow A = 0, \tag{3.210}$$

  $$X(L) = 0 \Rightarrow B = 0 \quad \text{or} \quad \sinh(\sqrt{K}L) = 0 \tag{3.211}$$

  We easily realize that neither of these options is acceptable: (1) the first option leads to X identically zero and (2) a quick look at the graph of $\sinh(x)$ shows that no such positive value of K exists. We therefore conclude that for these boundary conditions the constant K cannot be positive.

- **Case 2 —** if $K = 0$, the solution of (3.208) is given by

$$X(x) = ax + b. \tag{3.212}$$

Again, if we apply the boundary conditions $X(0) = X(L) = 0$, we clearly see that no non-zero solution is possible.

- **Case 3 —** if $K < 0$, it is convenient to set $K = -\lambda^2$. In this case, the general solution of (3.208) is given by

$$X(x) = A\cos\lambda x + B\cos\lambda x \tag{3.213}$$

Applying the boundary conditions, we find that

$$X(0) = 0 \Rightarrow A = 0 \tag{3.214}$$

as before, but the second condition imposes

$$X(L) = 0 \Rightarrow \sin\lambda L = 0 \tag{3.215}$$

for which there are an infinite number of solutions

$$\lambda = \frac{n\pi}{L}, \quad n = \pm 1, \pm 2, \cdots \tag{3.216}$$

The solutions for (3.208) is therefore

$$X_n = B_n \sin(n\pi x/L) \tag{3.217}$$

We now turn to the equation for T which takes the form

$$T'' + c^2\lambda^2 T = 0 \tag{3.218}$$

and therefore has the general solution

$$T = C\cos(\lambda ct) + D\sin(\lambda ct) \tag{3.219}$$

The initial conditions imply that

$$\frac{\partial u}{\partial t}(x, 0) = 0 \Rightarrow T'(0) = 0 \Rightarrow D = 0 \tag{3.220}$$

Substituting for λ we are left with the following family of solutions

$$T_n = C_n \cos(n\pi ct/L) \tag{3.221}$$

A solution that satisfies the wave equation (3.200) and the associated conditions (3.201) and (3.202) is then given by

$$u_n = X_n T_n = \beta_n \sin(n\pi x/L)\cos(n\pi ct/L) \tag{3.222}$$

where we have introduced $\beta_n = B_n C_n$. Since the wave equation is linear and homogeneous it follows that any linear combination of the solutions for different n is also a solution. The most general solution is therefore of the form

$$u(x, t) = \sum_{n=-\infty}^{\infty} \beta_n \sin(n\pi x/L)\cos(n\pi ct/L) \tag{3.223}$$

which can be expressed more succinctly as

$$u(x,t) = \sum_{n=1}^{\infty} b_n \sin(n\pi x/L)\cos(n\pi ct/L) \tag{3.224}$$

where we have introduced $b_n = \beta_n - \beta_{-n}$. So far, we have not used the following initial condition $u(x,0) = f(x)$. Imposing this condition, we see that $f(x)$ is related to the unknown coefficient b_n in the following way

$$f(x) = \sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi x}{L}\right) \quad (0 < x < L) \tag{3.225}$$

We recognize this expression as the half-range Fourier sine series for $f(x)$ and so

$$b_n = \frac{2}{L}\int_0^L f(x)\sin\left(\frac{n\pi x}{L}\right)dx \tag{3.226}$$

These coefficients can thus be computed for a given $f(x)$. The required solution to the wave equation is then given by the infinite sum (3.223), with coefficients b_n calculated using (3.226).

Example

> Solve the wave equation subject to the following associated conditions
>
> $$u(0,t) = u(L,t) = 0 \quad (t \geq 0), \tag{3.227}$$
> $$u(x,0) = 0 \quad (0 \leq x \leq L), \tag{3.228}$$
> $$\frac{\partial u}{\partial t}(x,0) = g(x) \quad (0 \leq x \leq L). \tag{3.229}$$

Normal modes of vibration

The solution we just exhibited [see (3.223)] is a superposition of so-called **standing waves**; i.e. waves of the form

$$f(x,t) = f(x)\left[A\cos(\omega t) + B\sin(\omega t)\right] \tag{3.230}$$

These type of wave are not travelling, they do not propagate disturbances; rather, they are composed of spatial perturbations whose amplitude is modulated in time by a time dependent sinusoidal oscillation. Further, we saw that imposing fixed ends boundary conditions constrained the form of the standing wave and the values that the wave number k and angular frequency ω take. Said differently, we saw that a string of finite length fixed at both ends can support waves of only specific wavelengths. These are called **normal modes** of the string.

For the vibrating string with fixed ends and zero initial velocity, the normal modes of vibrations were given by

$$u_n(x,t) = A_n \sin(k_n x)\cos(\omega_n t), \quad n \in \mathbb{N}^* \tag{3.231}$$

with

$$k_n = \frac{n\pi}{L} \quad \text{and} \quad \omega_n = \frac{n\pi c}{L} \tag{3.232}$$

The frequency ω_n at which the motion takes place for a given mode is called the **natural (or resonant) frequency**. In sound waves, each frequency can be understood as a

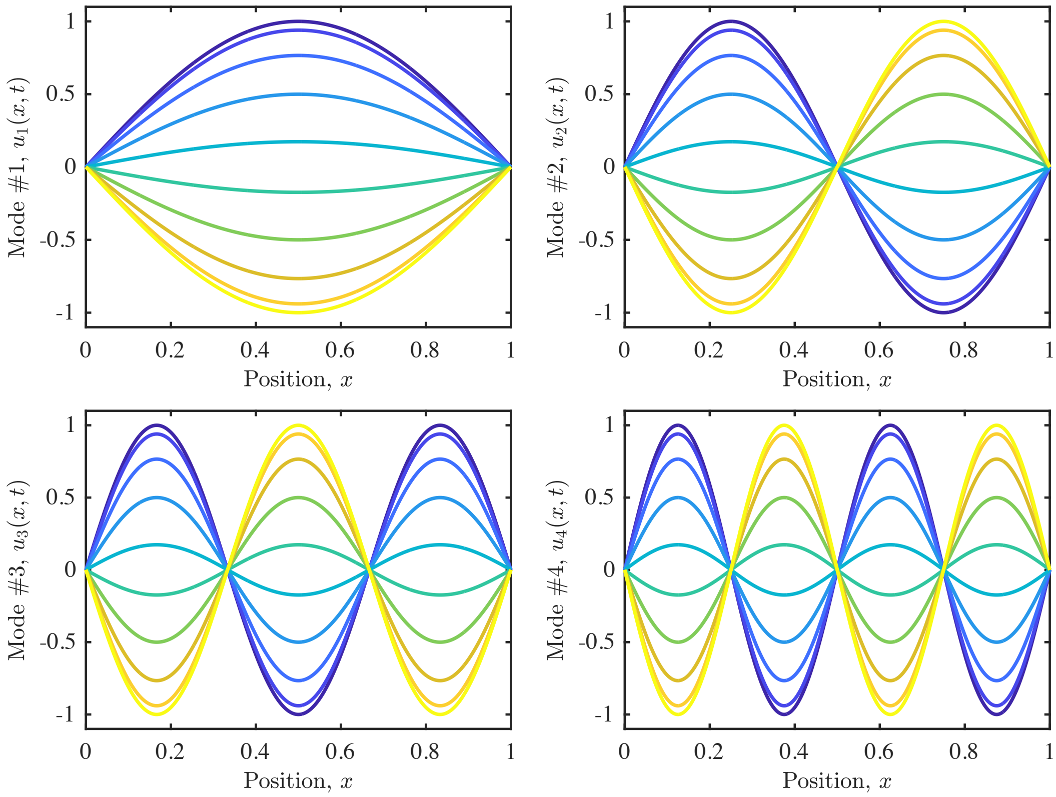

Figure 3.11 First four modes of a vibrating string with fixed ends with $L = 1$. In each case, we show time evolution over half a period of the oscillation (from blue to yellow).

single pitch. In music, these normal modes are also called **harmonics or overtones**. In Fig. 3.11, we show the time evolution of the first four normal modes of the vibrating string with fixed ends. In these 1D normal modes, we observe that the displacement is zero at a finite number of points, these are called **nodes**. These points are found at location $x_k = kL/n$ with $k = 1, 2, \dots, n$.

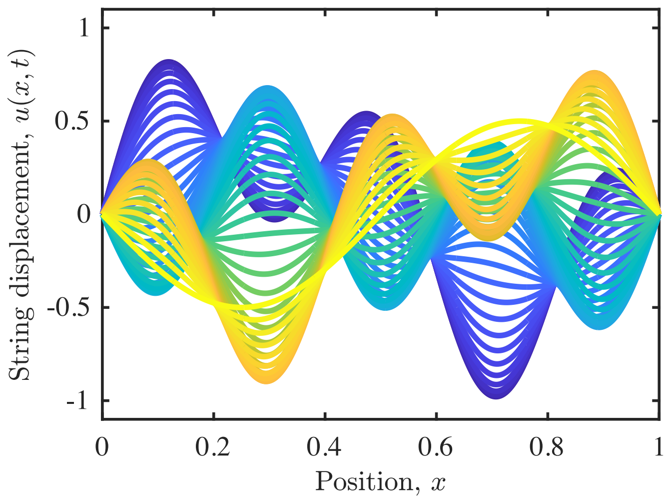

Figure 3.12 Short time evolution of the string vertical displacement given by (3.233) with time increasing from blue to yellow.

