Modelling and Analysis of Continuous Real-world Problems

Colin Please

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Contents

Introduction

This course consists of 16 one-hour lectures with associated classes and runs for two weeks. The course has two main parts. The first is analytical methods for

describing continuum problems, the second is examples of mathematical modelling of practical situations where continuum models may be appropriate. This set of lecture notes supports both parts.

The course will introduce a number of key methods for studying continuum models. Each week will be focused around various real-world problems, including heat diffusion, acoustics, viscous flow and liquid crystals, to motivate relevant analytical and computational methods. Analytical methods will include well-posedness, linear stability, resonance, high frequency asymptotics, regularisation, and weakly nonlinear theory. There are exercises sheets to work through during each week and assessment will be a challenge centred around real-world problems. We assume that the 2 week introductory session has covered basic modelling skills, dimensional analysis, basic Matlab. Each week we start by discussing how to derive mathematical models for particular types of real world problems. We then use these models as a vehicle to demonstrate the relevant analytical methods. At the end of each week, you should have the complete set of tools needed to set up, analyse and solve a class of mathematical models.

Outline of course:

Diffusion problems
Modelling problems: heat flow, diffusion, chemical reactions, pattern formation, thermal runaway.
Analytical methods: conservation laws, heat equation, well-posedness, separation of variables, transforms, nonlinear equilibria, linear stability.

Linear waves
Modelling problems: elastic waves, acoustics, Stokes waves, electromagnetism, optics.
Analytical methods: characteristics, separation of variables, eigenvalue problems, resonance, high-frequency asymptotics.

Nonlinear waves
Modelling problems: traffic, river flow, porous-medium flow, two-phase flow.
Analytical methods: characteristics, shocks, causality, regularisation, weakly nonlinear theory.

Energy minimisation
Modelling problems: capillary statics, elasticity, buckling, liquid crystals, image analysis Analytical methods: calculus of variations, bifurcations, weakly nonlinear analysis

1 Diffusion problems

Physical problems that can be described by a diffusion type equation are many and varied. These include heat flow in a solid, movement of populations across a surface, transport of a chemical species in a gas all of which have some underlying random walk phenomena. However, equations of this type can also arise from different physics such as spreading viscous films. In this section we will give a derivation of the underlying equation, give some of its properties, identify various methods of solution. We then explore behaviour of solutions to systems of such equations and to special nonlinear problems.

1.1 The heat equation and separation of variables

1.1.1 Derivation of the equation

We start by considering the flow of heat through a solid material in which a chemical reaction is creating heat. Such a situation might arise in a large pile of sawdust where the heat is generated by slow oxidation of the wood. We will derive a simple model of this behaviour. We derive the underlying equation in two ways to illustrate possible approaches, one that considers an infinitesimal region of the sawdust pile and the other that considers an arbitrary region.

In the simplest case consider a single spatial dimension, x (measured in m), and with time t (measured in s). The temperature, which we seek to find, is then $T(x,t)$ (measured in K) and the flux of heat, which we also seek, is $q(x,t)$ (measured in $J/m^2/s$). We also presume that heat is generated by the chemical reaction that creates heat at a rate given by $f(x,t,T)$ (measured in $J/m^3/s$). The total heat per unit volume, or enthalpy, at any point in the pile is defined to be

$$H(T) = \int_0^T \rho c_p(T)\, dT$$

where ρ (measured in kg/m^3) is the density of the sawdust and $c_p(T)$ (measured in $J/kg/K$ is the specific heat at constant pressure of the sawdust. Note that typically ρ is nearly constant, and $c_p(T)$ is constant over large ranges of temperature but can varying dramatically near temperatures where there are changes in phase of a material.

To derive the governing equation we need to first consider conservation of heat in a very small region extending from x to $x+\Delta x$. The total heat per crossectional

area in this region is then

$$\int_x^{x+\Delta x} H(T)\, dx\ .$$

The balance equation is then derived by requiring that the change in this total heat can only be due either to flow of heat into the region from either boundary of the region or by generation of heat within the region. This gives us

$$\frac{\partial}{\partial t}\left(\int_x^{x+\Delta x} H(T)\, dx\right) = q(x+\Delta x,t) - q(x,t) + \int_x^{x+\Delta x} f(x,t,T)\, dx$$

Change in heat with time = heat in from left - heat out to right + heat generated

Using the definition of H this gives us

$$\frac{\partial T}{\partial t}\left(\int_x^{x+\Delta x} \rho c_p(T(x,t))\, dx\right) = q(x,t) - q(x+\Delta x,t) + \int_x^{x+\Delta x} f(x,t,T)\, dx$$

To complete the derivation we now take the limit $\Delta x \to 0$. In doing this we make the assumption that both $c_p(T(x,t))$ and $f(x,t)$ are continuous so that

$$\frac{\partial T}{\partial t}\Delta x \rho c_p(T(x,t)) = q(x,t) - q(x+\Delta x,t) + \Delta x f(x,t,T)$$

and then assume that $q(x,t)$ is differentiable so that

$$\rho c_p(T(x,t))\frac{\partial T}{\partial t} = -\frac{\partial q(x,t)}{\partial x} + f(x,t,T)$$

This is the equation of conservation of heat and is central to all such modelling. Note the assumptions of continuity and differentiability are not trivial aspects and there are many common situations where these may not be valid (eg models of melting ice) and great care must then be taken.

To complete the model of the temperature movement within the sawdust pile we need to add an equation that determines $q(x,t)$. To make the model simple we first note that the sawdust is not moving and also will use an empirical law that states that heat travels from hot regions to cold regions. Specifically we write

$$q(x,t) = -k\frac{\partial T}{\partial x}$$

where k (measured in $J/s/m/K$) is the thermal diffusivity of the sawdust. This empirical law is called "Fick's law" and there are similar laws for other physical situations. In practice k may depend on: x due to inhomogeneities in the sawdust pile; t due to changes in the pile structure over time; and T due changes in transport

mechanisms such as radiation at high temperatures. Hence we have that the temperature within the sawdust pile is governed by

$$\rho c_p \frac{\partial T}{\partial t} = \frac{\partial}{\partial x}\left(k\frac{\partial T}{\partial x}\right) + f(x,t,T)$$

In the simplest case where the density, the specific heat and the diffusivity can adequately be assumed to be constant and no heat is generated this gives the classical diffusion equation

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial^2 T}{\partial x^2}$$

where $\kappa = k/\rho/c_p$ (measured in m^2/s) is the thermal diffusivity.

The mathematical problem is finally completed by specifying the region in which the problem is to be solved, imposing conditions at the boundary of this region which describe the interaction of the system with the outside world and what the temperature in the region is initially. Hence for example the sawdust pile may be taken to extend from $x-0$ to $x = L$ with both of these surfaces held at a constant, due to surrounding air, with $T(0,t) = T_a$ and $T(L,t) = T_a$. In addition we will assume that the sawdust pile was put in place at some time $t - 0$ and that it was at a spatially uniform temperature then $T(x,0) = T_0$.

An alternative derivation of the diffusion equation is to consider an arbitrary fixed region V of the sawdust pile where the outer surface of this region is denoted by ∂V. We consider the three dimension problem with the spatial variable $\mathbf{x}$, and introduce $\mathbf{q}(\mathbf{x},\mathbf{t})$ as a vector quantity describing the flux of heat. Conservation of heat then requires

$$\frac{\partial}{\partial t}\iiint_V H(T)\, dV = \iint_{\partial V} -\mathbf{q}\cdot d\mathbf{S} + \iiint_V f(\mathbf{x},t,T)\, dV$$

where $d\mathbf{S}$ is a surface area vector pointing out of V. Using the previous definition of $H(T)$ and making assumptions about continuity of H and f and differentiability of $\mathbf{q}$ we can now exploit the divergence theorem to find that

$$\iiint_V \rho c_p \frac{\partial T}{\partial t}\, dV = \iiint_V -\nabla\cdot\mathbf{q}\, dV + \iiint_V f(\mathbf{x},t,T)\, dV\ .$$

Since this holds for all possible V it follows that

$$\rho c_p \frac{\partial T}{\partial t} = -\nabla\cdot\mathbf{q} + f(\mathbf{x},t,T)\ .$$

To this we then add Fick's law that

$$\mathbf{q} = -k\nabla T$$

and this gives the three dimensional heat diffusion equation

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + f(\mathbf{x}, t, T) \ .$$

A condition then needs to be given at all points of the outer surface of the sawdust pile to describe the interaction with the outside world and a condition to describe the temperature distribution at some initial time.

1.1.2 Chemical reactions

When modelling chemical reactions it is common to consider the various species to be dilute in a fluid or gas. A good example of such a dilute system is the movement and reaction of oxygen and a fuel in air. Here these species are in relatively small concentrations compared to nitrogen which is dominant and in this case nonreacting. For dilute gases the species can be taken to have concentration $c_i(\mathbf{x}, t)$ for various i and a simple model of their movement is to take the underlying dominant gas to move with velocity $\mathbf{v}$ and for the species to diffusive relative to this gas. Hence the flux of each species is given by

$$\mathbf{q}_i = \mathbf{v} c_i + D_i \nabla c_i$$

where D_i is the diffusivity of that species in the dominant background gas. If there are no reactions the governing equation for each species comes from considering conservation of that species and is

$$\frac{\partial c_i}{\partial t} + \nabla \cdot (c_i \mathbf{v}) = \nabla \cdot (D_i \nabla c_i) \ .$$

If there are reactions in the bulk of the fluid, as opposed to reactions at a surface, then these can be included by a source term. If the reaction is

$$c_1 + c_2 \leftrightharpoons c_3$$

then typically the reaction rate depends on the local concentration of the species and the local temperature. For a simple reaction this might be modelled using a simple probability argument so that the forward reaction would depend linearly on concentrations c_1 and on c_2, while the reverse reaction would be proportional to the concentration of c_3. For more complex reaction, where there are intermediate species that are not modelled, the effective reaction rates are usually made proportional to some power of the various species. The reaction rate is typically highly dependent on the temperature and a common model is to use a Arrhenius form for this dependence. The reactions may also release or absorb heat as they

progress and hence may alter the temperature. Hence a model of the reaction above might take the form

$$\frac{\partial c_1}{\partial t} + \nabla \cdot c_1 \mathbf{v} = \nabla \cdot (D_1 \nabla c_1) - k_1 c_1 c_2 e^{-E_1/(RT)} + k_2 c_3 e^{-E_2/(RT)} \ .$$

$$\frac{\partial c_2}{\partial t} + \nabla \cdot c_2 \mathbf{v} = \nabla \cdot (D_2 \nabla c_2) - 2k_1 c_1 c_2 e^{-E_1/(RT)} + 2k_2 c_3 e^{-E_2/(RT)}$$

$$\frac{\partial c_3}{\partial t} + \nabla \cdot c_3 \mathbf{v} = \nabla \cdot (D_3 \nabla c_3) + k_1 c_1 c_2 e^{-E_1/(RT)} - k_2 c_3 e^{-E_2/(RT)}$$

$$\rho c_p \left(\frac{\partial T}{\partial t} + \nabla \cdot T \mathbf{v} \right) = \nabla \cdot (k \nabla T) + \Delta H_1 \left(k_1 c_1 c_2 e^{-E_1/(RT)} + k_2 c_3 e^{-E_2/(RT)} \right) \ .$$

where the constants E_1 and E_2 are the activation energies of the forward and reverse reactions, k_1 and k_2 are prefactors of the reaction rates and, ΔH_1 is the heat of the reaction. Such a model requires initial data for all the species and the temperature and one boundary condition on each boundary for each of the dependent variables.

Some common approximations to simplify this model are:

1) No flow of the dominant gas ($\mathbf{v} \approx 0$), no heat of reaction ($\Delta H_1 \approx 0$), and all chemical species diffuse at the same rate ($D_1 = D_2 = D_3$, the "Lewis number" is unity). Here there is no need to solve for the temperature and the equation for the third chemical species can be replaced by an equations for the variable $C = c_1 + c_3$ (or some other appropriate combination of species) which is given by

$$\frac{\partial C}{\partial t} = \nabla \cdot (D_3 \nabla C)$$

(note the lack of a source term). This can then be solved and subsequently the other species solved for. For the simplest case where the boundary conditions are such that C is a constant the nondimensional problem is then

$$\frac{\partial c_1}{\partial t} = \nabla^2 c_1 - \alpha c_1 c_2 e^{E_1/(RT)} + \beta(1 - c_1)$$

$$\frac{\partial c_2}{\partial t} = \nabla^2 c_2 - 2\alpha c_1 c_2 e^{E_1/(RT)} + 2\beta(1 - c_1)$$

which is pair of diffusion equations coupled by a nonlinear source term (in this case it may also be possible to further simplify the problem by considering the variable $(c_1 - c_2)$ and, if the boundary conditions for this quantity are constant, then the entire dynamics is governed by a single diffusion equation. Similar problems appear in many situations such as population dynamics.

2) No flow of the dominant gas ($\mathbf{v} \approx 0$), no reverse reaction ($k_2 = 0$) large concentrations of the two reacting species so we can take c_1, c_2 both as constants. The problem is then simply one of finding the temperature which is governed by the single equation

$$\rho c_p \frac{\partial T}{\partial t} = \nabla \cdot (k \nabla T) + \Delta H_1 k_1 c_1 c_2 e^{-E_1/(RT)} \ .$$

The nondimensional version of this equation is:

$$\frac{\partial T}{\partial t} = \nabla^2 T + \nu e^{-\gamma/T} \ .$$

This nonlinear diffusion equation is commonly approximated because the main issue is about how the temperature moves from its initial condition (such as modelling ignition of a reaction). Typically γ is a relatively large number and we take the initial temperature to be $T = 1$. we scale the problem with $T = 1 + \hat{T}/\gamma$ so that

$$\frac{\partial \hat{T}}{\partial t} = \nabla^2 \hat{T} + \gamma \nu e^{-\gamma/(1+\hat{T}/\gamma)} \ .$$

We now expand the function in the exponential, in the limit $\gamma \to \infty$, assuming that $\hat{T} = \mathcal{O}(1)$ so that

$$\frac{\gamma}{(1 + \hat{T}/\gamma)} \sim \gamma(1 - \hat{T}/\gamma + (\hat{T}/\gamma)^2 + \ldots) \sim \gamma - \hat{T} + \ldots$$

The approximate equation is therefore

$$\frac{\partial \hat{T}}{\partial t} = \nabla^2 \hat{T} + \lambda \nu e^{\hat{T}}$$

where $\lambda = \nu\gamma \exp(\gamma)$. This simple model is used to explore ignition phenomena and shows that the temperature dependence of the reaction rate can be approximated, at least in the early stages of a reaction, by a simple exponential.

1.1.3 Separation of variables

We will consider a method for solving the diffusion equation that can be used in simple cases. Specifically we will look at the case of no heat generation, where ρ, c_p and k are constants, the boundary conditions are linear, and the geometry of the region is particularly simple. The method can be extended in some cases and these are left as exercises.

The main idea of separation of variables is to seek a solution that is a linear sum of functions of a separated form. Hence if we look for solutions $u(x,t)$ to the PDE

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

we seek them in the form of a sum of solutions of the type

$$u(x,t) = X(x)T(t). \tag{1.1}$$

Furthermore we need the region for the solution to be bounded by surfaces each defined by one of the independent variables being constant (for Cartesian coordinates this requires regions with boundaries that are stationary eg ($x = a$, $x = b$). In higher dimensions Cartesian coordinates can be used for rectangular region while different coordinate systems eg cylindrical or spherical regions can be used for rods and balls). Note that there are problems where other special geometries allow separation of variables (such as a wedge when studying small water waves) but these are not encountered very often. Finally the boundary conditions must be linear and homogeneous (if there are forcing terms at the boundaries then these need to be removed by finding a suitable particular integral for the problem. Typically this is done by seeking a steady state solution, independent of t, that satisfies the boundary conditions). For the case here we take

$$u(0,t) = 0 \qquad \text{and} \qquad u(L,t) = 0$$

with initial conditions

$$u(x,t) = g(x)\ .$$

Putting the assumed form (1.1) for the solution into the equation gives us

$$X\frac{dT}{dt} = \kappa \frac{d^2X}{dx^2}T$$

and we can then separate this equation to find that

$$\frac{1}{\kappa}\frac{dT}{dt}\frac{1}{T} = \frac{d^2X}{dx^2}\frac{1}{X}$$

and since each side of this equation is a function of only one independent variable the two sides much be constant. Hence we write

$$\frac{1}{\kappa}\frac{dT}{dt}\frac{1}{T} = \frac{d^2X}{dx^2}\frac{1}{X} = \nu\ .$$

where ν is any constant. This gives us two ODE's for the functions $T(t)$ and $X(x)$ which in this simple case are

$$\frac{dT}{dt} - \nu\kappa T = 0 \qquad \text{and} \qquad \frac{d^2X}{dx^2} - \nu X = 0\ . \tag{1.2}$$

For the boundary conditions to hold we require

$$X(0)T(t) = 0 \qquad \text{and } X(L)T(t) = 0$$

and since we need $T(t) \not\equiv 0$ in order to avoid the trivial solution $u \equiv 0$ we require

$$X(0) = 0 \qquad \text{and } X(L) = 0.$$

This then creates an eigenvalue of problem for $X(x)$ where there are a set of eigenvalues ν_j, $j = 1, 2, \ldots$ for which there exists eigensolutions $X_j(x)$. In this case we find

$$X_j(x) = \sin\left(x\sqrt{-\nu_j}\right) \qquad \text{where} \qquad \nu_j = -(j\pi/L)^2 \qquad j = 1, 2, 3, \ldots$$

Solving (1.2) for $T(t)$ we find that we can write

$$u(x,t) = \sum_{j=1}^{\infty} A_j \sin\left(2j\pi x/L\right) \exp(-(j\pi/L)^2\kappa t)$$

where the A_j are constants still to be found. The final step is to satisfy the initial condition and here we find this requires

$$g(x) = \sum_{j=1}^{\infty} A_j \sin\left(2j\pi x/L\right)$$

Because of orthogonality conditions satisfied by trigonometric functions this can be solved using the usual Fourier series methods to find that the coefficients are given by

$$A_n = \frac{2}{L}\int_0^L g(x) \sin\left(n\pi x/L\right)\ dx$$

The method outlined above can be used in other coordinate systems, for different linear boundary conditions and in each case there is a linear ODE eigenvalue problem to be solved that may require some numerical approaches in order to find solutions.

Note that this method gives the solution as a infinite sum of eigenfunctions. In many cases these are difficult to find, particularly if they need calculating numerically and so the series is truncated, sometimes to include just the first term! Such approximations can be very useful, for example, since the first term dominates as t get large due to the exponential decay of the $T(t)$ functions,

1.1.4 Particular coordinate systems

Note it is often useful to exploit some geometric symmetry of a problem to reduce the number of dimensions that need to be analysed or to easily define a particular boundary. Two common examples are cylindrical polar coordinates and spherical polar coordinates where radial symmetry might be able to be exploited. Note that in these cases

Cylindrical polar coordinates (r, θ, z)

$$\nabla^2 T = \frac{1}{r}\frac{\partial}{\partial r}\left(r\frac{\partial T}{\partial r}\right) + \frac{1}{r^2}\frac{\partial^2 T}{\partial \theta^2} + \frac{\partial^2 T}{\partial z^2}$$

and separation of variables in this coordinate system requires analysis of various Bessel functions. Useful for modelling wires, cables, pipes etc.

Spherical polar coordinates (r, θ, ϕ) (beware there are different similar confusing notations used for these coordinates - here $x = r\cos\phi\sin\theta$, $y = r\sin\phi\sin\theta$, $z = r\cos\theta$ so that θ is the polar angle $0 \le \theta \le \pi$, and ϕ is the azimuthal angle $0 \le \phi \le 2\pi$)

$$\nabla^2 T = \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial T}{\partial r}\right) + \frac{1}{r^2\sin\theta}\frac{\partial}{\partial \theta}\left(\sin\theta\frac{\partial T}{\partial \theta}\right) + \frac{1}{r^2\sin^2\theta}\frac{\partial^2 T}{\partial \phi^2}$$

and separation of variables in this coordinate system requires analysis of various Legendre functions. Useful for modelling bubbles, droplet, particles, the "spherical cow", etc.

Note there are just 11 different coordinate systems in which the three dimensional operator Laplace operator is separable. Cartesian, cylindrical and spherical are the most common but occasionally others can be useful eg: prolate or oblate spherical coordinates.

1.2 Properties of the heat equation and solution methods

1.2.1 Maximum principle

A very powerful property of diffusion problems can be found by considering the heat diffusion equation with constant coefficients and no heat generation, in a finite region, with given initial temperature and given temperature along the boundary ie.

$$\frac{\partial u}{\partial t} = \kappa\frac{\partial^2 u}{\partial x^2} \qquad \text{for } t \ge 0, \quad 0 \le x \le L$$

with $u(0,t) = u_r(t)$, $u(L,t) = u_L(t)$, $u(x,0) = u_0(x)$. We then find that if we consider the solution $u(x,\tau)$ at a time $\tau \geq 0$ then this solution is bounded by the maximum value that occurred either initially or on either the boundary in the interval $0 \leq t \leq \tau$. Similarly the minimum of $u(x,\tau)$ is also bounded by the minimum initially or on the boundary. Specifically

$$u_{min}(\tau) \leq u(x,\tau) \leq u_{max}(\tau) \qquad \text{for } \tau \geq 0 \text{ and } 0 \leq x \leq L$$

where

$$u_{max} = \max\left\{ \max_{0\leq x\leq L} u_0(x),\ \max_{0\leq t\leq \tau} u_r(t),\ \max_{0\leq t\leq \tau} u_L(t) \right\}$$

$$u_{min} = \min\left\{ \min_{0\leq x\leq L} u_0(x),\ \min_{0\leq t\leq \tau} u_r(t),\ \min_{0\leq t\leq \tau} u_L(t) \right\}.$$

This property can be extended readily to multiple spatial dimensions and to more general diffusion problems and is a useful tool in determining bounds on the solution. Note that the idea also extends to the steady problem where the solution of the steady state heat equation is then bounded by the values of the function on the surface (this is a well known property of Laplace's equation).

Note that one immediate consequence of the maximum principle is that the solution to the heat equation is unique. We can show this by contradiction by considering that there are two different two solutions for $u(x,t)$ given by $U(x,t)$ and $W(x,t)$. Since each of these satisfies the problem it follows that the problem for $U(x,t) - W(x,t)$ is

$$\frac{\partial(U-W)}{\partial t} = \kappa \frac{\partial^2(U-W)}{\partial x^2} \qquad \text{for} t \geq 0, \quad 0 \leq x \leq L$$

with $U(0,t) - W(0,t) = 0$, $U(L,t) - W(L,t) = 0$, $U(x,0) - W(x,0) = 0$. By the maximum principle it follows that $0 \leq U(x,\tau) - W(x,\tau) \leq 0$ for $\tau \geq 0$ so the two functions are identical and the solution $u(x,t)$ is therefore unique.

1.2.2 Wellposedness

In studying PDE problems we are interested in determining if the problem is "well-posed" since we would hope that a model of a physical problem should sufficiently well defined for the behaviour of the solution to represent the behaviour of the physical system. Hence we explore whether the PDE problem (the PDE and its associated region of solution and the specified boundary and initial conditions) is well posed. One common assessment of wellposedness is consider it in the sense of Hadamard and to ask the following the three questions

- Does a solution to the problem exist?
- Is a solution unique?
- Does the solution depend continuously on the problem data (the initial data, the boundary conditions and any forcing terms)?

The previous section showed one method for determining uniqueness an alternative method of showing the function $\phi(x,t) = U(x,t) - W(x,t)$ must be zero, and hence the solution $u(x,t)$ is unique is to use an energy method. Multiplying the PDE for ϕ by ϕ and integrating over the region $0 \leq x \leq L$ gives, after integrating by parts and using the boundary conditions,

$$\frac{\partial}{\partial t}\left(\int_0^L (\phi(x,t))^2 dx\right) = -2\kappa \int_0^L \left(\frac{\partial \phi(x,t)}{\partial x}\right)^2 dx \; . \tag{1.3}$$

Since $\int (\phi(x,0))^2 dx$is obviously non-negative and (1.3) implies that it is nonincreasing we can use the initial data

$$\int_0^L (\phi(x,0))^2 dx = 0$$

to conclude that

$$\int_0^L (\phi(x,t))^2 dx = 0 \; .$$

This then shows how the L_2 norm of the function is a natural measure in assessing how close two functions are in this case. The method of separation of variables or other steps can be use to demonstrate a solution exists.

The final "wellposedness" question is commonly answered using the L_2 norm to measure how sensitive the solution is to the problem data. One simple method of assessment valid for linear equations is to consider a Fourier representation of the solution. Hence solving in the region $0 \leq x \leq L$ take

$$u(x,t) = \sum_{k=-\infty}^{k=+\infty} e^{i2\pi kx/L} u_k(t)$$

Here k is the wave number and indicates one mode of the spatial distribution of the solution. Putting this into the PDE and using the fact that the Fourier modes, $\exp(i2\pi kx/L)$, are linearly independent then this indicates that the solution can be written in the form

$$u(x,t) = \sum_{k=-\infty}^{k=+\infty} A_k e^{i2\pi kx/L} e^{i\omega t}$$

where ω must be related to k by

$$i\omega = \kappa(2\pi ik/L)^2 \qquad \rightarrow \qquad \omega = -i(2\pi/L)^2k^2 \; . \tag{1.4}$$

and the constants A_k can be determined by initial data. This relation (1.4) between ω and k is called the "dispersion relation" of the PDE. In this case it shows that all the Fourier modes of the solution will decay as time increases (taking k to be real the imaginary part of ω is negative) except the mode $k = 0$ which will remain constant in time. Because modes decay the PDE is called dissipative and we can conclude that small changes to the initial data will result in small (decaying) changes in the solution. Hence this Fourier analysis indicates that the heat diffusion PDE is well posed (note that this method only considers wellposedness due to initial data and makes no statement about the wellposedness of the boundary conditions). Note a problem is not well posed (ie it is illposed) if there are Fourier modes that grow with time (ie the imaginary part of ω is positive for some real value of k). A PDE which has the imaginary part of ω equal to zero for all k is called conservative.

The energy method can also be use to determine the sensitivity of the solution to the problem data. The ODE (1.3) for the L_2 norm of ϕ shows that if the initial value of the solution is changed by a small amount (as measured by it L_2 norm) then the later solution will also have a small change. Similarly the method can account for different boundary conditions and assess their effect on the wellposedness.

When considering the heat diffusion problem on an infinite spatial region it is necessary to impose conditions at infinity to ensure the solution exists and is unique. In particular a condition that ensures grow is less than $\exp x^2$ is typically sufficient and unfortunately seldom indicated in many practical problems, so care should be taken.

1.3 Fourier and Laplace transforms

A useful method for studying the solution behaviour of the heat equation is to solve the problem using a transform. This method is typically used because it can transform the problem from a partial differential equation in two dimensions to a differential equation in one dimension with the other dimension acting purely algebraically. This resulting transformed problem can hopefully then be solved using ODE methods. The main difficulty in the method usually arises in reversing the transform process to find the solution. In some cases this can be done but in many cases some approximation can be made such as finding what the solution does at a particular special point, as a function of time, or to find what the solution does after a long or short time. Note here we only briefly discuss Fourier and Laplace

transforms but there are many related transforms which can be exploited effectively, for example, when using other coordinate systems (eg Hankel transforms for cylinders, Mellin transforms for spheres, etc.)

1.3.1 Laplace Transforms

The Laplace transform of a function $f(t)$ is defined by

$$\bar{f}(p) = \int_0^\infty f(t)e^{-pt}dt.$$

Note that

- the over-bar does **not** indicate complex conjugate;
- a convenient notation is to write $\bar{f} = \mathcal{L}[f]$;
- we shall often allow p to be complex and then be interested in where $\bar{f}$ is defined in $\mathbb{C}$;
- if $|f(t)| \leq Me^{ct}$ for some positive M, c then the integral is defined at least for some p (in fact for all complex p with $Re(p) > c$); such f is said to have *exponential growth* and examples of such f are any polynomial in t, or any exponential but not e.g. e^{t^2}.

A short standard list of Laplace transforms

The following is a list of standard Laplace transforms, with corresponding domain of definition:

	$f(t)$	$\bar{f}(p)$	Domain of definition
1.	1	$\frac{1}{p}$	$Re(p) > 0$
2.	t	$\frac{1}{p^2}$	$Re(p) > 0$
3.	t^n	$\frac{n!}{p^{n+1}}$	$Re(p) > 0$
4.	$e^{at},\ a \in \mathbb{C}$	$\frac{1}{p-a}$	$Re(p) > Re(a)$
5.	$\sin \omega t$	$\frac{\omega}{p^2+\omega^2}$	$Re(p) > 0$
6.	$\cos \omega t$	$\frac{p}{p^2+\omega^2}$	$Re(p) > 0$
7.	$\sinh at$	$\frac{a}{p^2-a^2}$	$Re(p) > \|a\|$
8.	$\cosh at$	$\frac{p}{p^2-a^2}$	$Re(p) > \|a\|$

Properties of the Laplace transform

1. Linearity: $\mathcal{L}[\lambda f + \mu g] = \lambda\mathcal{L}[f] + \mu\mathcal{L}[g]$, for $\lambda, \mu \in \mathbb{C}$;
2. If $g(t) = e^{at}f(t)$, then $\bar{g}(p) = \bar{f}(p-a)$;
3. If $g(t) = f'(t)$, then $\bar{g}(p) = p\bar{f}(p) - f(0)$;
4. If $g(t) = \int_0^t f(s)\,ds$, then $\bar{g}(p) = \frac{\bar{f}(p)}{p}$;
5. Define the *convolution* $f * g$ of f and g by $f * g(t) = \int_0^t f(t-s)g(s)ds$, then $\mathcal{L}[f * g] = \mathcal{L}[f]\mathcal{L}[g]$ or $\overline{f * g} = \overline{f}\ \overline{g}$;
6. If $g(t) = tf(t)$, then $\bar{g}(p) = -\frac{d}{dp}\bar{f}(p)$.

It is worth outlining why property 5 is valid. Starting from the definition of convolution

$$\mathcal{L}[f * g] = \int_0^\infty \int_0^t f(t-s)g(s)\ ds\ e^{-pt}\ dt$$

and changing the order of integration gives

$$= \int_0^\infty \int_s^\infty f(t-s)g(s)e^{-pt}\ dtds.$$

Then making a change variable from t to $u = t - s$ gives

$$= \int_0^\infty \int_0^\infty f(u)g(s)e^{-ps}e^{-pu}\ duds$$

$$= \bar{f}(p)\bar{g}(p) = \mathcal{L}[f]\mathcal{L}[g].$$

The convolution operator appears in many practical situations and when such problems are linear the use of Laplace transforms may enable solutions to be found.

Note property 3 allows us to take Laplace transforms of higher derivatives such as

$$\text{If } g(t) = f''(t) \quad \text{ then } \quad \bar{g}(p) = p^2\bar{f}(p) - pf(0) - f'(0)$$

Example
Solve the IVP

$$x'' - 3x' + 2x = 4e^{2t}; \quad x(0) = -3; \quad x'(0) = 5.$$

Taking Laplace transforms of the ODE using the conditions

$$(p^2\bar{x} + 3p - 5) - 3(p\bar{x} + 3) + 2\bar{x} = \frac{4}{p-2}$$

where the RHS comes from the standard list; so

$$\bar{x}(p^2 - 3p + 2) = \frac{4}{p-2} - 3p + 14 = \frac{-3p^2 + 20p - 24}{p-2}$$

which can be solved algebraically for $\bar{x}$ as

$$\bar{x} = \frac{-3p^2 + 20p - 24}{(p-1)(p-2)^2}.$$

To invert this transform use partial fractions (split into fractions)

$$= \frac{-7}{p-1} + \frac{4}{p-2} + \frac{4}{(p-2)^2},$$

and use the standard list to give

$$x = -7e^t + 4e^{2t} + 4te^{2t}$$

where the last term needs $\mathcal{L}[e^{2t}] = \frac{1}{p-2}$, so $\frac{1}{(p-2)^2} = -\frac{d}{dp}\mathcal{L}[e^{2t}] = \mathcal{L}[te^{2t}]$ by property 6.

1.3.2 The Fourier Transform

Much of the study of this transform can proceed by analogy with the previous. First the definition of the Fourier transform of $f(t)$ is

$$f(t) \to \hat{f}(\omega) = \int_{-\infty}^{\infty} e^{-i\omega t} f(t) dt.$$

Then note

- existence needs only $\int_{-\infty}^{\infty} |f(t)| dt < \infty$
- $\hat{f}$ is complex from the start, so we may as well take $f \in \mathbb{C}$ (for f real, $\hat{f}(-\omega) = \bar{\hat{f}}$;
- some authors include a factor $\frac{1}{\sqrt{2\pi}}$ in the definition;
- we shall write $\hat{f} = \mathcal{F}[f]$.

Properties of the Fourier Transform

1. linearity:
$$\mathcal{F}[\lambda f + \mu g] = \lambda \mathcal{F}[f] + \mu \mathcal{F}[g]$$
2. if $g(t) = f'(t)$, then $\hat{g}(\omega) = i\omega \hat{f}(\omega)$ (so no "$f(0)$" as compared to the Laplace transform);
3. $$\mathcal{F}[f * g] = \mathcal{F}[f]\mathcal{F}[g]$$
with the definition $f*g(t) = \int_{-\infty}^{\infty} f(t-s)g(s)ds$ (this definition of convolution agrees with the earlier one if $f = g = 0$ for $t < 0$, but otherwise is different.)