What we have seen here is that the superposition principle dictates that the most general motion of an oscillating system is a superposition of its normal modes. These are called normal modes because they are orthogonal to each other (e.g. for the vibrating string they are given by sinusoidal functions). As they are orthogonal from each other, they can move independently, or said differently, they form a basis on which we can decompose the motion of the solid. We saw in the previous section that the amplitudes of each of the modes are determined by the initial conditions of the problem (through the coefficients of the half-range Fourier sine series of the initial profile). For example, we can imagine that the initial conditions we picked are such that our solution is only a superposition of the 2^{nd} and 5^{th} normal modes with equal amplitudes

$$u(x,t) = 1/2\left[\sin(2\pi x/L)\cos(2\pi ct/L) + \sin(5\pi x/L)\cos(5\pi ct/L)\right] \tag{3.233}$$

Fig. 3.12 shows the time evolution of the displacement of the string in this case.

The concept of normal mode is very general and we will explore the modes of vibration of a rectangular plate in problem sheet #5. A more complicated example is that of the modes of vibration of a circular membrane (e.g. vibrations of a drumhead, a stretched circular membrane attached on a rigid frame). Solving this problem requires finding the solutions of a 2D wave equation in cylindrical coordinates. This can be solved using the method of separation of variables and one can show that the separated solutions can be expressed in terms of Bessel functions. Namely, the solutions of the vibrating drumhead

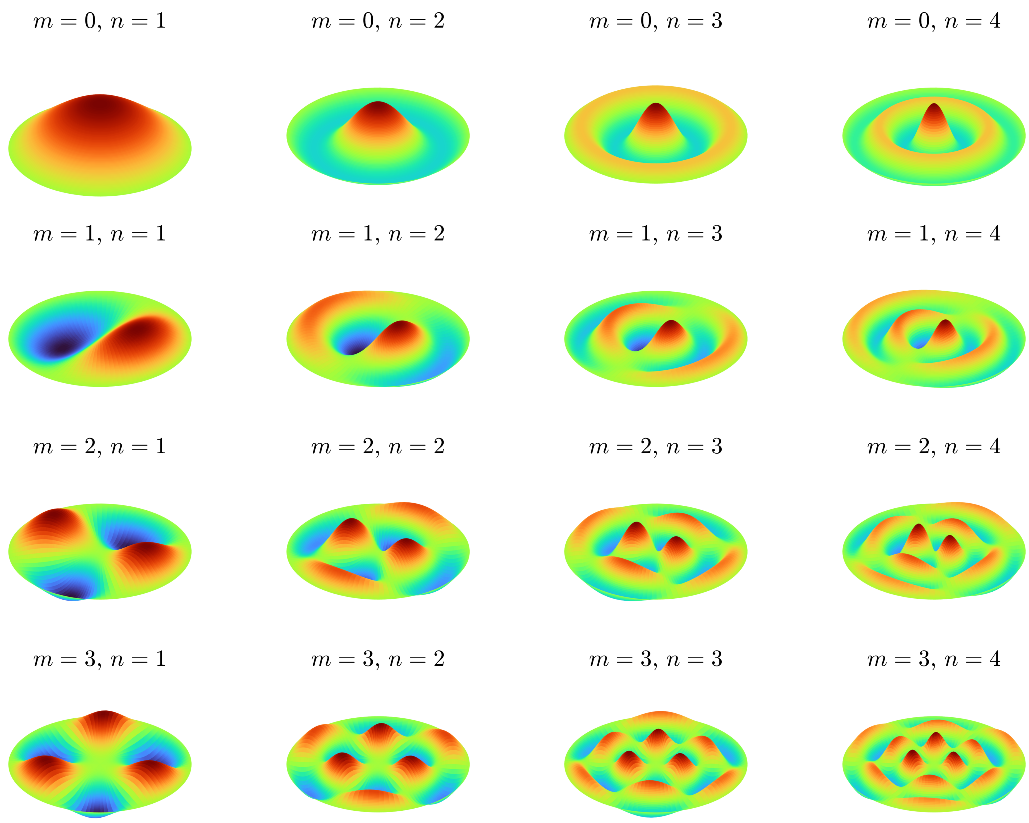

Figure 3.13 Normal modes of the circular drumhead of radius $R = 1$. Modes shapes are given by $u_{mn}(r,\theta) = J_m(\lambda_{mn} r)\cos(m\theta)$, with J_m the Bessel function of first kind of order m and λ_{mn} its n^{th} root.

problem are given in terms of the normal modes

$$u_{mn}(r,\theta,t) = [A_{mn}\cos c\lambda_{mn}t + B_{mn}\sin c\lambda_{mn}t]\, J_m(\lambda_{m,n}r)\,[C_{mn}\cos m\theta + D_{mn}\sin m\theta] \tag{3.234}$$

with $\lambda_{mn} = \gamma_{mn}/R$ where γ_{mn} is the n-th root of J_m the Bessel function of the first kind of order m and R is the radius of the drumhead. In Fig. 3.13, we show several normal modes of the vibrating drumhead. We can generalize the concept of **nodes** to this two dimensional system; indeed, in two dimensional systems, the nodes become lines where the displacement is always zero (these are called nodal lines). In Fig. 3.13, these would correspond to the location where the surface color is light green.

In practice, one can visualize the nodal lines in experimental systems quite easily. As early as 1787, Ernst Chladni invented a technique to visualize the various modes of vibration of rigid plates of various geometries. To do so, Chladni would draw a violin bow over the edge of the plate whose surface was lightly covered with sand, until it entered in resonance. The vibration of the plate would cause the sand to migrate away from the regions where vibration amplitudes are the largest to accumulate at the nodal lines. The figures that one obtains in this process are direct visual representations of the nodal pattern of the modes of vibrations of the plate; these are now known as **Chladni figures**. This technique has been used for instance in designing acoustic instruments like guitars, violins and cellos.

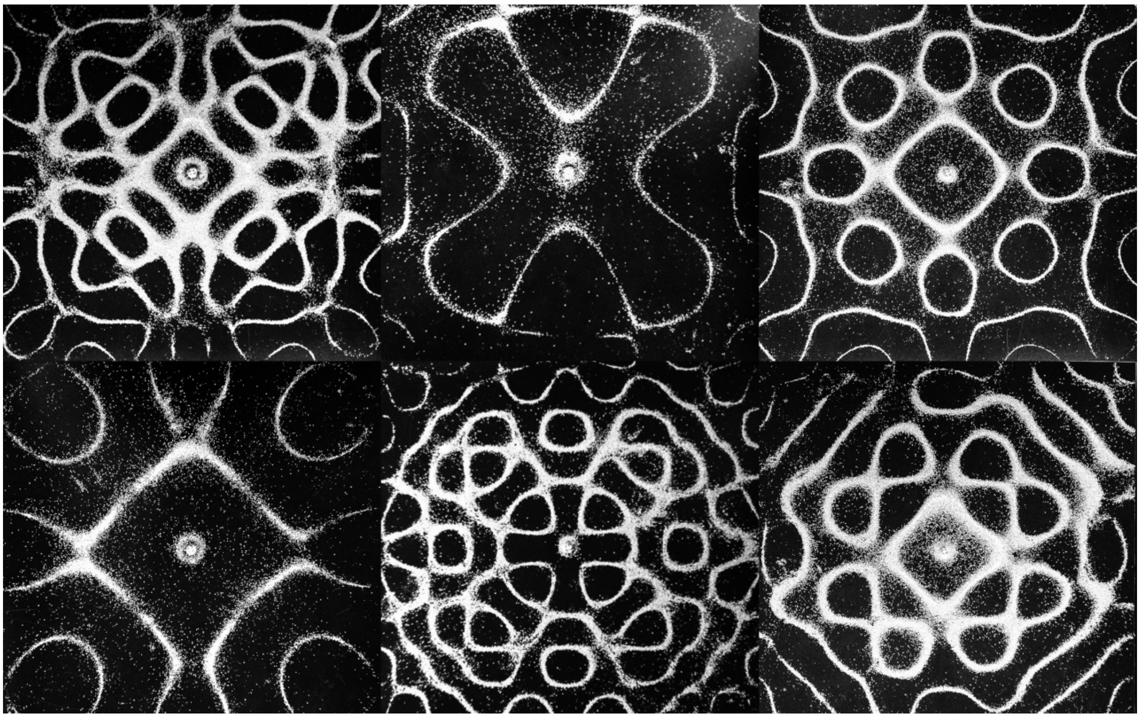

Figure 3.14 Example of Chladni figures for a rigid square plate.

Remark. *You are not expected to know the normal modes of the vibrating drumhead by heart as we have not derived these solutions in detail. This is merely an interesting example of vibration phenomena going beyond the 1D vibrating string.*

Uniqueness of the solution of the wave equation

Finally, note that one can show uniqueness of the solution of the wave equation using a similar method to what was done in Section 3.3.3. This will be done in Problem Sheet #5.

3.4.4 Solution on an infinite domain: Fourier transforms

On an infinite domain, we have previously seen that we can use a method based on Fourier transforms. Consider the general initial-value problem problem

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \quad t > 0, -\infty < x < \infty \tag{3.235}$$

$$u(x,0) = f_1(x) \quad -\infty < x < \infty \tag{3.236}$$

$$\frac{\partial u}{\partial t}(x,0) = f_2(x) \quad -\infty < x < \infty \tag{3.237}$$

This is a pure initial-value problem; the initial conditions can be interpreted as the initial position and velocity of an infinite vibrating string.