Inversion of the Fourier Transform

This is given by the *Inversion Formula*:

$$\frac{1}{2}[f(t_-) + f(t_+)] = \frac{1}{2\pi} \lim_{R\to\infty} \int_{-R}^{R} e^{i\omega t} \hat{f}(\omega) d\omega \tag{1.5}$$

where the expression on the left is the average of the limits of f approaching t from above and below. If f is continuous at t this is just $f(t)$.

Note that if the factor of $1/\sqrt{2\pi}$ is used in the definition of the Fourier transform the inversion transform appears more symmetric.

Example

Invert
$$\hat{f} = \frac{2}{1+w^2}.$$
The Inversion Formula (1.5) gives
$$f(t) = \frac{1}{2\pi} \lim_{R\to\infty} \int_{-R}^{R} \frac{2e^{i\omega t}}{1+\omega^2} d\omega$$
which we shall evaluate by closing the contour with a semi-circle of radius R centred at the origin. If $t > 0$ we choose the semi-circle in the upper-half-plane, and conversely if $t < 0$ we take it in the lower-half-plane. Call these contours C_+ and C_- respectively. Poles of the integrand are only at $\pm i$ so for positive t, Cauchy's integral formula gives:
$$\int_{C_+} \frac{e^{i\omega t}}{1+\omega^2} d\omega = 2\pi i \times \frac{1}{2i} e^{-t} = \pi e^{-t},$$
while if $t < 0$, we obtain
$$\int_{C_-} = -2\pi i \times (-\frac{1}{2i} e^{t}) = \pi e^{t},$$

the extra minus sign coming from the fact that the contour is traversed clockwise. Putting these together we obtain $f(t) = e^{-|t|}$.

Inversion of Laplace Transform From (1.5), we can obtain an inversion formula for the Laplace transform as follows:

$$\frac{1}{2}(f(t_-) + f(t_+)) = \frac{1}{2\pi i} \lim_{R\to\infty} \int_{\gamma-iR}^{\gamma+iR} e^{pt} \bar{f}(p) dp \tag{1.6}$$

where γ is chosen as follows: if $|f(t)| \leq Me^{ct}$ then $\gamma > c$. This means that the line along which the integration is carried out is to the right of any singularities of $\bar{f}$. As before, if f is continuous at t then (1.6) gives $f(t)$.

When it comes to examples, we often evaluate the integral by closing the contour to the left.

1.3.3 Examples

(a) Invert

$$\bar{f}(p) = \frac{1}{p^2(p-1)}.$$

This example can be done by partial fractions and the standard list, but we shall use the Inversion Formula. Poles of $\bar{f}$ are at 0 and 1 so we need $\gamma > 1$, and we shall close the contour to the left, with an arc of a circle centred at the origin. Write Γ_1 for the straight part of the contour, Γ_2 for the curved arc and Γ for the union. By (1.6), at points of continuity of f,

$$f(t) = \frac{1}{2\pi i} \lim_{R\to\infty} \int_{\Gamma_1} e^{pt} \frac{dp}{p^2(p-1)}$$

and we claim that, as $R \to \infty$

$$\int_{\Gamma_2} e^{pt} \frac{dp}{p^2(p-1)} \to 0,$$

so consider

$$\oint_{\Gamma} e^{pt} \frac{dp}{p^2(p-1)} = 2\pi i \times \text{ sum of residues.}$$

Calculate

$$Res|_1 = e^t; \quad Res|_0 = -(1+t),$$

and take the limit to find that $f = -(1+t) + e^t$.

(b) Invert $\bar{f}(p) = \frac{1}{p^{1/2}}$.

This has a branch point at the origin. We proceed as before, closing the contour to the left with a circular arc centred at the origin, but we need a 'key-hole', excluding the negative real axis and the origin.

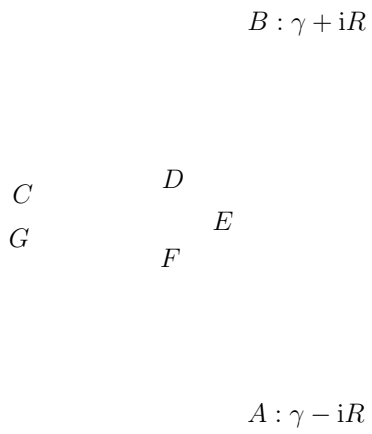

Figure 1.1: The contour for inverting $p^{-1/2}$

Then we may define $p^{1/2} = r^{1/2}e^{i\theta/2}$ for $-\pi < \theta < \pi$ and consider the integral $\oint_\Gamma e^{pt}\frac{dp}{p^{1/2}}$. With points as labelled on the diagram and DEF a circle of radius ϵ, we claim that

$$\oint_\Gamma = 0; \text{ while } \int_B^C, \quad \int_G^A, \quad \int_{DEF} \to 0$$

$$\int_C^D e^{pt}\frac{dp}{p^{1/2}} \to \int_0^\infty e^{-rt}\frac{dr}{ir^{1/2}}$$

$$\int_F^G e^{pt}\frac{dp}{p^{1/2}} \to \int_0^\infty e^{-rt}\frac{dr}{ir^{1/2}}$$

so

$$\int_A^B \to -\frac{2}{i}\int_0^\infty \frac{e^{-rt}}{r^{1/2}}dr$$

and

$$f(t) = \frac{1}{\pi}\int_0^\infty e^{-rt}\frac{dr}{r^{1/2}}.$$

To evaluate this integral, put $rt = s^2$,

$$= \frac{1}{\pi}\int_0^\infty e^{-s^2}\frac{2sds}{t}\frac{t^{1/2}}{s}$$

$$= \frac{1}{\pi\sqrt{t}} \int_{-\infty}^{\infty} e^{-s^2} ds$$

which is a standard integral:

$$= \frac{1}{\sqrt{t\pi}}.$$

With the aid of this example and property 6 of the Laplace transform, we can also invert $p^{-3/2}$, $p^{-5/2}$, etc.

The next two examples show how transforms can help transform PDE problems to ODE problems.

(c) Consider the following problem describing the heating an initially uniform temperature bar by a constant heat source from one end.

$$\kappa\, u_{xx} = u_t \qquad \text{in } \geq 0, t \geq 0$$

$$u = 0 \text{ at } t = 0, \qquad \left.\begin{array}{ll} -\kappa u_x = Q & \text{at } x = 0, \\ u \to 0 & \text{as } x \to \infty \end{array}\right\}$$

Note we are only interested in finding the surface temperature $u(0, t)$ for $t \geq 0$ (and not the entire solution).

We Laplace transform in t only with

$$\bar{u}(x, p) = \int_0^{\infty} u(x, t) e^{-pt} dt.$$

The transformed PDE and initial condition becomes

$$p\bar{u} = \kappa \bar{u}_{xx}.$$

This is an ODE in x for $\bar{u}$ which we can solve to give

$$\bar{u} = A(p) e^{x\sqrt{p/\kappa}} + B(p) e^{-x\sqrt{p/\kappa}}$$

(note here that the square root refers to root with non-negative real part). Then imposing $\bar{u} \to 0$ as $x \to \infty$ implies $A = 0$. and then using

$$\bar{u}_x(0, p) = \int_0^{\infty} u_x(0, t) e^{-pt} dt$$

gives

$$B = \frac{Q\sqrt{\kappa}}{k} p^{-3/2}.$$

Hence the solution is

$$\bar{u}(x,p) = \frac{Q\sqrt{\kappa}}{k} p^{-3/2} e^{-x\sqrt{p/k}}.$$

Inverting this would give us $u(x,t)$, but we are only asked for $u(0,t)$. Looking at the transform at $x = 0$ we have

$$\bar{u}(0,p) = \frac{Q\sqrt{\kappa}}{k}\ p^{-3/2}.$$

and this can be easily inverted to find

$$u(0,t) = \frac{4Q}{k}\sqrt{\frac{\kappa t}{\pi}}$$

(d) Consider the heat equation in an infinite bar:

$$u_{xx} = u_t; \quad -\infty < x < \infty, \quad t \geq 0$$

with initial conditions

$$u(x,0) = f(x).$$

we could attempt to solve this by Laplace transforms but a better approach, as we are on an infinite region, is to take a Fourier transform in x:

$$\hat{u}(\omega,t) = \int_{-\infty}^{\infty} u(x,t) e^{-i\omega x} dx$$

so

$$\hat{u}_t = \int u_t e^{-i\omega x} dx = \int u_{xx} e^{-i\omega x} dx = -\omega^2 \hat{u},$$

an ODE we can solve:

$$\hat{u}(\omega,t) = A(\omega) e^{-\omega^2 t}$$

but

$$\hat{u}(\omega,0) = \hat{f}(\omega) \text{ therefore } A = \hat{f}$$

and hence the solution is

$$\hat{u}(\omega,t) = \hat{f}(\omega) e^{-\omega^2 t}.$$

This is a product of Fourier transforms, so corresponds to a convolution:

$$u(x,t) = \int_{-\infty}^{\infty} K(x-y,t)\ f(y)\ dy \quad \text{where} \quad \hat{K}(\omega,t) = e^{-\omega^2 t}. \tag{1.7}$$

To invert $\hat{K}$ we use the inversion formula (1.6)

$$K(x,t) = \frac{1}{2\pi} \lim_{R\to\infty} \int_{-R}^{R} e^{i\omega x} e^{-\omega^2 t}\, d\omega$$

so with $s = \omega\sqrt{t}$ this is

$$= \frac{1}{2\pi\sqrt{t}} \lim_{R\to\infty} \int_{-R}^{R} e^{-s^2 + isx/\sqrt{t}}\, ds.$$

and this integral can be calculated using the result that, for real a,

$$\int_{-\infty}^{\infty} e^{-s^2+2Ha's}\, ds = \int_{-\infty}^{\infty} e^{-(s-ia)^2}\, e^{-a^2}\, ds = \sqrt{\pi} e^{-a^2}$$

Hence we have

$$K(x,t) = \frac{1}{2\pi\sqrt{t}} \cdot \sqrt{\pi} e^{-x^2/4t} = \frac{e^{-x^2/4t}}{2\sqrt{\pi t}}, \tag{1.8}$$

and therefore

$$u(x,t) = \frac{1}{2\sqrt{\pi t}} \int_{-\infty}^{\infty} e^{-\frac{1}{4t}(x-y)^2} f(y)\, dy. \tag{1.9}$$

1.4 Coupled diffusion problems

We might expect that solutions to problems governing by diffusion might become smooth as time progresses. However, there is a very interesting phenomena that occurs when there are a number of different things that diffuse that interact. The most common example is a mixture of reacting chemicals but similar behaviour is also observed when signalling information is passed between various cells in a tissue.

As an example consider two different chemicals which are reacting with reactions that are linearly proportional to the concentration of each species. We imagine that there may be some steady distribution of the species and we are interested in any small deviation away from this steady state. We take the variables c_1 and c_2 to be difference between the actual concentration and the static underlying distribution. Hence a one-dimensional model would be

$$\frac{\partial c_1}{\partial t} = D_1 \frac{\partial^2 c_1}{\partial x^2} + \alpha c_1 + \beta c_2$$

$$\frac{\partial c_2}{\partial t} = D_2 \frac{\partial^2 c_2}{\partial x^2} + \gamma c_1 + \delta c_2$$

The boundary of the region is taken to have no reactants so that $c_1 = c_2 = 0$

Such a problem can of course be solved by separation of variables or suitable transform method. Here however, we note that there is obviously a solution $c_1 = c_2 = 0$ and ask if this is stable.

An obvious question is whether the basic reaction is in a stable state. This can be determined by studying the ODE system

$$\frac{dc_1}{dt} = \alpha c_1 + \beta c_2$$

$$\frac{dc_2}{dt} = \gamma c_1 + \delta c_2$$

where standard methods then require $\alpha + \delta < 0 < \alpha\delta - \beta\gamma$ for stability. The interesting observation is that such a stable situation can be destabilised simply by diffusion, which might be anticipated to simply smooth behaviour.

Taking a Fourier transform, or separating variables and looking at the time-dependent part, we find that

$$\frac{\partial c_1}{\partial t} = D_1 \frac{\partial^2 c_1}{\partial x^2}(-D_1 k^2 + \alpha)c_1 + \beta c_2$$

$$\frac{\partial c_2}{\partial t} = D_2 \frac{\partial^2 c_2}{\partial x^2}\gamma c_1 + (-D_2 k^2 + \delta)c_2$$

and, for stability we now require that

$$\alpha + \delta - (D_1 + D_2)k^2 < 0 < (\alpha - D_1 k^2)(\delta - D_2 k^2) - \beta\gamma$$

for all real values of k. Such stability is possible for example so long as $\alpha\delta < 0$, $\beta\gamma < 0$ and, depending on whether $\alpha < 0$ or $\delta < 0$, D_1/D_2 is respectively less than or greater that the smaller root D^* of

$$(D^*\alpha - \delta)^2 + 4d^*\beta\gamma = 0.$$

The behaviour of systems where the diffusion act to destabilise the behaviour is of great interest and is commonly referred to as a Turing instability.

1.5 Nonlinear Diffusion behaviour

In many cases it can be highly instructive to have exact solutions to a problem in order both to understand the general behaviour and to compare and validate numerical results. For partial differential equation problems a common method

for seeking special solutions is to try to reduce the dimensionality (eg reduce the problem to an ODE) where standard solution methods might be applicable. For the heat diffusion problem there are two obvious examples, namely steady state solutions where we consider $u(x,t) = U(x)$ and spatially uniform problems were we assume that $u(x,t) = \mathcal{U}(t)$. Obviously in each case the resulting solution will only be valid for certain special forms of initial and boundary conditions. If these special cases are relevant to the physical problem then examining these steady-state or spatially-uniform solutions can be very informative about possible behaviour of the more complicated case, even if these still require numerical solution, since it reduces the dimensionality of the problem.

This idea can be extended to consider other special forms for solution to the original problem and each will be valid for special forms of the boundary and initial conditions conditions. In this section we consider two of these cases, travelling waves and similarity solutions using nonlinear diffusion problems as examples, but we note here that a general approach to finding such special forms of solution can be done using Lie groups.

1.5.1 Fisher equation and travelling waves

A very common simple model of the dynamics of a single population of animals or bacteria is the logistic model. Taking the population to be of size $N(t)$ the dynamics are taken to be governed by the ODE

$$\frac{dN}{dt} = rN\left(1 - \frac{N}{k}\right) \ .$$

is has the property that the growth rate is proportional to the population for when the size is small (the growth rate is approx rN) which describes unrestricted growth but that the death rate (approx rN^2/K) increases and becomes a limiting factor as the population approaches the "carrying capacity" k. The main property of this system is that there are two steady states $N = 0$ and $N = k$ where the first is unstable and the second is stable. This simple model has been extensively studied and extended to account for more detailed phenomena.

One interesting practical issue is to model populations that vary spatially. For example squirrels that may have very different dynamics in open farm land compared to woods and hedges. In this case a simple model is to use logistic dynamics, with spatially dependent coefficients r and k and to allow the population to move by a simple diffusion process. The variable of interest is the $n(x,t)$, the population density. The governing PDE in one-dimension is then

$$\frac{dn}{dt} = \frac{\partial}{\partial x}\left(D\frac{\partial n}{\partial x}\right) + rn\left(1 - \frac{n}{k}\right) \ .$$

This is commonly called Fisher's equation. This nonlinear PDE can be studied using numerical methods to explore behaviour of a moving population in one or more dimensions.

An interesting analytical approach to the problem arises by exploiting the two steady states for the logistic part of the problem. Hence consider the problem in a very long one dimensional region in which the population has reached is carrying capacity, $n = k$, to the far left but is unpopulated, $n = 0$, to the far right. We then expect an "invasion wave" that propagates from the highly populated region into the unpopulated region. The speed of this wave is of considerable interest.

To study this consider the case where all the parameters are constant, so we can nondimensionalised using $n = k\hat{n}$, $t = \hat{t}/r$, $x = \hat{x}\sqrt{D/r}$ and then immediately neglect the "hat" notation from hereon for simplicity. Mathematically we then pose the question as finding a solution to the problem

$$\frac{dn}{dt} = \frac{\partial^2 n}{\partial x^2} + n(1-n) \qquad -\infty < x < +\infty$$

with

$$n \to 1 \quad \text{as } x \to -\infty, \qquad n \to 0 \quad \text{as } x \to +\infty \, .$$

We could impose initial data on this problem but this will make the problem only accessible by numerical methods so an alternative approach is consider that any initial data may result in a wave that propagates at a steady speed. Note we cannot be sure that this is a valid assumption and need to consider this later. Hence we seek a "travelling wave" solution.

To find the solution we take all the parameters to be constants and assume that

$$n(x,t) = f(x-ct), \qquad x - ct = \eta$$

where c is a constant to be found (the nondimensional wave speed). Then the PDE problem becomes

$$cf' = f'' + f\,(1-f)$$

with

$$f \to 1 \quad \text{as } \eta \to -\infty, \qquad f \to 0 \quad \text{as } \eta \to +\infty \, .$$

We cannot completely solve this ODE problem analytically but we can find out a considerable amount about the solution by studying it in the phase plane (ie. in the plane (f, f')).

We note there are two critical points ($f = 0$, $f' = 0$) and ($f = 1$, $f' = 0$). Studying each of these locally by linearising we find that $(1, 0)$ is a saddle point for all values of c. The behaviour near $(0, 0)$ changes it nature as c goes through

the value $c = 2$. For values of $c < 2$ it is a unstable spiral while for values greater than 2 it is an unstable node. (use a standard direction-field plotting program in order to see the global behaviour). The solution we seek goes from $(0, 0)$ to $(1, 0)$. We can see that such a solution exists for all values of c and so there appears to be no specific c to choose. However, we need to consider the physical problem and since we are interested in populations it is not reasonable to have the solution that become negative, hence we see that we need to take $c \geq 2$.

This still does not completely answer the question we originally posed, which was to find the speed of the travelling wave. To find this we have to use some additional information and it turns out this comes from the behaviour as $\eta \to 0 + \infty$ and comes from the initial conditions of the original time dependent problem. If the initial condition is monotone decreasing in x with $u(x, 0) \to 1$ as $x \to -\infty$ and $u(x, 0) \to 0$ as $x \to +\infty$ then the solution will tend to a travelling wave with the speed determined by the behaviour of $u(x, 0)$ as $x \to +\infty$. We now study the behaviour of f in this region to find this dependency.

The analysis near $(0, 0))$ shows that $f \sim \exp(-a\eta)$ where $a = (c + \sqrt{c^2 - 4})/2$ and hence if the initial condition has the population decaying by a rate that makes is smaller than $\exp(-a\eta)$ then the wave travels at $\sqrt{2}$ but if the initial decay is slower then the decay rate dictates the value of c. This type of behaviour, where we seek a particular special solution of a problem and find the resulting problem insufficiently posed occurs quite often and care must be taken to analysing such cases. An example is the long time behaviour of the heat equation with Neumann boundary conditions

$$u_t = u_{xx} \qquad u_x(0, t) = 0 \qquad u_x(1, t) = 0$$

with initial date $u(x, 0) = g(x)$. The solution tends to steady state at very long time so satisfies

$$0 = u_{xx} \qquad u_x(0, t) = 0 \qquad u_x(1, t) = 0$$

and the solution to this requires looking carefully at the initial data to find what value the resulting constant solution takes.

1.5.2 Similarity solutions

The previous discussion considered possible simple forms for the solution of the problem and required special initial or boundary conditions to ensure that the resulting problem was of reduced dimensionality. We now seek a further set of such special solutions which exploit symmetries of the governing PDE.

A simple problem for the diffusion equation is to consider a bar at an initial uniform temperature and then linearly increase the temperature at one end. If

we assume that the bar is long (or we only consider a short time so the that the temperate only changes over a short length of the bar) then the problem is

$$\frac{\partial T}{\partial t} = \frac{\partial^2 T}{\partial x^2} \qquad 0 \le x < +\infty$$

with

$$T = 0 \text{ at } t = 0, \qquad T = t \text{ at } x = 0, \qquad T \to 0 \text{ as } x \to +\infty.$$

We might then observe that if we change the variables from T, x, t to $\mathbf{T}, \mathbf{x}, \mathbf{t}$ where

$$T = a\mathbf{T}, \qquad x = b\mathbf{x}, \qquad T = c\mathbf{T}$$

then if we choose $b = c$ and $c = b^2$ the problem for the new variables is identical to the original problem for all constants $a > 0$. Hence the problem is invariant under this rescaling. Obviously not all PDE problems have such invariant properties but we exploit this to find a solution. This will be a special "similarity" solution and one of the ways of studying PDE problems is to try to find any such invariants of the PDE and then see if physically reasonable boundary and initial conditions allow the same invariants for these conditions. Note for the diffusion equation above we only require $c = b^2$ with no restriction on a, and hence there are many boundary conditions that can be considered which remain invariant but we do require an infinite or semi-infinite spatial region (in order that the position of the boundaries is invariant under the change of variable).

We now seek a "similarity solution" which will have the property that it is "self-similar" in a manner outlined by the invariant property above. An ad hoc method for finding such a solution is to consider $T(x, t)$ to have a special form namely

$$T(x, t) = t^\alpha \phi(x/t^\beta)$$

where we will call the new variable $\eta = x/t^\beta$ and hope we can choose the two constants α and β so that the PDE becomes an ODE for ϕ and the boundary and initial condition can be satisfied by the ODE. Using this special form the PDE becomes

$$\alpha t^{\alpha-1}\phi(x/t^\beta) - \beta x t^{\alpha-\beta-1}\phi'(x/t^\beta) = t^{\alpha-2\beta}\phi''(x/t^\beta).$$

or

$$\alpha t^{\alpha-1}(\alpha\phi(x/t^\beta) - \beta\eta\phi'(x/t^\beta)) = t^{\alpha-2\beta}\phi''(x/t^\beta).$$

We want this to be an ODE in η and hence we must choose $\alpha - 1 = \alpha - 2\beta$ implying $\beta = 1/2$ which agrees with our observation $c = b^2$.

Turning to the boundary and initial conditions we find these become

$$\phi \to 0 \text{ as } \eta \to \infty, \qquad t^\alpha\phi = t \text{ at } \eta = 0, \qquad \phi \to 0 \text{ as } \eta \to +\infty.$$

Note that two of these conditions collapse to the same ODE condition. Finally we see that if we choose $\alpha = 1$ then we have the ODE problem

$$\phi - \frac{\eta}{2}\phi' = \phi''.$$

with

$$\phi \to 0 \text{ as } \eta \to \infty, \qquad \phi = 1 \text{ at } \eta = 0.$$

In this case unfortunately the ODE cannot be readily solved analytically but a simple numerical solution can be determined and hence the solution for all time and space found.

1.5.3 Degenerate diffusion equations, moving boundaries and similarity solutions

We now consider three different physical situations where diffusion occurs but has a nonlinear behaviour. The first is heat flow in in a bed of coal. Here the temperatures are extremely large and the dominant mechanism for heat flow is not conventional diffusion but rather radiation. Each small block of coal receives heat from the surrounding region by radiation and simultaneously emits radiation. Such a bed of material is called "optically thick" since radiation is absorbed in a distance much shorter than the region of interest. Assuming that the radiative energy density is given by the Stephan-Boltzmann law, where the energy flux from any surface is proportional to T^4, then the nett flux between two adjacent surfaces (at x and $x + dx$) is the difference in these so that

$$q = \beta T^4(x, t) - \beta T^4(x + dx, t)$$

and taking the limit $dx \to 0$ gives

$$q = -\gamma \frac{\partial T^4}{\partial x} \ .$$

Hence the conservation of heat equation gives

$$\frac{\partial T}{\partial t} = \kappa \frac{\partial}{\partial x}\left(T^3 \frac{\partial T}{\partial x}\right) \ .$$

for some constant κ.

A second situation is the flow of groundwater in unconfined aquifers. Here water flows in an aquifer which, for simplicity of modelling, has a flat layer of impermeable clay underlying it and the aquifer is saturated to a height of H above

this layer. The region containing the water is assumed to be very long and thin so that the pressure in the water is dominated by hydrostatic pressure and the upper surface of the water, is assumed to be at atmospheric pressure. The speed of the fluid in the porous aquifer is proportional to the pressure gradient (and hence the gradient of H and the flux is therefore proportional to H times this gradient. To lowest order in the aspect ratio of the region this results in a classical model that is called the "Dupuit approximation" and using conservation of water has a governing equation

$$\frac{\partial H}{\partial t} = \gamma \frac{\partial}{\partial x}\left(H \frac{\partial H}{\partial x} \right) .$$

The final case happens when you spill a beer on a table. Can we find a model that will allow us to predict how long it will take for the beer to get to the edge of the table? Note the same modelling applies to spreading glass during float glass production, chocolate dripping over a Magnum ice cream, or to lava flowing from a volcano.

The governing equation can be deduced in a systematic manner using asymptotic methods from Newtonian flow of a viscous fluid over a flat surface acted upon by gravity. This full model can then be studied approximately exploiting the thinness of the layer relative to the distance it spreads (small aspect ratio). In summary, if we consider the beer just to spread in one dimension on a flat horizontal table and take $h(x,t)$ to be the thickness of the beer at each point on the table and $q(x,t)$ to be the flux of beer, then we get two equations. Firstly conservation of mass

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

and the second a force balance (momentum equation)

$$q = -h^3 \frac{\rho}{6\mu} \frac{\partial h}{\partial x}$$

where ρ is the beer density and μ is its viscosity. If we suitably nondimensionalise the equation then the governing PDE becomes

$$\frac{\partial h}{\partial t} = \frac{\partial}{\partial x}\left(h^3 \frac{\partial h}{\partial x} \right) .$$

This is a diffusion equation but the "conductivity", h^3, is now a function of the unknown solution $h(x,t)$. This PDE has most of the properties of the diffusion equation but an additional difficulty due to the fact that we anticipate that the initial data for the problem (the height of the beer on the table when it first splashes down) will be zero over much of the table and hence the "diffusivity"

will be zero here - such a diffusion equation is called "degenerate". In fact we might anticipate that, if we specify the initial region of the beer and its height the PDE should then tell us how the beer spreads, without the need for additional boundary conditions. This is precisely what occurs but we need to be very careful in solving near the point where h goes to zero (ie a the edge of the beer). There are two approaches to this complication. Firstly we can consider the concept of a "weak solution" to the PDE where we allow h to do something special at the edge but require that momentum and mass are conserved but not proceed in the usual way because here the flux is not differentiable. Secondly we can solve the PDE in a region where $h > 0$ and insist that h is zero on the boundary and find some additional condition to determine how the interface moves (hence change the problem into a "moving boundary" problem). The extra condition comes from studying conservation of mass and momentum at the boundary. Note that the two approaches are equivalent although the former is better mathematically and quite often the way computations are done. Note also the moving boundary method assumes that we know where the boundary is and may not be able to detect the generation or removal of new boundaries where $h = 0$. A quick way to generate this extra condition is to note that q/h is the velocity of the beer and nondimensionally the PDE tell us $q = -h^3 \partial h/\partial x$ so the extra condition must be that the boundary, where $h = 0$, moves at a nondimensional velocity given by

$$-h^2 \frac{\partial h}{\partial x} \, .$$

We could seek steady, spatially independent or travelling wave solutions to this equation if they were useful but it can also be very instructive to seek other similarity solutions. In particular we seek some solution that spreads out but conserves the total amount of beer (rather than a solution that has some influx at a fixed boundary for example). Such a solution will satisfy

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

and we will hope that there is some special initial data that allows this. Additionally we hope that the only boundary conditions needed are that $h = 0$ for sufficiently large x.

We therefore seek a "similarity solution" by the ad hoc methods by assuming

$$h(x,t) = t^\alpha \phi(x/t^\beta)$$

where $\eta = x/t^\beta$. The PDE becomes

$$t^{\alpha-1}(\alpha\phi - \eta\beta\phi') = t^{(4\alpha-2\beta)}(\phi^3\phi')'$$

so, in order to make this an ODE, we need $\alpha - 1 = 4\alpha - 2\beta$ and

$$\int_{-\infty}^{+\infty} t^{\alpha}\phi(x/t^{\beta})\, dx = 1 \qquad \rightarrow \qquad \int_{-\infty}^{+\infty} t^{\alpha+\beta)}\phi(\eta)\, d\eta = 1.$$

Hence we need $\alpha + \beta = 0$ giving $\alpha = -1/5$, $\beta = 1/5$. This choice of constants will make the PDE into an ODE and allow us to impose the integral constraint. However, we also need to impose the condition at the moving boundaries $x = \pm s(t)$ (note we shall assume that the fluid is spreading symmetrically from $x = 0$). In the new coordinates this is $t^{1/5}\eta = \pm s(t)$ and hence for ϕ to only depend on η we require that $s(t)$ have the form $s(t) = t^{1/5}\lambda$ where λ, is a constant to be found. Using these changes of variable the conditions at $x = \pm s(t)$ can be converted to conditions at $\eta = \pm\lambda$.

In outline we then seek a solution to

$$1/5(\phi + \eta\phi') - (\phi^3\phi')' = 0$$

by integrating once to get

$$1/5\ \eta\phi - \phi^3\phi' = A$$

where we need to choose $A = 0$ in order that we can impose the condition $h = 0$ at the boundary. This integrated ODE then has two possible solutions

$$\phi = 0 \qquad \text{or } 1/5\ \eta - \phi^2\phi' = 0$$

To find the complete solution to the problem we need to fit together the solution $\phi = 0$ to the solution of the ODE and choose the resulting arbitrary constant to satisfy both the condition at the interface $\eta = \lambda$ and the integral constraint. These two conditions allow us to find the arbitrary constant from the ODE and λ and hence the entire solution.

Note that in many cases the resulting ODE may require numerical solution. However, identifying the similarity variable can, in itself, provide great insight. For example here we know that the boundary of the beer will travel like $\lambda t^{1/5}$ without solving the ODE and this might be compared to experimental evidence to see if the model is adequate for predicting behaviour.

2 Linear waves

There are numerous physical situations in which waves form and propagate. In this chapter we examine some of the physical mechanisms underlying such behaviour and the mathematical model that have been used to describe them.

We will then explore methods for studying linear waves by studying the underlying properties of the PDE problems

2.1 Strings and membranes

The simplest wave equations arise in situations where a very thin materials, a string or a membrane which can sustain tension but requires negligible force to bend, is held taut at its ends (at the boundary) and allowed to vibrate.

The classical problem of the small transverse movement of a string can be modelled using Newton's law for a string with a linear density ρ (mass/unit length) and a constant tension T force) along the string. Taking x to be the distance along the string (in the case of small displacements this is same as the distance along the string when it is straight and hence undeformed) and u as the transverse displacement from a straight string we have

$$\frac{\partial}{\partial t}\left(\rho\frac{\partial u}{\partial t}\right) = \frac{\partial}{\partial x}\left(T\frac{\partial u}{\partial x}\right)$$

and for constant T and ρ this gives the classic wave equation

$$\frac{\partial^2 u}{\partial t^2} = \frac{T}{\rho}\frac{\partial^2 u}{\partial x^2}$$

In a similar manner we can consider the tangential displacement of a thin membrane with undeformed membrane in the x, y plane and u as the transverse displacement. Assuming the membrane is under uniform stress σ_0 in all direction we find

$$\frac{\partial^2 u}{\partial t^2} = \frac{h\sigma_0}{\rho}\nabla^2\mathbf{u}.$$

where h is the membrane thickness and ρ is the area density (mass /unit area).

2.2 Elastic waves

We now consider the motion of a block of elastic material and how deformations within such a material can propagate as waves. In deriving the equations we shall assume that the deformations of the material from its initial state are small (nonlinear theories that account for large displacements, or for large strains, or for growth of a material can be found but are much more complicated)

Newton's law ($F = ma$) can be applied to a small element of an elastic material V with the assumption that the only forces acting are those on the surface to give

$$\frac{\partial^2}{\partial t^2}\int_V \rho\mathbf{u}\,\mathrm{d}V = \int_{\partial V} \boldsymbol{\sigma}\cdot\mathbf{n}\,\mathrm{d}S$$

where ρ is the density, $\mathbf{u}$ the displacement of a point in the material from its original position, and $\boldsymbol{\sigma}$ the stress tensor. Assuming that $\boldsymbol{\sigma}$ is differentiable and using Green's theorem (divergence theorem) it then follows that

$$\frac{\partial^2}{\partial t^2}\int_V \rho\mathbf{u}\,\mathrm{d}V = \int_V \nabla\cdot\boldsymbol{\sigma}\,\mathrm{d}V,$$

Hence since V is arbitrary we have

$$\rho\frac{\partial\mathbf{u}}{\partial t^2} = \nabla\cdot\boldsymbol{\sigma}.$$

We now need a constitutive law describing how a particular material acts by prescribing the relationship between the stress and the strain. For a simple linear elastic material (acting like a linear spring) we take Hooke's law where

$$\boldsymbol{\sigma} = \lambda\,\mathrm{tr}(\boldsymbol{\epsilon})\mathbf{I} + 2\mu\boldsymbol{\epsilon}, \qquad \sigma_{ij} = \lambda\delta_{ij}\epsilon_{kk} + 2\mu\epsilon_{ij},$$

and $\boldsymbol{\epsilon}$ is the Strain tensor,

$$\boldsymbol{\epsilon} = (\nabla\mathbf{u})^S, \qquad \epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)$$

Note in these we have used summation convention over repeated indices, we have taken the superscript S to indicate symmetric part of of the strain, and the constants λ and μ are the Lamé constants which can be determined by measurements on any particular material. Thus (again using summation convention)

$$\begin{aligned}
\rho\frac{\partial u_i}{\partial t^2} &= \frac{\partial\sigma_{ij}}{\partial x_j} \\
&= \frac{\partial}{\partial x_j}\left(\lambda\delta_{ij}\epsilon_{kk} + 2\mu\epsilon_{ij}\right) \\
&= \frac{\partial}{\partial x_j}\left(\lambda\delta_{ij}\frac{\partial u_k}{\partial x_k} + \mu\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right)\right) \\
&= (\lambda+\mu)\frac{\partial}{\partial x_i}\frac{\partial u_k}{\partial x_k} + \mu\frac{\partial^2 u_i}{\partial x_j^2}.
\end{aligned}$$

In vectorial form this is

$$\rho\frac{\partial^2\mathbf{u}}{\partial t^2} = (\lambda+\mu)\nabla(\nabla\cdot\mathbf{u}) + \mu\nabla^2\mathbf{u}$$

which is commonly referred to as Navier's equation.