To solve (3.235), we introduce the Fourier transforms

$$\widehat{f}_k(x) = \int_{-\infty}^{+\infty} f_k(x) e^{-i\omega x} dx \tag{3.238}$$

and the inversion formulas

$$f_k(x) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \widehat{f}_k(\omega) e^{i\omega x} d\omega \tag{3.239}$$

The Fourier representation of the solution to (3.235) is given by

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \widehat{u}(\omega,t) e^{i\omega x} d\omega \tag{3.240}$$

with $\widehat{u}(\omega,t)$ a solution of the following equation

$$\frac{1}{2\pi} \int_{-\infty}^{+\infty} \left[\frac{\partial^2 \widehat{u}}{\partial t^2} + c^2\omega^2 \widehat{u}\right] e^{i\omega x} d\omega = 0 \tag{3.241}$$

which implies that $\widehat{u}$ is a solution to the following ODE

$$\frac{\partial^2 \widehat{u}}{\partial t^2} + c^2\omega^2 \widehat{u} = 0 \tag{3.242}$$

The general solution of this equation is given by

$$\widehat{u}(\omega,t) = A(\omega)\cos(\omega ct) + B(\omega)\sin(\omega ct) \tag{3.243}$$

and we set $t = 0$ to determine $A(\omega)$ and $B(\omega)$ and obtain

$$u(x,0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} A(\omega) e^{i\omega x} d\omega \quad \text{and} \quad \frac{\partial u}{\partial t}(x,0) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \omega c B(\omega) e^{i\omega x} d\omega \tag{3.244}$$

Comparing this with the initial conditions (3.236) and (3.237), we conclude that

$$\begin{cases} \widehat{f}_1(\omega) = A(\omega) \\ \widehat{f}_2(\omega) = \omega c B(\omega) \end{cases} \tag{3.245}$$

Finally, we substitute this into (3.243) to conclude that the Fourier representation of the solution of the problem (3.235)-(3.237) is given by

$$u(x,t) = \frac{1}{2\pi} \int_{-\infty}^{+\infty} \left[\widehat{f}_1(\omega)\cos(\omega ct) + \widehat{f}_2(\omega)\frac{\sin(\omega ct)}{\omega c}\right] e^{i\omega x} d\omega \tag{3.246}$$

Example

Let us have a look at an example. Suppose that we have the following problem

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \quad t > 0, -\infty < x < \infty \tag{3.247}$$

$$u(x,0) = 4e^{-5|x|} \quad -\infty < x < \infty \tag{3.248}$$

$$\frac{\partial u}{\partial t}(x,0) = 0 \quad -\infty < x < \infty \tag{3.249}$$

with u bounded as $x \to \pm\infty$ for all t.

We take the Fourier transform in x of the PDE and obtain

$$\frac{\partial^2 \widehat{u}}{\partial t^2} = -c^2\omega^2\widehat{u} \tag{3.250}$$

whose general solution can be written

$$\widehat{u}(\omega,t) = A(\omega)\cos(\omega ct) + B(\omega)\sin(\omega ct) \tag{3.251}$$

The initial condition (3.249) implies that $\partial\widehat{u}/\partial t = 0$ at $t = 0$, and so we conclude that $B(\omega) = 0$. Then applying condition (3.248), we see that

$$A(\omega) = \mathcal{F}\left\{4e^{-5|x|}\right\} = \int_{-\infty}^{\infty} 4\exp(-5|x|)e^{-i\omega x}dx \tag{3.252}$$

$$= 4\left[\int_{-\infty}^{0} e^{(5-i\omega)x}dx + \int_{0}^{\infty} e^{-(5+i\omega)x}dx\right] \tag{3.253}$$

$$= 4\left[\frac{1}{5-i\omega} + \frac{1}{5+i\omega}\right] = \frac{40}{25+\omega^2} \tag{3.254}$$

Hence, we have

$$\widehat{u}(\omega,t) = \frac{40}{25+\omega^2}\cos(\omega ct) \tag{3.255}$$

We can invert this expression by using the convolution theorem, since $\widehat{u}$ is the product of two terms for which it is easier to obtain inverses. We proceed as follows

$$u(x,t) = \mathcal{F}^{-1}\left\{\frac{40}{25+\omega^2}\cos(\omega ct)\right\} \tag{3.256}$$

$$= \mathcal{F}^{-1}\left\{\frac{40}{25+\omega^2}\right\} * \mathcal{F}^{-1}\left\{\cos(\omega ct)\right\} \tag{3.257}$$

$$= 4e^{-5|x|} * \mathcal{F}^{-1}\left\{\cos(\omega ct)\right\} \tag{3.258}$$

The second term is obtained by remembering that

$$\mathcal{F}\{\cos(\omega_0 x)\} = \pi\delta(\omega+\omega_0) + \pi\delta(\omega-\omega_0) \tag{3.259}$$

where δ is the Dirac delta function. It thus follows from the symmetry formula

$$\mathcal{F}\{\pi\delta(x+\omega_0) + \pi\delta(x-\omega_0)\} = 2\pi\cos(-\omega_0\omega) \tag{3.260}$$

and hence, we obtain

$$\mathcal{F}^{-1}\{\cos(\omega_0\omega)\} = \frac{1}{2}\delta(x+\omega_0) + \frac{1}{2}\delta(x-\omega_0) \tag{3.261}$$

Thus, we conclude that

$$u(x,t) = 2e^{-5|x|} * (\delta(x+ct) + \delta(x-ct)) \tag{3.262}$$
$$= 2\int_{-\infty}^{\infty} e^{-5|x-s|}\delta(s+ct)ds + 2\int_{-\infty}^{\infty} e^{-5|x-s|}\delta(s-ct)ds \tag{3.263}$$
$$= 2e^{-5|x+ct|} + 2e^{-5|x-ct|} \tag{3.264}$$

where we have used the sifting property of the delta function. We represent the function $u(x,t)$ for various times in Fig. 3.15.

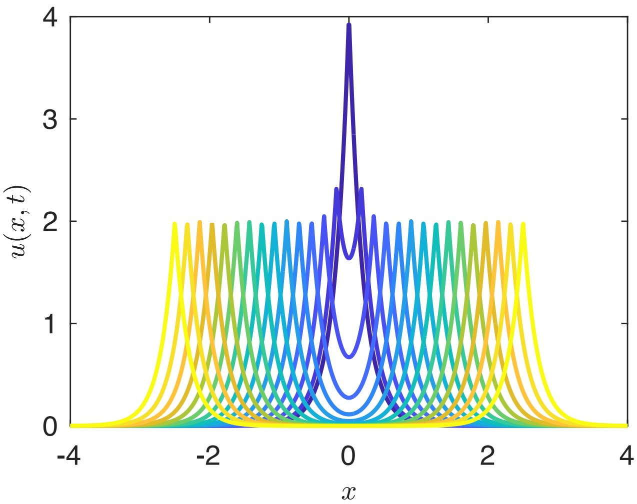

Figure 3.15 Solution of problem (3.247)-(3.249) $u(x,t)$ as a function of x for increasing times from $t = 0$ (blue) to $t = 2.5$ (yellow). Here, we used $c = 1$.

3.4.5 D'Alembert's solution for the wave equation

In the previous section, we obtained that the Fourier representation of the solution to the following problem

$$\frac{\partial^2 u}{\partial t^2} = c^2\frac{\partial^2 u}{\partial x^2} \quad t > 0, -\infty < x < \infty \tag{3.265}$$
$$u(x,0) = f_1(x) \quad -\infty < x < \infty \tag{3.266}$$
$$\frac{\partial u}{\partial t}(x,0) = f_2(x) \quad -\infty < x < \infty \tag{3.267}$$

was given by

$$u(x,t) = \frac{1}{2\pi}\int_{-\infty}^{+\infty}\left[\widehat{f}_1(\omega)\cos(\omega ct) + \widehat{f}_2(\omega)\frac{\sin(\omega ct)}{\omega c}\right]e^{i\omega x}d\omega \tag{3.268}$$

Using this, we can also obtain an explicit representation in terms of the functions $f_1(x)$ and $f_2(x)$. To do this, recall that

$$\cos(\theta) = \frac{1}{2}\left(e^{i\theta} + e^{-i\theta}\right) \quad \text{and} \quad \sin(\theta) = \frac{1}{2i}\left(e^{i\theta} - e^{-i\theta}\right) \tag{3.269}$$

Thus, we can write

$$\int_{-\infty}^{+\infty} \widehat{f_1}(\omega)\cos(\omega ct)e^{i\omega x}d\omega = \frac{1}{2}\int_{-\infty}^{+\infty} \widehat{f_1}(\omega)\left(e^{i\omega ct} + e^{-i\omega ct}\right)e^{i\omega x}d\omega \tag{3.270}$$

$$= \frac{1}{2}\int_{-\infty}^{+\infty} \widehat{f_1}(\omega)\left(e^{i\omega(x+ct)} + e^{i\omega(x-ct)}\right)d\omega \tag{3.271}$$

$$= \frac{2\pi}{2}\left[f_1(x-ct) + f_1(x+ct)\right] \tag{3.272}$$

Similarly, we write

$$\int_{-\infty}^{+\infty} \widehat{f_2}(\omega)\frac{\sin(\omega ct)}{\omega c}e^{i\omega x}d\omega = \frac{1}{2}\int_{-\infty}^{+\infty} \widehat{f_2}(\omega)\frac{e^{i\omega ct} - e^{-i\omega ct}}{i\omega c}e^{i\omega x}d\omega \tag{3.273}$$

$$= \frac{1}{2}\int_{-\infty}^{+\infty} \widehat{f_2}(\omega)\frac{e^{i\omega(x+ct)} - e^{i\omega(x-ct)}}{i\omega c}d\omega \tag{3.274}$$

$$= \frac{1}{2c}\int_{-\infty}^{+\infty} \widehat{f_2}(\omega)\left(\int_{x-ct}^{x+ct} e^{i\omega\xi}d\xi\right)d\omega \tag{3.275}$$

$$= \frac{1}{2c}\int_{x-ct}^{x+ct}\left(\int_{-\infty}^{+\infty} e^{i\omega\xi}\widehat{f_2}(\omega)d\xi\right)d\omega \tag{3.276}$$

$$= \frac{2\pi}{2c}\int_{x-ct}^{x+ct} f_2(\xi)d\xi \tag{3.277}$$

Combining these terms gives us what is known as **d'Alembert's formula**:

$$\boxed{u(x,t) = \frac{1}{2}\left[f_1(x-ct) + f_1(x+ct)\right] + \frac{1}{2c}\int_{x-ct}^{x+ct} f_2(\xi)d\xi} \tag{3.278}$$

This formula is named after the French mathematician and music theorist **Jean le Rond d'Alembert**, who derived it in 1747 as a solution to the problem of a vibrating string. Considering the applications of wave theory to music, it is not surprising that d'Alembert would make progress in this field.