Now we can use the vector identity

$$\nabla^2\mathbf{u} = \nabla(\nabla\cdot\mathbf{u}) - \nabla\wedge\nabla\wedge\mathbf{u},$$

to rewrite Navier's equation as

$$\rho\frac{\partial^2\mathbf{u}}{\partial t^2} = (\lambda+2\mu)\nabla(\nabla\cdot\mathbf{u}) - \mu\nabla\wedge\nabla\wedge\mathbf{u}.$$

We now examine properties of this Navier equation. Start by noting that the dilation (the volume change from the initial state) of the material is given by $\Delta = \nabla\cdot\mathbf{u}$ and the rotation of the material from its initial state is given by $\mathbf{r} = \frac{1}{2}\nabla\times\mathbf{u}$. Here $\mathbf{r}$ might be thought of as the elastic equivalent of vorticity in fluid dynamics.

By taking the divergence and then the crossproduct of the governing Navier equation we now find that

$$\begin{aligned}\rho\frac{\partial^2\Delta}{\partial t^2} &= (\lambda+2\mu)\nabla^2\Delta,\\ \rho\frac{\partial^2\mathbf{r}}{\partial t^2} &= -\mu\nabla\wedge\nabla\wedge\mathbf{r} = \mu\nabla^2\mathbf{r}.\end{aligned}$$

Thus both Δ and $\mathbf{r}$ satisfy a wave equation, but with different wavespeeds. The function Δ is a P-wave and represents a dilation or primary wave (also called a pressure wave or longitudinal wave in special circumstances) and the corresponding wavespeed is denoted c_P. The function $\mathbf{r}$ is an S-wave and represents a rotational or secondary wave (also called a transverse or shear wave in special circumstances), and the corresponding wavespeed is denoted c_s. Thus

$$c_p = \sqrt{\frac{\lambda+2\mu}{\rho}}, \qquad c_s = \sqrt{\frac{\mu}{\rho}}.$$

A very useful physical property of these waves comes from noting that since λ and μ are both positive, $c_p > c_s$ and so those deformations described by P-waves always travel faster than the deformations related to S-waves.

2.3 Acoustic waves

Next we consider the motion of a compressible gas and explore how the resulting behaviour gives rise to acoustic waves. The underlying model considers the gas to be homentropic (the entropy at any point or at any time remains constant) and that it is inviscid (no significant viscous dissipation).

Conservation of mass gives

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\rho \mathbf{u}) = 0,$$

where ρ is the fluid density and $\mathbf{u}$ is the fluid velocity (note the easy confusion between $\mathbf{u}$ as used in elasticity and $\mathbf{u}$ as used in fluid!!). Conservation of momentum gives

$$\rho \left(\frac{\partial \mathbf{u}}{\partial t} + (\mathbf{u} \cdot \nabla)\mathbf{u} \right) = -\nabla p.$$

For conservation of energy our assumption of homentropic flow gives

$$p = p(\rho)$$

where the precise form of this relationship depends on a constitutive relation describing the gas properties. We now linearise about a uniform steady the ambient state by setting

$$\rho = \rho_0 + \delta \bar{\rho}, \qquad p = p(\rho_0) + \delta \bar{p}, \qquad \mathbf{u} = \delta \bar{\mathbf{u}},$$

where $0 < \delta \ll 1$. Keeping only leading order terms in δ gives (dropping the overbar notation),

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \rho_0 \nabla \cdot \mathbf{u} &= 0, \\ \rho_0 \frac{\partial \mathbf{u}}{\partial t} &= -\nabla p, \\ p &= \frac{\mathrm{d}p}{\mathrm{d}\rho} \rho, \end{aligned}$$

where $\mathrm{d}p/\mathrm{d}\rho$ in the last equation is evaluated at $\rho = \rho_0$. Eliminating ρ and $\mathbf{u}$ gives

$$\frac{1}{c^2} \frac{\partial^2 p}{\partial t^2} = \nabla^2 p,$$

where

$$c^2 = \frac{\mathrm{d}p}{\mathrm{d}\rho}$$

and c is the wave speed,

2.4 Stokes waves

We now consider a large class of problems that arise in situations where there are waves at the interface between a dense incompressible inviscid fluid (eg water) and a gas. Typical examples are waves on the sea, ripples on a pond, waves in a teacup etc. In these situations it is reasonable to neglect the role of the gas except that this imposes a constant pressure and no tangential stress on the interface and to assume the the only external force on the system is gravity which acts on the dense fluid (extensions are well known that include other mechanisms such as surface tension etc.). The conventional terminology used for such waves on an inviscid irrotational incompressible fluid is Stokes waves or surface gravity waves.

Consider an inviscid, irrotational incompressible fluid occupying the region $-H < z < h(x, y, t)$, where the bottom surface, $z = -H$, is rigid, but the top surface, $z = h(x, y, t)$, is a free boundary. Irrotationality implies $\nabla \wedge \mathbf{u} = \mathbf{0}$, which implies the existence of a velocity potential ϕ such that

$$\mathbf{u} = \nabla\phi.$$

Conservation of mass along with incompressibility (ρ =constant) implies $\nabla \cdot \mathbf{u} = 0$, giving

$$\nabla^2\phi = 0,$$

in the fluid. Since the bottom surface is impermeable, $\mathbf{u} \cdot \mathbf{n} = 0$ there, i.e.

$$\frac{\partial\phi}{\partial z} = 0 \qquad \text{on } z = -H.$$

On the free surface we have the kinematic condition that particles on the free surface must remain there, giving

$$\frac{\mathrm{D}}{\mathrm{D}t}(z - h) = 0 \qquad \text{on } z = h(x, y, t),$$

where $\mathrm{D}/\mathrm{D}t$ is the convective derivative. Thus this implies

$$\left(\frac{\partial}{\partial t} + \mathbf{u} \cdot \nabla\right)(z - h) = 0 \qquad \text{on } z = h(x, y, t),$$

and hence

$$-\frac{\partial h}{\partial t} + \frac{\partial\phi}{\partial z} - \frac{\partial\phi}{\partial x}\frac{\partial h}{\partial x} - \frac{\partial\phi}{\partial y}\frac{\partial h}{\partial y} = 0 \qquad \text{on } z = h(x, y, t).$$

On the free surface we also have the dynamic condition, which arises from Bernoulli's equation. Bernoulli's equation gives

$$\frac{\partial\phi}{\partial t} + \frac{1}{2}|\nabla\phi|^2 = -gz - \frac{p}{\rho}.$$

On the free surface the pressure is atmospheric (which we may take to be zero without loss of generality), giving the condition

$$\frac{\partial \phi}{\partial t} + \frac{1}{2}|\nabla \phi|^2 = -gh \qquad \text{on } z = h(x, y, t).$$

This system of equations and boundary conditions now describes the behaviour of the fluid and the interface.

Linearisation

We now consider a special limit of the Stokes wave problem and look at very small waves on a very deep stationary pool of water (other limits give various different equations for the surface with equally interesting behaviour).

Consider small perturbations to a flat free surface and a static fluid by setting

$$\phi = \delta\bar{\phi}, \qquad h = \delta\bar{h}.$$

Keeping only leading order terms in δ, and dropping the overbar notation, gives

$$\begin{aligned} \nabla^2\phi &= 0 \qquad \text{in } -H < z < 0, \\ \frac{\partial \phi}{\partial z} &= 0 \qquad \text{on } z = -H, \\ -\frac{\partial h}{\partial t} + \frac{\partial \phi}{\partial z} &= 0 \qquad \text{on } z = 0, \\ \frac{\partial \phi}{\partial t} &= -gh \qquad \text{on } z = 0. \end{aligned}$$

(note care has to be taken particularly when linearising the boundary condition on $z = \delta h$)

We now consider the behaviour of waves in this linear system by separating the variables. Hence we take

$$\phi = Z(z)\psi(x, y, t)$$

which gives

$$\frac{Z''}{Z} = -\frac{\nabla^2\psi}{\psi} = \lambda^2.$$

where λ is an arbitrary constant. Using this equation and the boundary condition on $z = -H$ we find

$$Z = \cosh(\lambda(z + H)).$$

The conditions on $z = 0$ then gives

$$\begin{aligned} -\frac{\partial h}{\partial t} + \psi\lambda \sinh \lambda H &= 0, \\ \frac{\partial \psi}{\partial t} \cosh(\lambda H) &= -gh. \end{aligned}$$

along with

$$\nabla^2 \psi = -\lambda\psi$$

(where the operator ∇^2 is only in the plane x, y).

This gives wave phenomena which we can easily see by looking for wave solutions (or doing separation of variables)

$$h = A(x, y)\mathrm{e}^{\mathrm{i}\omega t}, \qquad \psi = B(x, y)\mathrm{e}^{\mathrm{i}\omega t}.$$

Substituting these into the governing equations gives

$$\begin{aligned} -A\mathrm{i}\omega + B\lambda \sinh \lambda H &= 0, \\ B\mathrm{i}\omega \cosh(\lambda H) &= -gA. \end{aligned}$$

Hence a nonzero solution for A and B exists providing λ satisfies

$$\omega^2 = g\lambda \tanh(\lambda H).$$

The actual amplitude of the waves that occur then depend on solving

$$\nabla^2 A = -\lambda A$$

with suitable boundary conditions.

Note that if we just consider this problem in one dimension then the amplitude equation is

$$A = \mathrm{e}^{\mathrm{i}kx}$$

and substituting this into the governing equations gives

$$\lambda = k$$

so that we require

$$\omega = \sqrt{gk \tanh(kH)}.$$

This is the "dispersion relation" of the waves. It relates the frequency of the wave, ω to the wavelength, k. From this we can see that waves of different wavelength travel at different speeds.

2.5 Electromagnetism

Finally we consider the behaviour of electromagnetic waves by briefly deriving Maxwell's equations. These are given by Gauss's law, Gauss's law for magnetism, Faraday's law, Ampere's Law, conservation of charge and some constitutive equations to describe the material that the electromagnetic waves are moving through.

2.5.1 Gauss's Law

Gauss's law says that the integral of the electric displacement field over a surface S is given by the total net charge in the volume V enclosed within that surface:

$$\int_S \mathbf{D} \cdot \mathrm{d}\mathbf{S} = \int_V \rho \, \mathrm{d}V.$$

By Green's theorem there is an equivalent differential form

$$\nabla \cdot \mathbf{D} = \rho. \tag{2.1}$$

2.5.2 Gauss's Law for magnetism

Gauss's law for magnetism says that magnetic monopoles (the magnetic equivalent of electric charge) do not exist. Thus the integral of the magnetic induction around any closed surface is zero:

$$\int_S \mathbf{B} \cdot \mathrm{d}\mathbf{S} = 0.$$

By Green's theorem there is an equivalent differential form

$$\nabla \cdot \mathbf{B} = 0. \tag{2.2}$$

2.5.3 Faraday's Law

Faraday's Law states that the line integral of the electric field $\mathbf{E}$ around a closed curve C equals the negative of the integral of the time variation of the magnetic induction $\mathbf{B}$ through the surface S enclosed by C:

$$\oint_C \mathbf{E} \cdot \mathrm{d}\boldsymbol{s} = -\int_S \frac{\partial \mathbf{B}}{\partial t} \cdot \mathrm{d}\mathbf{S}.$$

By Stokes Theorem there is an equivalent differential form

$$\nabla \wedge \mathbf{E} = -\frac{\partial \mathbf{B}}{\partial t}. \tag{2.3}$$

2.5.4 Conservation of charge

An electric current is a flux of charge. Conservation of charge gives

$$\frac{\partial \rho}{\partial t} + \nabla \cdot \mathbf{J} = 0.$$

Combining this with Gauss's law gives

$$\nabla \cdot \left(\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} \right) = 0.$$

This implies the existence of a field $\mathbf{H}$ (the magnetic field) such that

$$\frac{\partial \mathbf{D}}{\partial t} + \mathbf{J} = \nabla \wedge \mathbf{H}. \tag{2.4}$$

This equation is known as Ampere's law.

The set of equations (2.1)-(2.4) are collectively referred to as Maxwell's equations.

2.5.5 Constitutive equations

It remains to relate the fields $\mathbf{J}$, $\mathbf{E}$, $\mathbf{D}$, $\mathbf{H}$ and $\mathbf{B}$ to each other. These relations depend on the particular material under consideration, and can be viewed as constitutive relations. Usually the magnetic field $\mathbf{H}$ and the magnetic induction $\mathbf{B}$ are proportional to each other, and the electric displacement field $\mathbf{D}$ and the electric field $\mathbf{E}$ are proportional to each other.

In free space we assume the linear relations between the fields but also assume no current can flowing and there is no charge. Hence have

$$\mathbf{D} = \epsilon_0 \mathbf{E}, \qquad \mathbf{B} = \mu_0 \mathbf{H}, \qquad \mathbf{J} = \mathbf{0}, \qquad \rho = 0,$$

where $\epsilon_0 \approx 8.854 \times 10^{-12}\ \mathrm{F\,m^{-1}}$ is the vacuum permittivity and $\mu_0 = 4\pi \times 10^{-7}\ \mathrm{V\,s\,A^{-1}\,m^{-1}}$ is the vacuum permeability.

Then Maxwell's equations can be manipulated to give

$$\frac{\partial^2 \mathbf{B}}{\partial t^2} = -\nabla \wedge \frac{\partial \mathbf{E}}{\partial t} = -\frac{1}{\mu_0 \epsilon_0} \nabla \wedge \nabla \wedge \mathbf{B} = \frac{1}{\mu_0 \epsilon_0} \nabla^2 \mathbf{B}.$$

$$\nabla^2 \mathbf{E} = -\nabla \wedge \nabla \wedge \mathbf{E} = \frac{\partial}{\partial t} \nabla \wedge \mathbf{B} = \mu_0 \epsilon_0 \frac{\partial^2 \mathbf{E}}{\partial t^2}.$$

This indicates that the components of **E** and **B** all satisfy the same wave equation. Hence in free space electromagnetic waves travel at a speed given by

$$c = \frac{1}{\sqrt{\mu_0 \epsilon_0}} \approx 3.00 \times 10^8 \mathrm{m\,s^{-1}}.$$

Note for more complex materials or situations the electric and magnetic fields may satisfy vector wave equations which can result in different types of behaviour.

2.6 Characteristics, Group and Phase velocities

Second order linear PDEs in two independent variables are often classified as elliptic, parabolic or hyperbolic based on the reduction of the PDE to a standard, canonical form. In this course we will address such classification later and by an alternative method. However we make the following observation based on the canonical approach. If we start with the wave equation

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

then the change of variables from x, t to

$$\eta = x + ct, \qquad \xi = x = ct$$

resulting in the PDE becoming

$$\frac{\partial^2 u}{\partial \xi \, \partial \eta} = 0.$$

Hence the general solution to the problem is

$$u - F(\xi) + G(\eta) = F(x - ct) + G(x + ct)$$

for arbitrary functions F and G (this is commonly called "D'Alembert's solution"). These special variables, η and ξ, are called characteristic variables with the curves in x, t space given by ξ=constant and η =constant representing two families of projected characteristics. Physically we see that "information" in the problem propagates along these characteristics with one representing waves travelling to the left and the other waves travelling to the right.

We now consider more general wave equations and some properties of the behaviour that help interpret observations. The role of the dispersion relation in wave equations can be given a special interpretation. Consider an initial shape

of the wave given by a "wave packet" with a wave form $u(x,t)$ as a function of position x and time t. Let $A(k)$ be its Fourier transform at time $t = 0$:

$$u(x,0) = \int_{-\infty}^{\infty} A_k e^{ikx}\, dk,$$

where k is the wave number of the modes. The wavepacket at any time t is then

$$u(x,t) = \int_{-\infty}^{\infty} A_k e^{i(kx-\omega t)}\, dk,$$

where ω and k are related by the dispersion relation of the governing equation. Now assume that the wave packet has a special form where the only modes in the wave are all almost at the same frequency (this corresponds to $A(k)$ being nonzero only in the vicinity of a central wavenumber k_0). We can then linearise the dispersion relation about this central wavenumber to give

$$\omega(k) \approx \omega_0 + (k - k_0)\omega_0'$$

where $\omega_0 = \omega(k_0)$ and $\omega_0' = \frac{\partial \omega(k)}{\partial k}|_{k=k_0}$. It then follows that

$$u(x,t) = e^{it(\omega_0' k_0 - \omega_0)} \int_{-\infty}^{\infty} A_k e^{ik(x-\omega_0' t)}\, dk.$$

and hence

$$|u(x,t)| = |u((x - \omega_0' t), 0)|.$$

Hence the wave packet, moves at speed ω_0' and this is called the "group velocity". If the dispersion relation has k linearly proportional to ω, such as in the 1-D wave equation, then the wave packet will travel at constant speed and the envelope of the wave will remain unchanged.

Note that "group velocity" is distinct from "phase velocity". The phase velocity is the speed at which a point of fixed phase (eg peaks) of a single mode k will travel. This is given by

$$v_{phase} = \frac{\omega}{k}.$$

To extend these ideas to more dimensions we need to introduce the idea that waves can be represented as a sum of plane waves. Each wave is therefore broken into waves of the form

$$u_{\mathbf{k}} = A_k e^{i\mathbf{k}\cdot\mathbf{x}}.$$

where the wave vector $\mathbf{k}$ gives the direction of travel of the plane wave. The PDE can then be used to find the dispersion relation between the scalar ω and $\mathbf{k}$. The group velocity can then be extended to give

$$\mathbf{v}_{group} = \vec{\nabla}_{\mathbf{k}}\, \omega$$

Similarly we have the phase velocity given by

$$\mathbf{v}_{phase} = \frac{\omega}{|k|^2}\mathbf{k}.$$

2.7 Eigenvalue problems and resonance

As we have seen, the propagation of sound or light waves in two spatial dimensions is governed by the wave equation

$$\frac{\partial^2\psi}{\partial x^2} + \frac{\partial^2\psi}{\partial y^2} = \frac{1}{c^2}\frac{\partial^2\psi}{\partial t^2},$$

where ψ is some state variable such as pressure or a scalar electric field and c is the wave speed (note that in general electromagnetic waves are governed by vector wave equations, rather than a scalar wave equation and there are situations where this creates behaviour that the scalar equation cannot mimic.

We look for time-periodic (or "monochromatic") solutions with constant frequency ω by setting

$$\psi(x, y, t) = \phi(x, y)\mathrm{e}^{-\mathrm{i}\omega t}.$$

Then ϕ satisfies the *Helmholtz equation*

$$\nabla^2\phi + k^2\phi = \frac{\partial^2\phi}{\partial x^2} + \frac{\partial^2\phi}{\partial y^2} + k^2\phi = 0, \tag{2.5}$$

where $k = \omega/c$ is the wavenumber (*i.e.* 2π divided by the wavelength).

One question we can then ask is what are the possible vibration modes within a region. Depending on the type of boundary we might take the boundary to be governed by simple Dirichlet conditions $\phi = 0$ and then the modes of vibration are the eigensolutions corresponding to the eigenvalues, k_n of the problem. For a simple region (eg a rectangle) these modes can be determined by separation of variables.

2.8 Green's functions

2.8.1 Green's Functions for Poisson and Helmholtz Equations

Introduction

The typical problem we want to consider is that of finding solutions $\phi(\mathbf{x})$ of

$$\mathcal{L}[\phi] = f(\mathbf{x})$$

where $\mathcal{L}$ is the Laplacian ∇ or the Helmholtz operator $\nabla + k^2$ and $f(\mathbf{x})$ is a given function.

The nature of the solution depends on the boundary conditions and in this section we start by assuming that solutions are required in unbounded space. We assume that $f(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$ so that there are no 'sources at infinity'. We will derive the Green's function for this problem in order to allow solutions to be found for any $f(\mathbf{x})$.

Three dimensional δ-function

We start by defining the three dimensional delta function by

$$\delta(\mathbf{x}) = \delta(x_1)\delta(x_2)\delta(x_3),$$

where the RHS has the conventional one-dimensional delta functions, or alternatively by the properties

$$\delta(\mathbf{x}) = 0 \text{ for } \mathbf{x} \neq \mathbf{0}, \quad \text{and} \quad \int \delta(\mathbf{x})\psi(\mathbf{x})\, d^3\mathbf{x} = \psi(\mathbf{0})$$

for all test functions[1] $\psi(\mathbf{x})$.

In spherical polar co-ordinates (with $r^2 = x_1^2 + x_2^2 + x_3^2$) we have

$$\delta(\mathbf{x}) = \frac{1}{4\pi}\frac{\delta(r)}{r^2}. \tag{2.6}$$

Note: Although we have said that

$$g(x)\delta(x) = g(0)\delta(x)$$

this only applies to functions $g(x)$ which are continuous at $x = 0$. An expression of the form $g(x)\delta(x)$ when $g(x)$ is not continuous at $x = 0$ must be interpreted as a generalised function in its own right. Thus $\delta(r)/r^2$ is a generalised function and it is most certainly not equal to $\delta(r)/0^2$.

Free space Green's function for the Poisson equation

Here we wish to solve the problem

$$\nabla\phi = f(\mathbf{x})$$

with $\phi(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$; that is, the effect of sources falls off far away from these sources. We can do this in much the same way as used when finding Green's functions for ODEs.

[1] In n dimensions, a test function is any infinitely differentiable function which vanishes together with all its partial derivatives of all orders as $|\mathbf{x}| \to \infty$.

Both Helmholtz and Poisson equations are self-adjoint so suppose we have a Green's function, $G(\mathbf{x}, \mathbf{y})$, that satisfies

$$\nabla_x G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}), \quad G(\mathbf{x}, \mathbf{y}) \to 0 \text{ as } |\mathbf{x} - \mathbf{y}| \to \infty$$

where ∇_x indicates differentiation with respect to $\mathbf{x} = (x_1, x_2, x_3)$ and not with respect to $\mathbf{y} = (y_1, y_2, y_3)$;

Then we will put

$$\phi(\mathbf{x}) = \int G(\mathbf{x}, \mathbf{y}) f(\mathbf{y})\, d^3\mathbf{y}$$

Note, since the integral is with respect to $\mathbf{y}$ and the derivatives are with respect to $\mathbf{x}$, if we want to put this into our PDE we will have

$$\nabla_x \phi = \int \nabla_x G(\mathbf{x}, \mathbf{y}) f(\mathbf{y})\, d^3\mathbf{y} = \int \delta(\mathbf{x} - \mathbf{y}) f(\mathbf{y})\, d^3\mathbf{y} = f(\mathbf{x}).$$

Hence if we can find a Green's function for the problem we can solve for general $f(\mathbf{x})$.

Now, we return to the question of finding G and observe that the Laplace operator ∇_x is independent of the origin of the $\mathbf{x}$-coordinates, so we can move these to $\mathbf{y}$. That is, if we put $\mathbf{x}' = \mathbf{x} - \mathbf{y}$ then the problem for G becomes

$$\nabla_{x'} G = \delta(\mathbf{x}') \tag{2.7}$$

Since the problem is posed over an infinite region and we only want decay at infinity we expect G to be radially symmetric, so we look for a function

$$G(\mathbf{x}') = G(r)$$

in which case (2.7) becomes

$$\frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2 \frac{\partial G}{\partial r}\right) = \frac{1}{4\pi}\frac{\delta(r)}{r^2}$$

For $r > 0$, $\delta(r) = 0$, so we find that

$$G = -\frac{A}{r} + B \quad (\text{for } r > 0)$$

where A and B are constants. Since $G \to 0$ as $r \to \infty$, $B = 0$.

To find A we argue as follows. Since $\nabla_{x'} G = \delta(\mathbf{x}')$ we must have

$$\int_V \nabla_{x'} G\, d^3\mathbf{x}' = 1$$

for any volume V that includes the origin. By the divergence theorem we also have

$$\int_S \frac{\partial G}{\partial n}\, d^2\mathbf{x}' = \int_V \nabla_{\mathbf{x}'} G\, d^3\mathbf{x}' = 1$$

where S is the surface of V.

Now, choose V to be a sphere of radius R. The outward normal to the surface is just the unit vector pointing from the origin to the point on the surface and so

$$\frac{\partial G}{\partial n} = \frac{\partial G}{\partial r} = \frac{A}{R^2}$$

on the surface $r = R$ of the sphere. Also, on the surface $r = R$, the unit of area $d^2\mathbf{x}'$ is given by $R^2 \sin\theta\, d\theta d\varphi$, so

$$\int_0^{\pi} \int_0^{2\pi} \left.\frac{\partial G}{\partial r}\right|_{r=R} R^2 \sin\theta\, d\theta d\varphi = 1$$

Thus

$$A \int_0^{\pi} \int_0^{2\pi} \sin\theta\, d\theta d\varphi = 1$$

and so

$$A = \frac{1}{4\pi}.$$

Thus

$$G = -\frac{1}{4\pi\, r} = -\frac{1}{4\pi}\frac{1}{|\mathbf{x}'|} = -\frac{1}{4\pi}\frac{1}{|\mathbf{x} - \mathbf{y}|}$$

or

$$G = -\frac{1}{4\pi}\frac{1}{\sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - y_3)^2}}$$

and the solution of the problem

$$\nabla\phi = f(\mathbf{x}), \quad \phi \to 0 \text{ as } |\mathbf{x}| \to \infty$$

is

$$\phi(\mathbf{x}) = -\frac{1}{4\pi} \int \frac{f(\mathbf{y})\, d^3\mathbf{y}}{|\mathbf{x} - \mathbf{y}|}$$

or

$$\phi(x_1, x_2, x_3) = -\frac{1}{4\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} \frac{f(y_1, y_2, y_3)\, dy_1\, dy_2\, dy_3}{\sqrt{(x_1 - y_1)^2 + (x_2 - y_2)^2 + (x_3 - y_3)^2}}.$$

Note that, strictly speaking, $G(\mathbf{x}, \mathbf{y})$ is not defined at $\mathbf{x} = \mathbf{y}$. We should interpret $G(\mathbf{x}, \mathbf{y})$ as some sort of generalised function. One useful interpretation uses the Heaviside function H with

$$G(\mathbf{x}, \mathbf{y}) = \lim_{\epsilon \to 0} -\frac{1}{4\pi} \frac{H(|\mathbf{x} - \mathbf{y}| - \epsilon)}{|\mathbf{x} - \mathbf{y}|}.$$

The Helmholtz equation

Consider the wave equation

$$\frac{\partial^2 \psi}{\partial t^2} = c^2 \nabla \psi.$$

with wave speed c.

If we look for time harmonic standing waves of frequency ω;

$$\psi(\mathbf{x}, t) = e^{-i\omega t} \phi(\mathbf{x})$$

we find that $\phi(\mathbf{x})$ satisfies the Helmholtz equation:

$$(\nabla + k^2)\phi = 0.$$

where $k = \omega/c$ is the wave number. The solutions of the Helmholtz equation represent (the spatial part of) standing wave solutions of the wave equation.

If there is a harmonic momentum source (i.e., a harmonic disturbance $f(\mathbf{x})e^{-i\omega t}$ which is producing the waves) then it appears on the right-hand-side of the Helmholtz equation,

$$(\nabla + k^2)\phi = f(\mathbf{x}).$$

We think of $f(\mathbf{x})$ as a wave source, see figure 2.1.

Physically we expect waves to propagate away from the disturbance generating them and not towards it. This gives us a *radiation condition* which replaces the condition that $\phi \to 0$ as $|\mathbf{x}| \to \infty$ used for Poisson's equation. (We shall describe this radiation condition shortly.)

The Green's function for the Helmholtz equation satisfies

$$(\nabla_x + k^2)G(\mathbf{x}, \mathbf{y}) = \delta(\mathbf{x} - \mathbf{y}).$$

subject a to suitable *radiation condition.* Then

$$\phi(\mathbf{x}) = \int G(\mathbf{x}, \mathbf{y}) f(\mathbf{y}) \, d^3\mathbf{y}$$

Figure 2.1: Radiation condition; waves move away from the source

is the solution of

$$(\nabla + k^2)\phi = f(\mathbf{x})$$

(subject to the same radiation condition as the Green's function).

As before, it is convenient to introduce $\mathbf{x}' = \mathbf{x} - \mathbf{y}$ in which case the problem becomes

$$(\nabla_{x'} + k^2)G = \delta(\mathbf{x}')$$

which clearly has spherical symmetry. So, we look for a solution with $G(\mathbf{x}') = G(r)$, and the problem is then

$$\frac{1}{r}\left(\frac{\partial^2}{\partial r^2}(rG) + k^2(rG)\right) = \frac{\delta(r)}{4\pi r^2}$$

since

$$\nabla \mapsto \frac{1}{r^2}\frac{\partial}{\partial r}\left(r^2\frac{\partial}{\partial r}\right) \equiv \frac{1}{r}\frac{\partial^2}{\partial r^2}\,(r\ )\,.$$

So for $r > 0$ we have

$$\frac{\partial^2}{\partial r^2}(rG) + k^2(rG) = 0$$

which implies that $rG = \alpha e^{ikr} + \beta e^{-ikr}$ or

$$G = \frac{A}{4\pi r}e^{ikr} + \frac{B}{4\pi r}e^{-ikr}$$

If we now consider Ge^{-jkt}, which is a solution of the wave equation, we have

$$Ge^{-ikt} = \frac{A}{4\pi r}e^{ik(r-t)} + \frac{B}{4\pi r}e^{-ik(r+t)}.$$

Now any function $f(r-t)$ represents a wave moving away from $r=0$ towards $r \to \infty$ as t increases (i.e., outward radiation). On the other hand a function $g(r+t)$ represents a wave moving in towards $r=0$ from $r \to \infty$ (i.e., inward radiation).

The δ-function in the problem for G represents a disturbance at the origin; physically we expect waves to propagate outward away from this disturbance and not inward from infinity. This gives us our *radiation condition*—there should only be waves moving away from the disturbance at the origin. Thus we must take $B=0$.

Hence we have

$$G = \frac{A}{4\pi r}e^{ikr}, \quad r > 0.$$

We can extend this to all values of r by defining G to be the generalised function

$$G = \lim_{\epsilon \to 0}\left(\frac{AH(r-\epsilon)}{4\pi r}e^{ikr}\right).$$

We compute the Laplacian of G to find

$$\nabla G = \frac{-Ak^2e^{ikr}}{4\pi r} - A\delta(\mathbf{x}')$$

so that

$$(\nabla + k^2)G = -A\delta(\mathbf{x}')$$

and hence we take $A=-1$:

$$G(\mathbf{x}') = -\frac{1}{4\pi r}e^{ikr} = -\frac{1}{4\pi\left|\mathbf{x}'\right|}e^{ik|\mathbf{x}'|}$$

Finally, recall that $G(\mathbf{x},\mathbf{y}) = G(\mathbf{x}')$ so

$$G(\mathbf{x},\mathbf{y}) = -\frac{1}{4\pi\left|\mathbf{x}-\mathbf{y}\right|}e^{ik|\mathbf{x}-\mathbf{y}|}$$

or

$$G(\mathbf{x},\mathbf{y}) = -\frac{1}{4\pi}\frac{\exp\left(ik\sqrt{(x_1-y_1)^2+(x_2-y_2)^2+(x_3-y_3)^2}\right)}{\sqrt{(x_1-y_1)^2+(x_2-y_2)^2+(x_3-y_3)^2}}$$

Note that as $k \to 0$ we recover the Green's function for the Poisson equation.

Inhomogeneous Helmholtz equation

The solution of the inhomogeneous Helmholtz problem

$$(\nabla + k^2)\phi = f(\mathbf{x})$$

(where we assume $f(\mathbf{x}) \to 0$ as $|\mathbf{x}| \to \infty$) which satisfies the outward radiation condition is given by

$$\phi(\mathbf{x}) = -\frac{1}{4\pi} \int \frac{f(\mathbf{y})}{|\mathbf{x}-\mathbf{y}|} e^{ik|\mathbf{x}-\mathbf{y}|}\, d^3\mathbf{y}$$

or

$$\phi(x_1, x_2, x_3) = -\frac{1}{4\pi} \int_{-\infty}^{\infty}\int_{-\infty}^{\infty}\int_{-\infty}^{\infty} f(y_1, y_2, y_3) \times \\ \times \frac{\exp\left(ik\sqrt{(x_1-y_1)^2 + (x_2-y_2)^2 + (x_3-y_3)^2}\right)}{\sqrt{(x_1-y_1)^2 + (x_2-y_2)^2 + (x_3-y_3)^2}} dy_1\, dy_2\, dy_3.$$

This represents the (spatial part of) an outgoing train of waves caused by a disturbance in the region where $f(\mathbf{x}) \neq 0$.