It is natural to wonder whether this formula is only valid for the solutions to the wave equation on an infinite domain; d'Alembert's formula is far more general and it can be shown that it is also a solution of the wave equation on a finite domain. For instance, let us revisit the solution we obtained in the case of a finite-sized domain. The particular solution we obtained by separation of variables read

$$u(x,t) = \sum_{n=1}^{\infty} b_n \sin(n\pi x/L)\cos(n\pi ct/L) \tag{3.279}$$

Above we introduce important combinations of variables $x-ct$ and $x+ct$. We can express the separated solution using those and write

$$u(x,t) = \frac{1}{2}\sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi}{L}(x+ct)\right) + \frac{1}{2}\sum_{n=1}^{\infty} b_n \sin\left(\frac{n\pi}{L}(x-ct)\right) \tag{3.280}$$

The functional dependence on these quantities indicates that in both cases the solution is the sum of a left-traveling ($x+ct$) and a right-traveling ($x-ct$) wave, with both waves propagating at speed c. This observation provides us with some motivation for the following study which results in the derivation of the general solution of the wave equation.

We introduce the following new variables

$$\xi = x + ct \quad \text{and} \quad \eta = x - ct \tag{3.281}$$

The partial derivatives transform as follows:

$$\frac{\partial}{\partial x} = \frac{\partial \xi}{\partial x}\frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial x}\frac{\partial}{\partial \eta} = \frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta}, \tag{3.282}$$

$$\frac{\partial}{\partial t} = \frac{\partial \xi}{\partial t}\frac{\partial}{\partial \xi} + \frac{\partial \eta}{\partial t}\frac{\partial}{\partial \eta} = c\frac{\partial}{\partial \xi} - c\frac{\partial}{\partial \eta}. \tag{3.283}$$

We can then calculate the second order partial derivatives

$$\frac{\partial^2 u}{\partial x^2} = \frac{\partial}{\partial x}\left(\frac{\partial u}{\partial x}\right) = \left(\frac{\partial}{\partial \xi} + \frac{\partial}{\partial \eta}\right)\left(\frac{\partial u}{\partial \xi} + \frac{\partial u}{\partial \eta}\right), \tag{3.284}$$

$$= \frac{\partial^2 u}{\partial \xi^2} + 2\frac{\partial^2 u}{\partial \xi \partial \eta} + \frac{\partial^2 u}{\partial \eta^2} \tag{3.285}$$

and

$$\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}\left(\frac{\partial u}{\partial t}\right) = \left(c\frac{\partial}{\partial \xi} - c\frac{\partial}{\partial \eta}\right)\left(c\frac{\partial u}{\partial \xi} - c\frac{\partial u}{\partial \eta}\right), \tag{3.286}$$

$$= c^2\left(\frac{\partial^2 u}{\partial \xi^2} - 2\frac{\partial^2 u}{\partial \xi \partial \eta} + \frac{\partial^2 u}{\partial \eta^2}\right) \tag{3.287}$$

Under this transformation, the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2\frac{\partial^2 u}{\partial x^2} \tag{3.288}$$

becomes

$$-4c^2\frac{\partial^2 u}{\partial \xi \partial \eta} = 0 \tag{3.289}$$

The equation is then said to be in its **canonical form**. This equation can be integrated once with respect to ξ to give

$$\frac{\partial u}{\partial \eta} = f'(\eta) \tag{3.290}$$

where f' is an arbitrary function of η. Integrating again, this time with respect to η, we obtain

$$u = f(\eta) + g(\xi) \tag{3.291}$$

where g is an arbitrary function of ξ. The general solution of the wave equation therefore has the form

$$\boxed{u(x,t) = f(x - ct) + g(x + ct)} \tag{3.292}$$

and so can always be written as the sum of right and left travelling waves.

3.4.6 Types of waves

At this point in the lectures, it may be useful to pause for a moment and take a step back. You may have realized that throughout the material so far, we have exhibited numerous wave phenomena. We talked about travelling waves (rarefaction/shock waves) in the context of traffic flow modelling. We are now closing a section on the wave equation which was said to governed the vibrations of elastic strings and membranes. But our experience of waves shows us that they are found in a lot of settings including: sound waves, electromagnetic waves (radio or light waves), water waves, elastic waves in solids. Further, as sufficiently small scales, quantum mechanics describes matter in terms of wave functions.

Although all these wave phenomena share similarities, they also show important differences. For instance, travelling waves (like in water waves or traffic flow) propagate a disturbance in space while standing waves do not. Further, sound waves need a supporting medium while electromagnetic waves do not.

While it seems too hard to give a general definition of a **wave**, it may be useful to clarify some terminology at this point.

1. **Progressive or travelling waves** are described by a function of the following form

$$u(x,t) = f(x - ct) \tag{3.293}$$

For $t = 0$, we have $u(x, 0) = f(x)$, which represents the initial profile of the perturbation. For travelling waves, the profile propagates without deformation with speed $|c|$, in the positive (respectively, negative) direction if $c > 0$ (resp., $c < 0$).

2. **Harmonic waves** are particular progressive waves of the form

$$u(x,t) = A\exp\left[i(kx - \omega t)\right], \quad A, k, \omega \in \mathbb{R} \tag{3.294}$$

The complex notation is often used because it simplifies the computations but one should understand that the real part (or the imaginary part) only are of interest. For harmonic waves, we denote

- the *wave amplitude* $|A|$;
- the *wave number* k (with $[k] = L^{-1}$) and the *wavelength*

$$\lambda = \frac{2\pi}{k} \tag{3.295}$$

which is the distance between successive maxima or minima of the waveform. The wave number can be interpreted as the number of complete oscillations in the interval $[0, 2\pi]$.

- the *angular frequency* ω and *frequency*

$$f = \frac{\omega}{2\pi} \tag{3.296}$$

which is the number of complete oscillations in one second (measured in Hertz) at a fixed position in space.

- the *wave (or phase) speed*

$$c = \frac{\omega}{k} \tag{3.297}$$

3. **Standing (or stationary) waves** are of the form

$$u(x,t) = f(x)\left[A\cos(\omega t) + B\sin(\omega t)\right] \tag{3.298}$$

An example of these was seen in the case of the vibrating string with fixed ends, there our standing waves were of the form

$$u(x,t) = A\sin kx \cos \omega t \tag{3.299}$$

In these waves, the basic sinusoidal wave $\sin kx$ is modulated by the time dependent oscillation $A\cos \omega t$. A standing wave may be generated by superposing two harmonic waves with the same amplitude and travelling in opposite directions (with same speed); indeed, for example, we can write

$$u(x,t) = \frac{A}{2}\sin(kx - \omega t) + \frac{A}{2}\sin(kx + \omega t) = A\sin kx \cos \omega t \tag{3.300}$$

4. **Plane waves** (scalar) are of the form

$$u(\mathbf{r},t) = f(\mathbf{k}\cdot\mathbf{r} - \omega t) \tag{3.301}$$

they generalize to higher spatial dimensions ($n > 1$) the concept of travelling waves. The disturbance propagates in the direction of $\mathbf{k}$ with speed $c = \omega/|\mathbf{k}|$. The planes of equation

$$\boldsymbol{\theta}(\mathbf{r},t) = \mathbf{k}\cdot\mathbf{r} - \omega t = C \tag{3.302}$$

where C is a constant are called *wave-fronts*. Among all plane waves, we distinguish *harmonic or monochromatic plane waves* as waves of the form

$$u(\mathbf{r},t) = A\exp\left[i(\mathbf{k}\cdot\mathbf{r} - \omega t)\right] \tag{3.303}$$

In this case, $\mathbf{k}$ is the wave number vector and ω the angular frequency. The vector $\mathbf{k}$ is orthogonal to the wave front and $|\mathbf{k}|/2\pi$ measures the number of waves per unit length, while $\omega/2\pi$ gives the number of oscillations per unit time at a fixed position (i.e. the number of oscillations in 1 sec, measured in Hertz).

5. **Spherical waves** are waves of the form

$$u(\mathbf{r},t) = v(r,t) \tag{3.304}$$

where $r = |\mathbf{r} - \mathbf{r}_0|$ with $\mathbf{r}_0 \in \mathbb{R}^n$ a fixed point. As indicated by their name, these waves are spherically symmetric. In particular, $u(\mathbf{r},t) = v(r - ct)$ is a travelling wave whose wavefronts are the spheres $r - ct = \text{constant}$, moving with speed $|c|$ (in an outward direction if $c > 0$ and an inward direction if $c < 0$).