2.8.2 Green's functions for Bounded Regions

In this section, we deal with the Helmholtz equation

$$(\nabla + k^2)\phi = f(\mathbf{x})$$

and determine Green's functions relevant to problems where the region of interest is bounded. Results for the Poisson equation follow by taking the limit $k \to 0$.

Interior problems for Helmholtz and Poisson equations

In the previous section we considered the free space problems of the form

$$(\nabla_x + k^2)\phi = f(\mathbf{x}), \tag{2.8}$$

and

$$(\nabla_x + k^2)G = \delta(\mathbf{x}-\mathbf{y}) \tag{2.9}$$

and expressed the solution of (2.8) in the form

$$\phi(\mathbf{x}) = \int f(\mathbf{y})G(\mathbf{x},\mathbf{y})\, d^3\mathbf{y}. \tag{2.10}$$

To deal with problems where boundaries are present, it is convenient to adopt a more general point of view. Suppose we regard the point $\mathbf{x}$ as fixed and $\mathbf{y}$ as the variable in the equation for the Green's function. That is, suppose the Green's function satisfies

$$(\nabla_y + k^2)G(\mathbf{x},\mathbf{y}) = \left(\frac{\partial^2}{\partial y_1^2} + \frac{\partial^2}{\partial y_2^2} + \frac{\partial^2}{\partial y_3^2} + k^2\right) G = \delta(\mathbf{x}-\mathbf{y}).$$

Now, write equations (2.8) and (2.9) as

$$(\nabla_y + k^2)\phi = f(\mathbf{y}) \tag{2.11}$$

and

$$(\nabla_y + k^2)G = \delta(\mathbf{x}-\mathbf{y}) \tag{2.12}$$

but regard $\mathbf{x}$ as the point in a bounded region V in $\mathbf{y}$-space where we want the solution ϕ.

Suppose that $G(\mathbf{x},\mathbf{y})$ is any solution of (2.11)); there are infinitely many solutions of (2.11) and specific forms for G are obtained only when we impose boundary conditions on the surface S of V.[2] Multiplying (2.11) by $G(\mathbf{x},\mathbf{y})$, multiplying (2.12) by $\phi(\mathbf{y})$ and subtracting these gives:

$$G\nabla_y\phi(\mathbf{y}) - \phi(\mathbf{y})\nabla_y G = f(\mathbf{y})G - \phi(\mathbf{y})\delta(\mathbf{x}-\mathbf{y}).$$

Integrate this with respect to $\mathbf{y}$ over V then gives

$$\begin{aligned}\int_V \Big(G(\mathbf{x},\mathbf{y})\nabla_y\phi(\mathbf{y}) - \phi(\mathbf{y})\nabla_y G(\mathbf{x},\mathbf{y})\Big)\, d^3\mathbf{y} \\ = \int_V f(\mathbf{y})G(\mathbf{x},\mathbf{y})\, d^3\mathbf{y} - \int_V \phi(\mathbf{y})\delta(\mathbf{x}-\mathbf{y})\, d^3\mathbf{y}.\end{aligned}$$

Using Green's theorem and the properties of $\delta(\mathbf{x}-\mathbf{y})$ we then find

$$\begin{aligned}\phi(\mathbf{x}) = \int_V f(\mathbf{y})G(\mathbf{x},\mathbf{y})\, d^3\mathbf{y} \\ + \int_S \left(\phi(\mathbf{y})\frac{\partial G}{\partial n_y}(\mathbf{x},\mathbf{y}) - G(\mathbf{x},\mathbf{y})\frac{\partial\phi}{\partial n_y}(\mathbf{y})\right) d^2\mathbf{y}\end{aligned} \tag{2.13}$$

where $\partial/\partial n_y$ denotes normal derivative with respect to the $\mathbf{y}$ variables, i.e.,

$$\frac{\partial G}{\partial n_y} = (\nabla_y G)\cdot\mathbf{n}_y.$$

[2]This is because to any solution of (2.12) we can add a solution ψ of (2.11) and then $(\nabla + k^2)(G+\psi) = (\nabla+k^2)G + (\nabla+k^2)\psi = \delta(\mathbf{x}-\mathbf{y})$.

The representation (2.13) is called the Kirchhoff–Helmholtz representation. It gives the value of $\phi(\mathbf{x})$ inside the region V in terms of the source distribution $f(\mathbf{x})$ in V and the values of ϕ and $\partial\phi/\partial n$ on the surface S. It is true for *any* $G(\mathbf{x},\mathbf{y})$ that satisfies (2.12).

When attempting to solve (2.8) analytically, we attempt to choose G so that we minimise the amount of information we need to know about ϕ and $\partial\phi/\partial n$ on the boundary. For example, if we are given a Dirichlet problem, so ϕ is prescribed on the boundary, then we try to find G so that $G(\mathbf{x},\mathbf{y}) = 0$ when $\mathbf{y}$ is on the boundary. This eliminates the unknown $\partial\phi/\partial n$ and allows us to calculate ϕ in terms of known quantities. Similarly, for the Neumann problem where we know $\partial\phi/\partial n$ on the boundary we try to find G so that $(\partial G/\partial n)(\mathbf{x},\mathbf{y}) = 0$ when $\mathbf{y}$ is on the boundary. This eliminates the unknown ϕ from the integral over the surface.

Note that (2.13) can also be used numerically. We choose a simple G, say a free space Green's function, and this gives us an integral equation to solve numerically. For example if we are given a Neumann problem with $\partial\phi/\partial n$ specified on the boundary (but we do not know ϕ on the boundary) then by choosing $\mathbf{x}$ to be a point on the boundary, (2.8) becomes an integral equation for the unknown $\phi(\mathbf{x})$ on the boundary. This is solved numerically, and once we know $\phi(\mathbf{x})$ on the boundary, then (2.8) tells us the value of $\phi(\mathbf{x})$ at all points inside the boundary. This is the essence of "boundary integral methods". Note that the integral equation is two dimensional whereas the original problem is three dimensional. This reduction in dimensionality is why boundary integral methods are powerful for efficiently solving problems.

The Dirichlet Problem This is the problem of finding ϕ in V given that

$$\begin{aligned}(\nabla + k^2)\phi &= f(\mathbf{x}) \quad \text{in } V\\ \phi &= g(\mathbf{x}) \quad \text{on } S.\end{aligned}$$

We solve this in terms of the Kirchhoff–Helmholtz representation by eliminating the unknown $\partial\phi/\partial n$ from the integral, that is, we attempt to find a Green's function such that

$$\begin{aligned}(\nabla_y + k^2)G(\mathbf{x},\mathbf{y}) &= \delta(\mathbf{x}-\mathbf{y}) \quad \text{in } V\\ G(\mathbf{x},\mathbf{y}) &= 0 \quad \text{when } \mathbf{y} \text{ on } S.\end{aligned}$$

In practice it may be difficult to find such a G, but assuming G is known the solution is then, from the Kirchhoff-Helmholtz representation,

$$\phi(\mathbf{x}) = \int_V f(\mathbf{y})G(\mathbf{x},\mathbf{y})d^3\mathbf{y} + \int_S g(\mathbf{y})\frac{\partial G}{\partial n}(\mathbf{x},\mathbf{y})\,d^2\mathbf{y}.$$

The Neumann problem

This is the problem of finding ϕ in V given that

$$\begin{aligned}(\nabla + k^2)\phi &= f(\mathbf{x}) \quad \text{in } V \\ \frac{\partial \phi}{\partial n} &= g(\mathbf{x}) \quad \text{on } S.\end{aligned}$$

We solve this in terms of the Kirchhoff–Helmholtz representation by eliminating the unknown ϕ from the integral, that is, we attempt to find a Green's function such that

$$\begin{aligned}(\nabla_y + k^2)G(\mathbf{x},\mathbf{y}) &= \delta(\mathbf{x}-\mathbf{y}) \quad \text{in } V \\ \frac{\partial G}{\partial n}(\mathbf{x},\mathbf{y}) &= 0 \quad \text{when } \mathbf{y} \text{ on } S.\end{aligned}$$

Assuming G can be found, the solution is then

$$\phi(\mathbf{x}) = \int_V f(\mathbf{y})G(\mathbf{x},\mathbf{y})d^3\mathbf{x} - \int_S g(\mathbf{y})G(\mathbf{x},\mathbf{y})\, d^2\mathbf{y}.$$

Robin boundary conditions

This is the problem of finding ϕ in V given that

$$\begin{aligned}(\nabla + k^2)\phi &= f(\mathbf{x}) \quad \text{in } V \\ \frac{\partial \phi}{\partial n}(\mathbf{x}) + \lambda(\mathbf{x})\phi(\mathbf{x}) &= g(\mathbf{x}) \quad \text{on } S\end{aligned}$$

where $f(\mathbf{x})$, $g(\mathbf{x})$ and $\lambda(\mathbf{x})$ are all given functions.

We solve this in terms of the Kirchhoff–Helmholtz representation by eliminating the unknown $\partial\phi/\partial n$ from the problem using the fact that

$$\frac{\partial \phi}{\partial n}(\mathbf{x}) = g(\mathbf{x}) - \lambda(\mathbf{x})\phi(\mathbf{x}) \quad \text{on } S.$$

so the Kirchhoff-Helmholtz representation (2.13) becomes

$$\begin{aligned}\phi(\mathbf{x}) = &\int_V f(\mathbf{y})G(\mathbf{x},\mathbf{y})\, d^3\mathbf{y} \\ &+ \int_S \phi(\mathbf{y}) \left(\frac{\partial G}{\partial n}(\mathbf{x},\mathbf{y}) + \lambda(\mathbf{y})G(\mathbf{x},\mathbf{y}) \right) d^2\mathbf{y} \\ &- \int_S g(\mathbf{y})G(\mathbf{x},\mathbf{y})\, d^2\mathbf{y}\end{aligned}$$

Then, as we do not know ϕ on the surface S, we choose G so that this term is eliminated. That is, we choose G to be a solution of

$$\begin{aligned}(\nabla_y + k^2)G(\mathbf{x},\mathbf{y}) &= \delta(\mathbf{x}-\mathbf{y}) \quad \text{in } V \\ \frac{\partial G}{\partial n}(\mathbf{x},\mathbf{y}) + \lambda(\mathbf{y})G(\mathbf{x},\mathbf{y}) &= 0 \quad \text{when } \mathbf{y} \text{ on } S.\end{aligned}$$

Assuming G can be found, the solution is then

$$\phi(\mathbf{x}) = \int_V f(\mathbf{y})G(\mathbf{x},\mathbf{y})d^3\mathbf{x} - \int_S g(\mathbf{y})G(\mathbf{x},\mathbf{y})\, d^2\mathbf{y}.$$

2.8.3 The Reciprocal Theorem

In all of the problems in this section, the Green's function is symmetric, that is

$$G(\mathbf{x},\mathbf{y}) = G(\mathbf{y},\mathbf{x}).$$

This is why the general method in which we find G by solving a partial differential equation in $\mathbf{y}$ variables (used in this section) is equivalent to the more naive method of the previous chapter where we found G by solving a partial differential equation in $\mathbf{x}$ variables.

We illustrate this symmetry for the Dirichlet problem for the Poisson equation:

Reciprocal Theorem

It is worth noting a mathematical property of the Green's function that may be exploited in certain situations. If $G(\mathbf{x},\mathbf{y})$ is the solution of

$$\begin{aligned} \nabla G(\mathbf{x},\mathbf{y}) &= \delta(\mathbf{x}-\mathbf{y}) \quad \text{in } V \\ G(\mathbf{x},\mathbf{y}) &= 0 \quad \text{for } \mathbf{x} \text{ on } S \end{aligned}$$

then

$$G(\mathbf{x},\mathbf{y}) = G(\mathbf{y},\mathbf{x}).$$

Hence physically the effect at a point $\mathbf{x}$ of imposing a force at point $\mathbf{y}$ is the same at the effect at a point $\mathbf{y}$ of imposing a force at point $\mathbf{x}$.

2.8.4 Exterior problems

The general Kirchhoff-Helmholtz solution (2.13) can be shown to be valid for exterior problems provided physical conditions ensure that ϕ decays at large distances (i.e, for $k = 0$ $\phi \to 0$ as $|\mathbf{x}| \to \infty$) or has outgoing wave behaviour (i.e, for $k \neq 0$ satisfies the radiation condition).

3 Nonlinear waves

3.1 Traffic flow, river flow, two-phase flow

A relative simple model of flow of traffic on a single lane road describes the density of traffic as a continuous variable and hence the movement as being like a fluid. Such models are rather over simplified since stochastic behaviour of drivers is a large element in the dynamics, however we present it here as it is easy to visualise. Taking the density to be ρ (cars/km) and the speed to be u (km/s) we exploit "conservation of cars" on a 1-D road to give

$$\frac{\partial \rho}{\partial t} + \frac{\partial (\rho u)}{\partial x} = 0$$

The simplest model is then completed by including a constitutive equation which, for example assumes that drivers travel at a speed determined by the density of traffic on the road. Such a constitutive relation might assume that cars have a maximum speed limit and they go slower the higher the traffic density and might take the form

$$u = u_{max}(1 - \rho/\rho_{max})$$

where, u_{max} is the maximum speed and ρ_{max} is a constant representing the maximum density cars will fit on the road (and at that density the traffic is stationary). The resulting equation for the traffic density is the kinematic equation

$$\frac{\partial \rho}{\partial t} + u_{max}\frac{\partial (\rho - \rho^2/\rho_{max})}{\partial x} = 0.$$

For flow in an estuary or a river we can return to the ideas of "Stokes waves" given earlier in the course. The main difference here is that the tidal variations on an estuary (the height variations) can get to be as large as the depth of the water. Hence a model should account for this rather than consider the very small waves that were analysed in the section on Stokes waves. The basic model assumes that in the inviscid fluid the velocity is approximately uniform with depth. Hence if h is the water depth, u is the average velocity, then the mass conservation equation can be integrated in the vertical direction between the estuary bed at $z = 0$ to the water surface $z = y$ to get

$$\frac{\partial h}{\partial t} + \frac{\partial (hu)}{\partial x} = 0$$

while conservation of momentum with just gravity acting on the inviscid fluid, again integrated from $z = 0$ to $z = h$, is

$$\frac{\partial (hu)}{\partial t} + \frac{\partial (hu^2)}{\partial x} + \frac{\partial (gh^2)}{\partial x} = 0$$

This system is typically referred to as the "shallow water equations". The previous two equations are in conservation form but quite often they are presented in a form found by subtracting u times the first equation from the second to give the system

$$\frac{\partial h}{\partial t} + +u\frac{\partial h}{\partial x} + h\frac{\partial u}{\partial x} = 0$$
$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} + g\frac{\partial h}{\partial x} = 0$$

In many oil fields, once the oil has finished coming out of wells under its own pressure, a second phase is reached as water is pumped into the oil reservoir to push a further significant fraction of the oil out (there are interesting problems to do with how to extract even more oil once the water pumping has ceased to be effective). To model water pushing oil out of rock we start by assuming both fluids are incompressible but that at any point there is a saturation, S, which is the volume fraction of water in the rock pores (and hence the volume fraction of oil in the pores is $(1-S)$). Conservation of mass for each fluid therefore gives

$$\frac{\partial(S\rho_{water})}{\partial t} + +\frac{\partial(S\rho_{water}\mathbf{q}_{water})}{\partial x} = 0, \qquad \frac{\partial((1-S)\rho_{oil}}{\partial t} + +\frac{\partial((1-S)\rho_{oil}\mathbf{q}_{oil})}{\partial x} = 0$$

where $\mathbf{q}_{water}$ and $\mathbf{q}_{oil}$ are the flow of the respective fluid phases (water or oil). For momentum balance we use "Darcy flow" to describe the flow of each phase.

$$\mathbf{q}_{oil} = \frac{-K_{oil}}{\mu_{oil}}\frac{\partial p_{oil}}{\partial x}, \qquad \mathbf{q}_{water} = \frac{-K_{ware}}{\mu_{water}}\frac{\partial p_{water}}{\partial x}$$

where K_{oil} and K_{water} are the "permeabilities" of the fluid and are strong function of S at any point (eg $K_{water} \to 0$ as $S \to 0$, $K_{oil} \to 0$ as $S \to 1$). The μ are the respective fluid viscosities and the p are the pressures in the fluids. If the capillary pressure between oil and water is small (not usually true) then we assume that

$$p_{oil} = p_{water}.$$

From this we find the following equations hold

$$S_t + (SK_{water}p_x)x = 0, \qquad ((SK_{water} + (1-S)K_{oil})p_x)_x = 0.$$

If we now integrate the final equation and impose a fixed total flux of fluid, Q at some point x, then

$$p_x = \frac{Q}{(SK_{water} + (1-S)K_{oil})}$$

and the saturation is governed by a single equation

$$S_t + \left(\frac{QSK_{water}}{(SK_{water} + (1-S)K_{oil})}\right)_x = 0.$$

This is called the Buckley-Leverett model of 2-phase flow.