3.5 Laplace equation and Poisson equation

Finally, we close this Chapter with the study of the main prototypes for **elliptic equations**,

$$\Delta\phi = 0 \tag{3.305}$$

introduced by the French mathematician Pierre-Simon Laplace (1749 – 1827). Note that a function ϕ that satisfies Laplace equation is called a **harmonic function**. This equation is a special case of a more general class of equations

$$\Delta\phi = f(\mathbf{r}) \tag{3.306}$$

where f is a prescribed function of position $\mathbf{r} = x\hat{\mathbf{i}} + y\hat{\mathbf{j}} + z\hat{\mathbf{k}}$ (in Cartesian coordinates). Equation (3.306) was introduced by the French mathematician Simeon Poisson (1781 – 1840), a student of Laplace, in the studies of diverse problems in mechanics and theoretical physics.

3.5.1 Applications of the Laplace/Poisson equation

You may wonder where one would encounter the Laplace or the Poisson equation. It is easy to see that Laplace equation does not depend explicitly on time: it describes **steady state phenomena**. Laplace equation appears in many branches of theoretical physics and mechanics. For instance, it can be seen as the steady-state limit of the heat/diffusion equation.

Indeed, consider the problem of heat conduction in a thin sheet of conducting material in which you set the temperature at the boundaries. We have seen that solving the (two-dimensional) heat equation would give you the evolution of two-dimensional temperature profile (i.e. the value of the temperature at each position in the material) starting from prescribed initial conditions. After a long time, the temperature field would normally converge to a stationary (i.e. time-independent profile) profile. In steady-state the temperature profile does not change with time anymore and so $\partial u/\partial t = 0$ and the heat equation reduces to the Laplace equation.

Poisson's equation, which is slightly more general, plays an important role in the **theory of conservative fields**, i.e. vector fields which are derived from the gradient of a potential. In particular, it appears in the following examples:

- In **fluid dynamics**, irrotational flows arise when the curl of the velocity field $\mathbf{u}(\mathbf{r}, t)$ of the fluid is zero, that is
$$\nabla \times \mathbf{u} = 0 \tag{3.307}$$
If one assumes that the fluid is incompressible (i.e. that the fluid density $\rho(\mathbf{r}, t)$ is constant), the continuity equation
$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0 \tag{3.308}$$
becomes
$$\nabla \cdot \mathbf{u} = 0 \tag{3.309}$$
Helmholtz's theorem dictates that we can write the velocity field as the sum of the gradient of a scalar potential ϕ and the curl of a vector potential $\mathbf{A}$:
$$\mathbf{u} = -\nabla\phi + \nabla \times \mathbf{A} \tag{3.310}$$
but imposing the fact that $\nabla \times \mathbf{u} = 0$ implies that $\nabla \times (\nabla \times \mathbf{A}) = 0$ (as the curl of a gradient is always zero). Now, as the curl of the curl of a vector field is only identically zero if the vector potential itself is zero; we find that $\mathbf{u} = -\nabla\phi$ and so using the continuity equation, we finally find that the scalar potential is governed by Laplace's equation for irrotational flows:
$$\nabla^2\phi = 0 \tag{3.311}$$

- In **electromagnetism**, one often denotes $\mathbf{E}$ the electric field, i.e. a force field due to a distribution of electric charges in a domain $\Omega \subset \mathbb{R}^3$. Maxwell's first equation (or Gauss law for electricity) states that *the total electric flux through any closed surface in free space of any shape drawn in an electric field is proportional to the total electric charge enclosed by the surface*, i.e.
$$\oint_{\partial\Omega} \mathbf{E} \cdot \hat{\mathbf{n}} dS = \int_{\Omega} \frac{\rho}{\varepsilon_0} dV \tag{3.312}$$
where ρ is the density of electric charges and ε_0 is a constant called the vacuum permittivity. Using the divergence theorem, we can write Gauss' law in differential form
$$\nabla \cdot \mathbf{E} = \frac{\rho}{\varepsilon_0} \tag{3.313}$$
Under what is called the electrostatic approximation, the electric field is irrotational and so $\nabla \times \mathbf{E} = 0$. In this case, we can express the electric field as the gradient of a scalar function ϕ called the **electrostatic potential** (also know as voltage). As it is observed that the electric field points from region of high voltage to regions of low voltage, we get that
$$\mathbf{E} = -\nabla\phi \tag{3.314}$$

Plugging this into Gauss' law, we can see that the **electrostatic potential** is governed by

$$\nabla^2\phi(\mathbf{r},t) = -\frac{\rho(\mathbf{r})}{\varepsilon_0} \tag{3.315}$$

which is Poisson's equation. In the absence of electric charges, $\rho(\mathbf{r},t) \equiv 0$ and we recover Laplace equation.

- as a final example, Gauss' law for the **gravitational field** $\mathbf{g}$ created by a density of mass $\rho(\mathbf{r},t)$ reads

$$\nabla \cdot \mathbf{g} = -4\pi G\rho \tag{3.316}$$

where G is the gravitational constant. Now, as you may have seen in mechanics, the work done in moving a particle in the gravitational field only depends on the start and end points (not on the path taken), it means that the gravitational field is a conservative field. Thus, we can define a function called the **potential energy** independent of the path that the particle takes such that

$$\int_a^b \mathbf{g} \cdot d\mathbf{r} = \phi(a) - \phi(b) \tag{3.317}$$

or equivalently

$$\mathbf{g} = -\nabla\phi \tag{3.318}$$

By definition, conservative fields are vector fields which represent forces of physical systems in which **energy is conserved**. Injecting this in Gauss' law of gravitation we obtain

$$\nabla^2\phi = 4\pi G\rho(\mathbf{r}) \tag{3.319}$$

which is a Poisson equation. Note that in empty space, $\rho = 0$ and we recover Laplace equation.

Remark. *The Laplacian operator appears very often in mathematical physics, partially because it is the only second-order linear differential operator which is invariant under the symmetries of Euclidean space, that is, translations and rotations*

$$\mathbf{r} \mapsto \mathbf{r} + \mathbf{a} \quad \textit{and} \quad \mathbf{r} \mapsto R\mathbf{r} \tag{3.320}$$

with the rotation R represented by an orthogonal matrix $R^T = R^{-1}$. This is one elementary manifestation of the principle of relativity, which is that equations which describe physical phenomena should be invariant under symmetries of the underlying space.

Boundary conditions

Thinking back to the problem of heat conduction, we have seen in Section 3.3 that to obtain a unique temperature distribution, we must provide boundary conditions for the temperature or the temperature flux. As on Fig. 3.16, we consider a domain V enclosed by a surface S_0. In general, boundary conditions will then be given on the surface S_0 which bounds There are several possible boundary conditions:

Definition 3.5.1: Dirichlet problem

The problem defined by Poisson's equation and the Dirichlet boundary condition

$$\begin{aligned} \Delta u = f(\mathbf{r}), &\quad \mathbf{r} \in V \setminus S \\ u(\mathbf{r}) = g(\mathbf{r}), &\quad \mathbf{r} \in S \end{aligned} \tag{3.321}$$

for a given function g is called the **Dirichlet problem**.

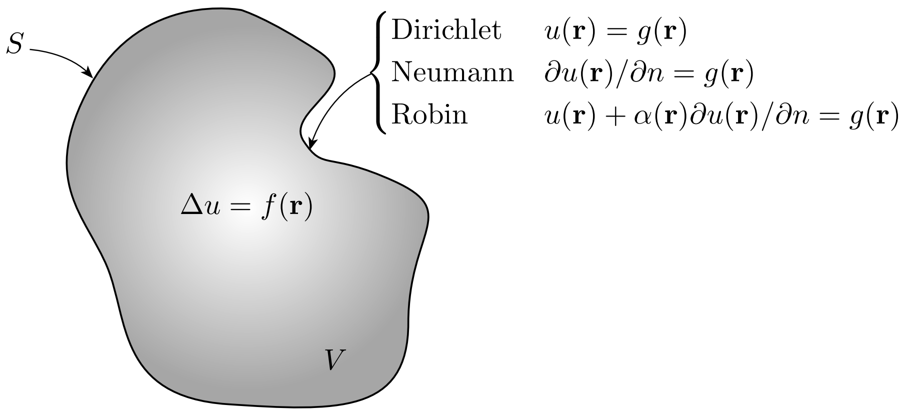

Figure 3.16 A volume V bounded on its exterior by the surface S.

Definition 3.5.2: Neumann problem

Let us define a problem by Poisson's equation and the Neumann boundary condition

$$\begin{aligned} \Delta u &= f(\mathbf{r}), \quad \mathbf{r} \in V \setminus S \\ \frac{\partial u(\mathbf{r})}{\partial n} &= g(\mathbf{r}), \quad \mathbf{r} \in S \end{aligned} \tag{3.322}$$

for a given function g, $\partial/\partial n$ denotes the normal derivative to the boundary, i.e. defining $\hat{\mathbf{n}}$ the unit outward normal to S_0, $\partial u/\partial n = \hat{\mathbf{n}} \cdot \nabla u$. This problem is called the **Neumann problem**.

Definition 3.5.3

The problem defined by Poisson's equation and the boundary condition of the third kind

$$\begin{aligned} \Delta u &= f(\mathbf{r}), \quad \mathbf{r} \in V \setminus S \\ u(\mathbf{r}) + \alpha(\mathbf{r})\frac{\partial u(\mathbf{r})}{\partial n} &= g(\mathbf{r}), \quad \mathbf{r} \in S \end{aligned} \tag{3.323}$$

for α and g are given functions and $\partial/\partial n$ denotes the normal derivative to the boundary, i.e. defining $\hat{\mathbf{n}}$ the unit outward normal to S_0, $\partial u/\partial n = \hat{\mathbf{n}} \cdot \nabla u$. This is called a **problem of the third kind** (or **Robin problem**).

Remark. *Note that a common notation for the domain of study is Ω; the boundary of the domain is then commonly denoted $\partial\Omega$. Using this notation, the domain of study can then be a segment (1D), an area (2D) or a volume (3D) without referring explicitly to variable names such as S, V etc.*

3.5.2 Separation of variables

The method of separation of variables, introduced earlier for the heat equation and for the wave equation, can in some cases also be applied to elliptic equations. Applying the method requires certain symmetries to hold, both for the equation and for the domain under study. Thus, the main limitations of these methods are the simple shapes of domain to which they can be applied (rectangles, disks, circular sectors,...), and the necessity for the variables in the boundary conditions to separate. There are examples of the use of these techniques on problem sheet #6.

In what follows we shall consider the three-dimensional form of the equations and apply some of the techniques and theorems you have learned during the first term of **MATH50004 - Multi-variable Calculus and Differential Equations** to formulate solutions. We will use a number of results from vector calculus and will also generalize the Dirac delta function.

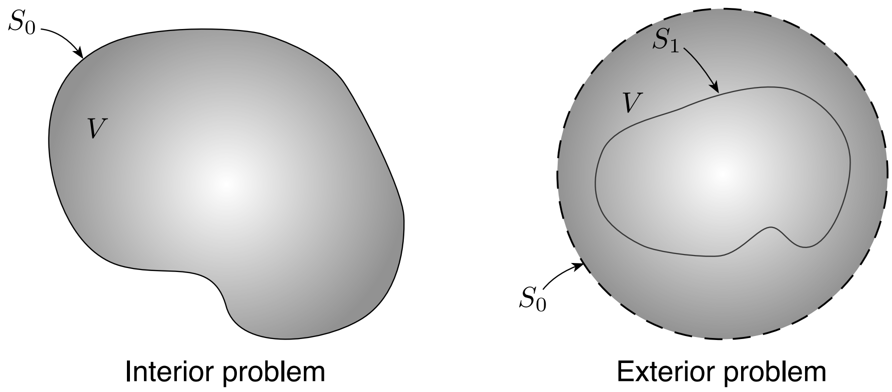

Figure 3.17 (*Left*) **Interior problem** — the volume V bounded on its exterior by the surface S_0; (*Right*) **Exterior problem** — An unbounded volume V with an inner boundary S_1. The dashed line representing the outer boundary S_0 is to be considered at infinity.

3.5.3 Uniqueness of solution for interior problems

Before we move on to introducing these new resolution techniques, let's first assume that we have found a solution and address the problem of its uniqueness!

Proposition 3.5.1

Let $\phi(\mathbf{r})$ satisfy Poisson's equation

$$\nabla^2\phi = f(\mathbf{r}) \tag{3.324}$$

in a volume V. Let the volume be bounded on its exterior by a surface S_0 (see Fig. 3.17). On the surface, we consider a Dirichlet boundary condition, i.e. that the value of ϕ is specified, namely $\phi(\mathbf{r}) = p(\mathbf{r})$ on S_0. **The solution ϕ to this problem is unique.**

Proof. We will suppose that two solutions to this problem exist and show that they are necessarily equal. Let the two solutions be ϕ_1 and ϕ_2. As they are solutions, we must both satisfy Poisson's equation and the same boundary condition. We define

$$\psi \equiv \phi_1 - \phi_2 \tag{3.325}$$

By definition, ψ is the solution to the following problem

$$\begin{aligned} \nabla^2\psi &= 0, \quad \mathbf{r} \in V \setminus S_0 \\ \psi(\mathbf{r}) &= 0, \quad \mathbf{r} \in S_0 \end{aligned} \tag{3.326}$$

Recall for two scalar fields u and v defined on $V \subset \mathbb{R}^3$ with boundary S_0 and with continuous second derivatives, we have the following relation

$$\int_{S_0} u\frac{\partial v}{\partial n}dS = \int_V \left\{v\nabla^2 u + (\nabla u)\cdot(\nabla v)\right\}dV \tag{3.327}$$

with $\partial v/\partial n = \hat{\mathbf{n}}\cdot\nabla v$ and $\hat{\mathbf{n}}$ the unit outward normal. This is called Green's first identity. Applying Green's first identity to $u = v = \psi$, we obtain

$$\int_{S_0} \psi\frac{\partial \psi}{\partial n}dS = \int_V \psi\nabla^2\psi dV + \int_V |\nabla\psi|^2 dV \tag{3.328}$$

Using the boundary condition, i.e. $\psi(\mathbf{r}) = 0$ on S_0, the LHS of this expression is zero. Since ψ satisfied Laplace's equation throughout V, the first term on the RHS is also zero. We are thus left with

$$\int_V |\nabla\psi|^2 dV = 0 \tag{3.329}$$

The volume integral of a positive quantity can only be zero if the integrand is identically zero, and so this implies that

$$\nabla\psi = 0 \tag{3.330}$$

which means that ψ is at most a constant throughout V, but because ψ is zero on the boundaries, it follows that ψ is identically zero throughout V. Hence, $\phi_1 = \phi_2$ and the solution is unique. ■

Remark. *The same reasoning applies if ϕ is a complex-valued function of position, if we have Neumann boundary conditions, and also if the volume V has holes in it.*

Example

Solve $\nabla^2\psi = 2$ inside the unit sphere $r \le 1$ with $\psi = 1$ on $r = 1$.

We note that this problem possesses a radial symmetry. It is therefore natural: (1) to work in spherical coordinates and (2) seek a radially symmetric solution $\psi = \psi(r)$ independent of θ and ϕ. Recall that the Laplacian in spherical coordinates is given by

$$\nabla^2\psi = \frac{1}{r^2\sin\theta}\left[\frac{\partial}{\partial r}\left(r^2\sin\theta\frac{\partial\psi}{\partial r}\right) + \frac{\partial}{\partial\theta}\left(\sin\theta\frac{\partial\psi}{\partial\theta}\right) + \frac{\partial}{\partial\phi}\left(\frac{1}{\sin\theta}\frac{\partial\psi}{\partial\phi}\right)\right] \tag{3.331}$$

Under the assumption of radial symmetry, our equation thus reduces to

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) = 2 \tag{3.332}$$

Integrating once, we obtain

$$r^2\frac{d\psi}{dr} = \frac{2}{3}r^3 + C \tag{3.333}$$

which we can integrate a second time to obtain

$$\psi = \frac{1}{3}r^2 - \frac{C}{r} + D \tag{3.334}$$

For ψ to remain finite at $r = 0$, we require that $C = 0$. Applying the boundary condition, we obtain that

$$\psi = 1, \text{ on } r = 1 \Rightarrow D = 2/3 \tag{3.335}$$

The required solution is then

$$\psi(r) = \frac{1}{3}r^2 + \frac{2}{3} \tag{3.336}$$

Due to the uniqueness theorem, this is the only possible solution to this problem.

3.5.4 Uniqueness of solution for exterior problems

Let us now move to what are called exterior problems.

Proposition 3.5.2

Consider an exterior problem as shown on Fig. 3.17, i.e. a problem in which we have an inner boundary S_1 but the outer boundary S_0 is taken to infinity so that V is an unbounded volume. Let $\phi(\mathbf{r})$ satisfy Poisson's equation

$$\nabla^2\phi = f(\mathbf{r}) \tag{3.337}$$

throughout V. On the inner surface, we consider a Dirichlet boundary condition, i.e. that the value of ϕ is specified, namely $\phi(\mathbf{r}) = p(\mathbf{r})$ on S_1. Suppose in addition that $\phi = \mathcal{O}(1/r)$, $\partial\phi/\partial r = \mathcal{O}(1/r^2)$ as $r \to \infty$. **Then the solution ϕ in V is unique.**

Proof. We start by considering the surface S_0 to be a large sphere of radius R. As in the previous section, we suppose that there exist two solutions ϕ_1 and ϕ_2 and form the difference $\psi \equiv \phi_1 - \phi_2$. Using Green's first identity as in the previous case, we obtain

$$\int_V |\nabla\psi|^2 dV = \sum_{i=0}^{1} \int_{S_i} \psi\frac{\partial\psi}{\partial n}dS = \int_{S_0} \psi\frac{\partial\psi}{\partial n}dS \tag{3.338}$$

where the second equality holds since the integral over S_1 is zero due to the boundary condition that ψ vanishes on S_1. Since S_0 is a sphere of radius R, we can write $dS = R^2 \sin\theta d\theta d\phi$ in spherical coordinates, and $\partial\psi/\partial n = \partial\psi/\partial r$. We therefore have

$$\int_V |\nabla\psi|^2 = R^2 \int_0^{2\pi} \int_0^{\pi} \psi\frac{\partial\psi}{\partial r}\sin\theta d\theta d\phi \tag{3.339}$$

Because we assumed that $\psi = \mathcal{O}(1/r)$ and $\partial\psi/\partial r = \mathcal{O}(1/r^2)$ as $r \to \infty$, the RHS of this expression is of order $1/R$ and hence tends to zero when $R \to \infty$. Thus, we see that for the exterior problem

$$\int_V |\nabla\psi|^2 dV = 0, \tag{3.340}$$

and hence, arguing as in the previous section, $\psi = 0$ and hence the solution is unique. ■

Remark. *The proof extends to Neumann boundary conditions as before, and to the situation where the volume V has any finite number of inner boundaries including no inner boundary.*

Example

Solve $\nabla^2\psi = f(\mathbf{r})$ for $0 \le r < \infty$, where

$$f(\mathbf{r}) = \begin{cases} f_0, & r \le a \\ 0, & r > a \end{cases} \tag{3.341}$$

We will assume that ψ is bounded throughout the region and that ψ and $\partial\psi/\partial r \to 0$ as $r \to \infty$ in order to guarantee a unique solution. Due to symmetry consideration, we seek once again a solution with radial symmetry and so

$$\frac{1}{r^2}\frac{d}{dr}\left(r^2\frac{d\psi}{dr}\right) = f(r) \tag{3.342}$$

Integrating first for $r \leq a$, we obtain

$$\psi = \frac{1}{6}f_0 r^2 - \frac{A}{r} + B \tag{3.343}$$

as before we require $A = 0$ to ensure that the solution is finite at $r = 0$. We can then solve (3.342) for $r > a$ and we obtain

$$\psi = \frac{C}{r} + D \tag{3.344}$$

As we require $\psi \to 0$ when $r \to \infty$, we can deduce that $D = 0$. To find the remaining constants, we impose continuity of both ψ and $d\psi/dr$ at $r = a$. This gives

$$\begin{cases} f_0 a^2/6 + B = C/a \\ f_0 a/3 = -C/a^2 \end{cases} \tag{3.345}$$

Substituting for B and C, we find that the resulting solution for ψ is

$$\psi(r) = \begin{cases} f_0 r^2/6 - f_0 a^2/2, & r \leq a \\ -f_0 a^3/(3r), & r > a \end{cases} \tag{3.346}$$

This solution is shown on Fig. 3.18.

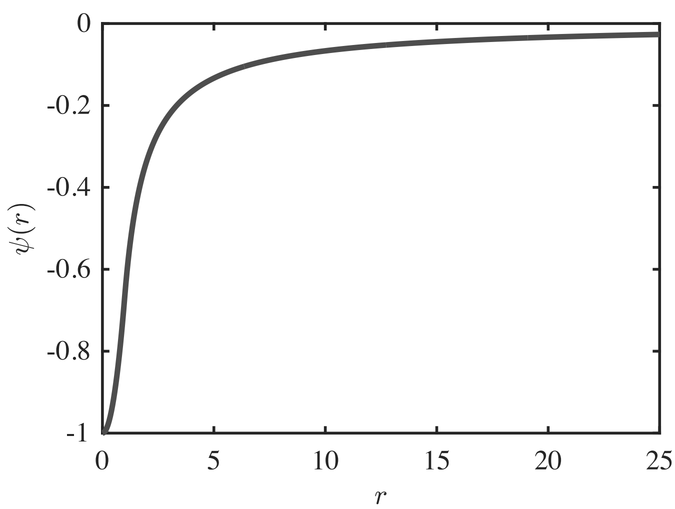

Figure 3.18 Solution to the exterior problem example.

3.5.5 Point sources and the Dirac delta function

In this section, we will consider the result obtained in the previous example in the limit where $a \to 0$. Remember that we considered the following problem

$$\nabla^2\psi = f(\mathbf{r}) \tag{3.347}$$

with $0 \le r \le \infty$, where

$$f(\mathbf{r}) = \begin{cases} f_0, & r \le a \\ 0, & r > 1 \end{cases} \tag{3.348}$$

Taking the limit $a \to 0$ implies that the function $f(r)$ becomes entirely concentrated at the origin $r = 0$. In addition, we will let $f_0 \to \infty$ in such a way that $(4/3)\pi a^3 f_0$ remains constant. We can call this constant K. In this limit, the solution we obtained above for ψ when $r > a$ becomes

$$\psi = -\frac{K}{4\pi r} \tag{3.349}$$

This function is thus solution to

$$\nabla^2\psi = f(r), \tag{3.350}$$

where the RHS is defined as

$$f(r) = \begin{cases} 0, & r \ne 0 \\ \infty, & r = 0 \end{cases} \tag{3.351}$$

Further, using the divergence theorem we can show that the volume integral of the function f over a sphere of radius R centered on the origin is equal to K; indeed, we have

$$\int_V f(r)dV = \int_V \nabla^2\psi dV = \int_V \nabla\cdot\nabla\psi dV \tag{3.352}$$

$$= \int_{r=R} \frac{\partial\psi}{\partial r} dS = \int_0^{2\pi}\int_0^{\pi} \frac{K}{4\pi R^2} R^2 \sin\theta d\theta d\phi \tag{3.353}$$

$$= K \tag{3.354}$$

The function defined by f/K is the extension of the Dirac delta function introduced previously to three dimensions. We denote it $\delta(r)$.

3.5.6 The Delta function with vector argument

We can extend the definition of the Dirac delta function to vectorial arguments. We define

$$\delta(\mathbf{r}) = 0 \quad \text{for } \mathbf{r} \ne \mathbf{0}, \tag{3.355}$$

and

$$\int_V \delta(\mathbf{r})dV = \begin{cases} 1, & \text{if } V \text{ contains the origin} \\ 0, & \text{otherwise} \end{cases} \tag{3.356}$$

Proposition 3.5.3

The solution of the Poisson equation

$$\nabla^2\psi = K\delta(\mathbf{r}) \tag{3.357}$$

is

$$\psi(\mathbf{r}) = -\frac{K}{4\pi|\mathbf{r}|} \tag{3.358}$$

Proof. First, we can easily show that $\nabla^2[-K/(4\pi|\mathbf{r}|)] = 0$ for $r \ne 0$. Indeed, the function $f : \mathbf{r} \mapsto 1/|\mathbf{r}|$ is radially symmetric, so denoting $r \equiv |\mathbf{r}|$, we have

$$\nabla^2(1/r) = 0 \tag{3.359}$$

Thus, we are only left with checking the solution for $r = 0$. To do so, we integrate both sides of (3.357) over a volume V containing $r = 0$ and get

$$\int_V \nabla^2 \psi dV = K \int_V \delta(\mathbf{r}) dV = K \tag{3.360}$$

We need to show that the LHS of this expression is indeed equal to K. Using the divergence theorem, the LHS can be rewritten as

$$\int_S \nabla\psi \cdot \hat{\mathbf{n}} dS \tag{3.361}$$

where the origin is interior to the closed surface S which bounds V. Now, we know that

$$\nabla(1/r) = -\frac{\mathbf{r}}{r^3} \tag{3.362}$$

so that the surface integral above can be rewritten as

$$\int_S \nabla\psi \cdot \hat{\mathbf{n}} dS = \frac{K}{4\pi} \int_S \frac{\mathbf{r} \cdot \hat{\mathbf{n}}}{r^3} dS \tag{3.363}$$

Using Gauss' flux theorem, one can easily show that

$$\int_S \frac{\mathbf{r} \cdot \hat{\mathbf{n}}}{r^3} dS = 4\pi \tag{3.364}$$

So, we have shown that

$$\int_V \nabla^2 \psi dV = K \tag{3.365}$$

and we have therefore verified that (3.358) is a solution to (3.357). ■

If we move the source to $\mathbf{r} = \mathbf{r}_0$ instead of the origin, then we can easily modify our analysis and show that:

Proposition 3.5.4

The solution of the Poisson equation

$$\nabla^2 \psi = K\delta(\mathbf{r} - \mathbf{r}_0) \tag{3.366}$$

is

$$\psi(\mathbf{r}) = -\frac{K}{4\pi|\mathbf{r} - \mathbf{r}_0|} \tag{3.367}$$

Finally, note that it can also be shown that the sifting property of the delta function carries over to three dimensions, i.e.

$$\int_V g(\mathbf{r})\delta(\mathbf{r} - \mathbf{r}_1) dV = g(\mathbf{r}_1) \tag{3.368}$$

for any continuous function g.

3.5.7 Green's functions

Definition 3.5.4

The Green's function $G(\mathbf{r}, \mathbf{r}_0)$ for the laplacian is defined as the solution of

$$\nabla^2 G = \delta(\mathbf{r} - \mathbf{r}_0) \tag{3.369}$$

subject to some appropriate boundary conditions.

For the three-dimensional problems we have studied, we have seen that the so-called "free-space" Green's function, i.e. the function that satisfies (3.369) and tends to zero as $r \to \infty$ is given by

$$\boxed{G(\mathbf{r}, \mathbf{r}_0) = -\frac{1}{4\pi|\mathbf{r} - \mathbf{r}_0|} = -\frac{1}{4\pi[(x - x_0)^2 + (y - y_0)^2 + (z - z_0)^2]^{1/2}}} \tag{3.370}$$

when expressed in Cartesian coordinates. In the next section, we will see that Green's functions will enable us to write down solutions to Poisson's and Laplace's equation in closed form.

3.5.8 Solutions to Poisson's equation using Green's functions

Suppose that ψ satisfies

$$\nabla^2 \psi = f(\mathbf{r}) \tag{3.371}$$

throughout some volume V. We will denote the boundary of V by the surface ∂V (Note that if the volume is unbounded, we will then assume that $\psi = \mathcal{O}(1/r)$ as $r \to \infty$, so that a unique solution is guaranteed). We suppose that the boundary condition is of Dirichlet-type, i.e.

$$\psi = p(\mathbf{r}) \quad \text{on } \partial V \tag{3.372}$$

Consider now the following associated problem for $G(\mathbf{r}, \mathbf{r}_0)$

$$\nabla^2 G = \delta(\mathbf{r} - \mathbf{r}_0) \quad \text{in } V \tag{3.373}$$

$$G = 0 \quad \text{on } \partial V \tag{3.374}$$

Applying Green's second identity to the functions ψ and G, we obtain

$$\int_V (\psi \nabla^2 G - G \nabla^2 \psi) dV = \int_{\partial V} \left(\psi \frac{\partial G}{\partial n} - G \frac{\partial \psi}{\partial n} \right) dS \tag{3.375}$$

Taking into account the boundary conditions, the RHS can be rewritten as

$$\int_{\partial V} p(\mathbf{r}) \frac{\partial G}{\partial n} dS \tag{3.376}$$

while after substituting for $\nabla^2 G$ and $\nabla^2 \psi$, the LHS reads

$$\int_V \psi(\mathbf{r}) \delta(\mathbf{r} - \mathbf{r}_0) dV - \int_V G(\mathbf{r}, \mathbf{r}_0) f(\mathbf{r}) dV \tag{3.377}$$

Using the sifting property of the Dirac delta function, we can finally write the solution ψ in the form

$$\psi(\mathbf{r}_0) = \int_V G(\mathbf{r}, \mathbf{r}_0) f(\mathbf{r}) dV + \int_{\partial V} p(\mathbf{r}) \frac{\partial G}{\partial n}(\mathbf{r}, \mathbf{r}_0) dS \tag{3.378}$$

In conclusion, if we can find the Green's function $G(\mathbf{r}, \mathbf{r}_0)$, then we can solve Poisson's equation for ψ.

Remark. *A similar approach can be taken if Poisson's equation is subject to Neumann conditions on the boundary.*

3.5.9 The method of images

We have just seen that solving Poisson's/Laplace's equation then boils down to finding the Green's function. It is often possible to determine explicitly the Green's function by so-called **method of images**. Here, we shall introduce it via the following Laplace equation example.

Suppose we wish to solve

$$\nabla^2 \psi = 0 \tag{3.379}$$

in the region $z > 0$ with the boundary condition

$$\psi(x, y, 0) = p(x, y) \tag{3.380}$$

and as usual, we will assume that $\psi = \mathcal{O}(1/r)$ as $z \to \infty$ to ensure uniqueness.

We tackle this problem by introducing the associated **Dirichlet Green's function** that satisfies the following problem

$$\nabla^2 G = \delta(\mathbf{r} - \mathbf{r}_0) \quad \text{for } z > 0 \tag{3.381}$$

$$G = 0 \quad \text{for } z = 0 \tag{3.382}$$

If the boundary condition at $z = 0$ is absent we know that the Green's function is given by

$$G(\mathbf{r}, \mathbf{r}_0) = -\frac{1}{4\pi|\mathbf{r} - \mathbf{r}_0|} \tag{3.383}$$

This solution is usually referred to as a source singularity of strength 1 situated at $\mathbf{r} = \mathbf{r}_0 = (x_0, y_0, z_0)$.

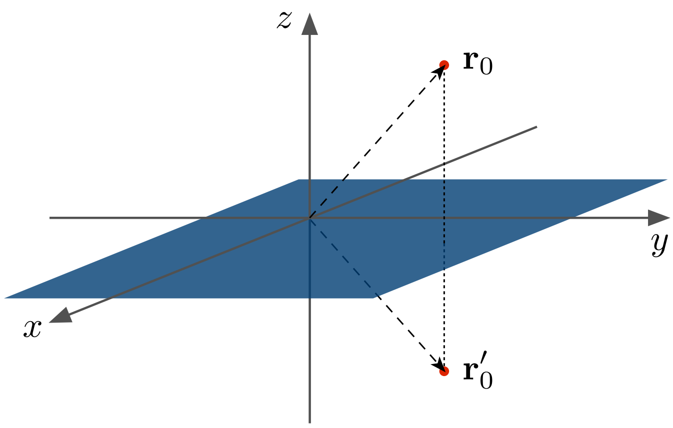

Figure 3.19 Method of images

Now we add another singularity of opposite strength at a location the same distance below the (xy)-plane, i.e. at $\mathbf{r}'_0 = (x_0, y_0, -z_0)$ — a mirror image of point $\mathbf{r}_0$ (see Figure 3.19). The modified Green's function is therefore

$$G(\mathbf{r}, \mathbf{r}_0) = -\frac{1}{4\pi|\mathbf{r} - \mathbf{r}_0|} + \frac{1}{4\pi|\mathbf{r} - \mathbf{r}'_0|} \tag{3.384}$$

When $z = 0$, we have by construction

$$|\mathbf{r} - \mathbf{r}_0| = |\mathbf{r} - \mathbf{r}'_0| \tag{3.385}$$

and so we see that $G = 0$ when $z = 0$ as required. Thus, the Green's function (3.384) satisfies both equation (3.381) and boundary condition (3.382). Now that we have explicitly determined the Green's function for this problem, we can apply the result in (3.378) with $f = 0$ to obtain the solution for ψ as

$$\psi(\mathbf{r}_0) = \int_{\partial V} p(x,y) \frac{\partial G}{\partial n}(\mathbf{r}, \mathbf{r}_0) dS \tag{3.386}$$

In this example, ∂V is the plane $z = 0$ and $\partial/\partial n = -\partial/\partial z$ (since n is the outward normal to the volume V). Using our expression for the Green's function:

$$\begin{aligned} G = -(4\pi)^{-1} \Big[&((x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2)^{-1/2} \\ &- ((x-x_0)^2 + (y-y_0)^2 + (z+z_0)^2)^{-1/2} \Big] \end{aligned} \tag{3.387}$$

we find that

$$\begin{aligned} \frac{\partial G}{\partial n} = (4\pi)^{-1} \Big[&-(z-z_0)((x-x_0)^2 + (y-y_0)^2 + (z-z_0)^2)^{-3/2} \\ &+ (z+z_0)((x-x_0)^2 + (y-y_0)^2 + (z+z_0)^2)^{-3/2} \Big] \end{aligned} \tag{3.388}$$

Evaluating this quantity at $z = 0$, we have

$$\left. \frac{\partial G}{\partial z} \right|_{z=0} = -\frac{2}{4\pi} \frac{z_0}{\left[(x-x_0)^2 + (y-y_0)^2 + z_0^2\right]^{3/2}} \tag{3.389}$$

and so the solution for ψ can be expressed in the form

$$\psi(x_0, y_0, z_0) = \frac{z_0}{2\pi} \int_{-\infty}^{+\infty} \int_{-\infty}^{+\infty} p(x,y) \left[(x-x_0)^2 + (y-y_0)^2 + z_0^2\right]^{-3/2} dx dy \tag{3.390}$$

Example

Suppose we wish to solve Laplace's equation for $z > 0$ with $\psi = p(x,y)$ on $z = 0$ where $p(x,y)$ is given explicitly by

$$p(x,y) = \begin{cases} 1, & x^2 + y^2 \leq 1 \\ 0, & x^2 + y^2 > 1 \end{cases} \tag{3.391}$$

Using the result derived above with this specific from for p:

$$\psi(x_0, y_0, z_0) = \frac{z_0}{2\pi} \int_{x^2+y^2 \leq 1} \left[(x-x_0)^2 + (y-y_0)^2 + z_0^2\right]^{-3/2} dx dy \tag{3.392}$$

$$= \frac{z_0}{2\pi} \int_0^{2\pi} \int_0^1 \left[\rho^2 + x_0^2 + y_0^2 + z_0^2 - 2x_0 \rho \cos\theta - 2y_0 \sin\theta\right]^{-3/2} \rho d\rho d\theta \tag{3.393}$$

where due to symmetry considerations, we switched to plane polar coordinates (ρ, θ). In particular, the solution along the z-axis is given by

$$\psi(0, 0, z_0) = \frac{z_0}{2\pi} \int_0^{2\pi} \int_0^1 \left(\rho^2 + z_0^2\right)^{-3/2} \rho d\rho d\theta \tag{3.394}$$

$$= -z_0 \left[(\rho^2 + z_0^2)^{-1/2} \right]_0^1 \tag{3.395}$$

$$= 1 - \frac{z_0}{\sqrt{1 + z_0^2}} \tag{3.396}$$

Remark. *Note that we can apply the method of images in a similar fashion to solve the same problem but with a Neumann condition on $z = 0$.*

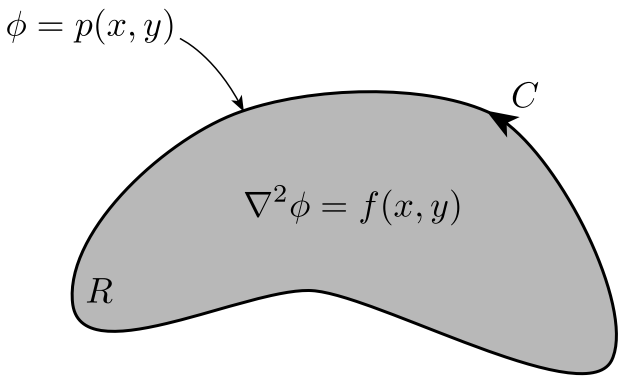

Figure 3.20 Two-dimensional Poisson Dirichlet problem

3.5.10 Poisson's equation in two dimensions

The Green's functions approach can also be used for two-dimensional problems. In this case, the Green's function has a different functional form (logarithmic). For a Dirichlet problem in which we wish to solve the following Poisson equation

$$\nabla^2\phi = f(\mathbf{r}) \tag{3.397}$$

in a region R of the (xy)-plane, with

$$\phi = p(\mathbf{r}) \tag{3.398}$$

on the boundary C of R (see Fig. 3.20)

We consider the Green's function problem

$$\nabla^2 G = \delta(\mathbf{r} - \mathbf{r}_0) \quad \text{in } R \tag{3.399}$$

$$G = 0 \quad \text{on } C \tag{3.400}$$

Applying Green's second identity in 2D, we find that

$$\phi(\mathbf{r}_0) = \int_R G(\mathbf{r}, \mathbf{r}_0) f(\mathbf{r}) dxdy + \int_C p(\mathbf{r}) \frac{\partial G}{\partial n}(\mathbf{r}, \mathbf{r}_0) ds \tag{3.401}$$

where now $\mathbf{r}_0 = (x_0, y_0)$. A similar expression can be derived for Neumann boundary conditions. By using the method of images as we did in three dimensions, Green's functions can be found explicitly for certain problems.

*[This version was compiled on **January 9, 2024**.]*