3.2 Classification of systems of PDEs

Throughout this course we have been looking at a number of different PDE problems. We now turn to discuss how to classify the different types of PDEs and to discuss the consequences in terms of the initial and boundary data that should be imposed to make the problem wellposed. When considering classifying PDEs the two approaches are to look at semi-linear second order equations or systems of quasi-linear first order equations. Here we adopt the latter method as it allows us to consider large systems and the former method can be put into this same framework. We shall simplify the discussion by working with just two independent variables x, y with a dependent vector $\mathbf{z}(x, y)$ of length n and make a few comments about how some of the ideas relate to systems in higher dimensions.

We consider the quasi-linear system

$$\mathbf{A}(x, y, \mathbf{z})\frac{\partial \mathbf{z}}{\partial x} + \mathbf{B}(x, y, \mathbf{z})\frac{\partial \mathbf{z}}{\partial y} = \mathbf{C}(x, y, \mathbf{z})$$

where $\mathbf{A}$, $\mathbf{B}$ are matrices of size $(n \times n)$ and $\mathbf{C}$ is a vector of length n.

Many second order linear equations can be written in this form but care must be taken to ensure the resulting system is just 2×2. There are many physical systems where the governing laws are derived using a number of first order equations although the result in often presented as a second order equation. (for example Newton's second law: $\dot{x} = v$, $\dot{v} = \text{Force}/m$).

Simple examples are:

Laplace's equation $z_{1_{xx}} + z_{1_{yy}} = 0$

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}_x + \begin{pmatrix} 0 & 1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}_y = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

The wave equation $z_{1_{xx}} = z_{1_{yy}}$

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}_x + \begin{pmatrix} 0 & -1 \\ -1 & 0 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}_y = \begin{pmatrix} 0 \\ 0 \end{pmatrix}$$

and the heat equation $z_{1_{xx}} - z_{1_y} = 0$

$$\begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}_x + \begin{pmatrix} 0 & 0 \\ 0 & -1 \end{pmatrix} \begin{pmatrix} z_1 \\ z_2 \end{pmatrix}_y = \begin{pmatrix} z_2 \\ 0 \end{pmatrix}$$

The classification of such equations is made by locally freezing the coefficient matrices $\mathbf{A}$ and $\mathbf{B}$ and examining the characteristics of the resulting linearised system.

Method of characteristics

For the simplest case of a single quasi-linear PDE the characteristics are relatively easy to find. Given

$$a(x,y,z)z_x + b(x,y,z)z_y = c(x,y,z)$$

we seek to change coordinates from x, y to s, r such that the PDE reduces to a PDE. Hence using the chain rule

$$x_s z_x + y_s z_y = z_s$$

we see this equivalent to the PDE if we choose

$$\frac{\partial x}{\partial s} = a(x,y,z) \qquad \frac{\partial y}{\partial s} = b(x,y,z) \qquad \frac{\partial z}{\partial s} = c(x,y,z).$$

We can then observe that the solution can be obtained by solving this system of ODES (the variable r is only a parameter in them). The system will require data at some point $s = 0$ and this is provided by the initial data where z is given on a curve $f(x, y) = 0$ which we can parametrises by the variable r.

The resulting curves (x, y), where r is constant, are the "projected characteristics" of the system and indicate the path along which the "information" from the initial data travels (formally the "characteristics" are the curves (x, y, u) where r is constant, but this distinction is seldom made) . The local slope of these projected characteristics is given by

$$\frac{dy}{dx} = \frac{y_s}{x_s} = \frac{b}{a} = \lambda$$

or

$$\lambda a - b = 0.$$

(note a simple check on what slope *lambda* represents is to note the operators are $\mathbf{A}\partial/\partial x$ and $\mathbf{B}\partial/\partial y$ so that the dimensions are $\mathbf{A}/dx$ and $\mathbf{B}/dy$ Hence dimensionally the equation for the slope must be $|\mathbf{A}dy/dx - \mathbf{B}| = 0$.)

This approach also demonstrated that the initial data must not be given along a line that is a characteristics (ie initial data must not a curve with a tangent vector $x_r = a$, $y_r = b$ as, unless we are very lucky, the data for z will be inconsistent with $z_r = c$.

One final note is that this method parametrises the solution by s, r and it is not obvious that we will have a 1-1 mapping of s, r to x, y. we revisit this problem later.

Example (this and others can be found in the notes for the Oxford Part B course B5b - Applied PDEs at
`https://www0.maths.ox.ac.uk/system/files/coursematerial/2014/3078/6/B5b1.pdf`

Solve the PDE

$$u_t + u\, u_x = 1$$

for $u(x,t)$ in $t > 0$, subject to the initial condition $u = x$ on $t = 0$. The characteristics are given by

$$\frac{dt}{dr} = 1, \qquad \frac{dx}{dr} = u, \qquad \frac{du}{dr} = 1$$

and the initial data may be parametrised by

$$t = 0, \qquad x = s, \qquad u = s \quad \text{at } r = 0.$$

Solving for t first, we see that $t = r + A(s)$ and the initial data then makes $t = r$ and thus we may replace r by t henceforth. The initial-value problem for u has the solution

$$u = s + t$$

so that the problem for x becomes

$$\frac{dx}{dt} = s + t \qquad \text{with } x = s \text{ when } t = 0$$

whose solution is

$$x = s + st + \frac{1}{2}t^2$$

Now we can now find s in terms of u, t, x and use it to obtain the solution in explicit form

$$u = \frac{x + t + \frac{1}{2}t^2}{1 + t}$$

Returning to the classification problem for a system of first order PDEs. we now perform a procedure similar to that for a single first order PDE. Note that if we had n independent PDEs then there would be n independent characteristics at each point in (x, y). Our approach is simply to find the slope of these characteristics at each point (x, y) and we denote this slope locally by $\lambda = dy/dx$. This slope must satisfy the condition

$$\|\mathbf{B} - \lambda \mathbf{A}\| = 0.$$

This is a polynomial for λ and the roots dependent of the coefficients and hence possibly on x, y and $\mathbf{z}$. We classify the local behaviour of the PDE based on these roots.

Hyperbolic

If all the roots are real and distinct (no repeated roots) then we can imagine that information is travelling in various directions at any point. Formally the

"information" is the set of left eigenvectors. Such a system is *hyperbolic* and exhibits wavelike behaviour with the waves travelling along the characteristics. Hence if data is specified on some curve it will only affect the solution in a limited region of x, y due to the wave behaviour. Typically we would have one of the variable being "time" and the other representing space. Note that a 'time-like" variable need not be actual time but can be a space coordinate.

Parabolic

Note if a degenerate case occurs and roots are equal then the system is *parabolic* if the eigenspace is also degenerate and hyperbolic otherwise.

Elliptic

If all the roots are complex (non-zero imaginary part) then there is no concept of propagating information. Such a system is *elliptic* and if data is specified on some curve then it will affect the solution everywhere in (x, y). This global influence of data makes such models very difficult to interpret as having a time-like variable since data affect both the future and the past. Such equations typically appear when considering steady state problems.

Mixed systems and other

There are of course a huge variety of other possible behaviours of the roots. A general rule is that a problem where one of independent variables is actually time then all the roots λ should be real, although not necessarily distinct, everywhere in (x, y) and $\mathbf{z}$.

Some general approximate rules for boundary conditions can be extracted from characteristics. If the system is hyperbolic then one variable is time-like and hence we want the problem to be posed so that events are not influenced by the future. This implies that as the time-like variable increases we want information to propagate along the characteristics from the past to future. At boundaries of the region this means that as time increases any characteristic entering the region from the boundary must be given data in the form of a boundary or initial condition. (General rule: the number of conditions needed at a boundary equals the number of characteristics entering the solution region at that point as time increases)
Note: there is a further complication that the information must include some aspect of the eigenvector related to the particular characteristic. Furthermore there the conditions at the boundary cannot specify values of the information of characteristics leaving the region. This tells us that all variables should be specified initially and at boundaries the number of variables will change as the number of characteristics entering or leaving the region changes. Hyperbolic systems, due to their time-like variable, are typically posed on finite regions in the space variable and semi-infinite regions in the time-like variable.

If the system is elliptic then the slope of the characteristics, λ, all appear in complex conjugate pairs (note this requires that there are an even number of variables and assumes all parameters in the equation are real). For these systems it is necessary to impose conditions equal to half the number variables at each point on the boundary. Such problems are typically posed on finite regions of (x, y) although this is not always necessary.

3.3 Shocks and causality

The method of characteristics can be used to find the solution to a single quasi-linear PDE in two dimensions. As we have seen the solution is found parametrised by the new variables r and s. We have seen that it can be difficult to find a explicit solution given the implicit function $x(r, s)$, $t(r, s)$ and $u(r, s)$. The more significant difficult is that the mapping between x, t and r, s may not be one-to-one. In particular the projected characteristics my intersect and then the solution is multivalued in x, t. Such behaviour can also occur for systems of quasi-linear PDEs. If the problem is hyperbolic we will assume that the solution to the PDE is valid up to the "time" when the intersection occurs. We now explore how we can extend the solution to the problem past such a point (formally the solution to the PDE problem ceases to exist)

Note there are two types of discontinuous behaviour in quasi-linear PDEs. The first type relates to discontinuities in the initial data that propagate but have differentiable behaviour along characteristics (see for example the equation of a string with discontinuous initial data) which are typically called contact discontinuities (they also occur commonly in gas dynamics). The second type relates to discontinuities that are created by the nonlinear behaviour of the problem which are commonly called shocks. Here we examine shocks.

We now consider, weak solutions of the PDE problem and allow the solution to have discontinuities. For these weak solutions to be physically reasonable we need to return to the original conservation laws that underlie the problem. (beware: the same PDE can be extended to have many possible different forms for the weak solution)

Previously we could have derived the conservation of mass in the form

$$\frac{\partial}{\partial t} \iiint_V \rho \, dV = \iint_{\partial V} \rho \mathbf{u} \cdot d\mathbf{S}$$

and we then integrate the surface integral by parts. However, we are now interested in the case where u may be discontinuous. Hence if there is a discontinuity we consider a region V that covers the discontinuity and allow this region to shrink

to the line containing the discontinuity. (see notes from Oxford's Part B B5b - Applied Differential Equations p6-18 for more details).

One alternative approach to finding the behaviour at a shock, and one then ensures that we only physically relevant shocks in the solution is the method of "viscous solutions" or "entropy". Consider the case where the physical conservation law is

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = \epsilon \frac{\partial^2 u}{\partial x^2}$$

for some "flux function" $f(u)$. Note that the crucial idea here is that there is some underlying dissipation due to diffusivity and that it is critical to have the correct form of the PDE as otherwise we can introduce discontinuities that only conserve other quantities across them and not the physically relevant one.

On physical grounds we assume that the parameter ϵ is extremely small and hence anticipate that we should be able to solve the simple hyperbolic equation

$$\frac{\partial u}{\partial t} + \frac{\partial f(u)}{\partial x} = 0$$

This is a valid approach in regions where the solution is smooth but if the hyperbolic equation predicts that the solution gradient gets large (and a discontinuity is forming) then we need to reconsider the problem. consider the discontinuity to be forming on a curve given locally by $x = Vt + C$, where V is the local speed of the shock. If we rescale to be near this point the we take

$$\eta = \epsilon(x - Vt + C)$$

and then seek a travelling wave solution with the properties that
i) as $\eta \to -\infty$ $u \to u^-$
ii) as $\eta \to +\infty$ $u \to u^+$
where u^- and u^+ are constants determined by the smooth behaviour of the hyperbolic equation. Using this variable and sending $\epsilon \to 0$ we get the ODE

$$-Vu_\eta + (f(u))_\eta = u_{\eta\eta}$$

which integrates to give

$$-Vu + f(u) = u_\eta + D \ .$$

Now we impose that boundary conditions noting that in both cases $u_\eta \to 0$ at large distances and hence we require

$$-Vu^+ + f(u^+) = D \text{ and } -Vu^- + f(u^-) = D \ .$$

Hence we conclude that such a travelling wave is only possible if

$$-Vu^+ + f(u^+) = -Vu^- + f(u^-).$$

If follows therefore that we need to have the speed of the shock V at any point determined by the behaviour on either side of the shock and that

$$V = \frac{[u]^+_-}{[f(u)]^+_-}$$

This relation is called the "Rankine-Hugoniot" condition and allows us to extend the solution of the conservation law to regions where the solution has discontinuities which travel at this speed V.

Note also that this derivation requires that the travelling wave satisfy the ODE

$$-Vu + f(u) = u_\eta + D \ .$$

and this will only hold for certain combinations of the u^+ and u^- because of the sign of u_η. There are physically irrelevant solutions which do not satisfy this ODE and typically these irrelevant solutions have characteristics that leave the shock as time increases (rather than the physically relevant solutions where characteristics enter the shock). For example if we linearise around u^+ and around u^- assuming $f(u)$ is differentiable we find that in order for a physically relevant travelling wave to exist we need at least to have

$$f'(u^-) > V \text{ and } f'(u^+) < V.$$

3.4 Charpit's method

The previous discussion was about quasi-linear systems of PDEs in two dimensions. We now turn to more complicated problems and consider a single dependent variable where the governing equations simply give a relation between the the two dependent variables, the dependent variable and the two partial derivatives. Such problems can be written in the form

$$F(p, q, u, x, y) = 0, \tag{3.1}$$

where we use the notation

$$\frac{\partial u}{\partial x} = p, \quad \frac{\partial u}{\partial y} = q$$

as shorthand. We now discuss how to solve such problems using Charpit's method. We start by noting the consistency condition that

$$\frac{\partial p}{\partial y} = \frac{\partial q}{\partial x} \qquad \text{from } u_{xy} = u_{yx}. \tag{3.2}$$

If we differentiate (3.1) with respect to x and y, we obtain

$$\begin{aligned}\frac{\partial F}{\partial p}\frac{\partial p}{\partial x}+\frac{\partial F}{\partial q}\frac{\partial q}{\partial x} &= -\frac{\partial F}{\partial x}-p\frac{\partial F}{\partial u},\\ \frac{\partial F}{\partial p}\frac{\partial p}{\partial y}+\frac{\partial F}{\partial q}\frac{\partial q}{\partial y} &= -\frac{\partial F}{\partial y}-q\frac{\partial F}{\partial u},\end{aligned}$$

or, using (3.2),

$$\frac{\partial F}{\partial p}\frac{\partial p}{\partial x}+\frac{\partial F}{\partial q}\frac{\partial p}{\partial y} = -\frac{\partial F}{\partial x}-p\frac{\partial F}{\partial u}, \tag{3.3}$$

$$\frac{\partial F}{\partial p}\frac{\partial q}{\partial x}+\frac{\partial F}{\partial q}\frac{\partial q}{\partial y} = -\frac{\partial F}{\partial y}-q\frac{\partial F}{\partial u}. \tag{3.4}$$

So, if we define *characteristics* or *rays* as curves $(x(\tau), y(\tau))$ satisfying

$$\frac{\mathrm{d}x}{\mathrm{d}\tau}=\frac{\partial F}{\partial p}, \quad \frac{\mathrm{d}y}{\mathrm{d}\tau}=\frac{\partial F}{\partial q}$$

then, along these curves,

$$\begin{aligned}\frac{\mathrm{d}p}{\mathrm{d}\tau} &= \frac{\partial p}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}\tau}+\frac{\partial p}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}\tau}=-\frac{\partial F}{\partial x}-p\frac{\partial F}{\partial u},\\ \frac{\mathrm{d}q}{\mathrm{d}\tau} &= \frac{\partial q}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}\tau}+\frac{\partial q}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}\tau}=-\frac{\partial F}{\partial y}-q\frac{\partial F}{\partial u},\end{aligned}$$

by (3.3), (3.4). We therefore have a system of four ODEs for x, y, p and q satisfied along the rays. Recall, though, that in general F depends on u also, so to close the system we also need an ODE for u along the rays, namely

$$\frac{\mathrm{d}u}{\mathrm{d}\tau}=\frac{\partial u}{\partial x}\frac{\mathrm{d}x}{\mathrm{d}\tau}+\frac{\partial u}{\partial y}\frac{\mathrm{d}y}{\mathrm{d}\tau}=p\frac{\partial F}{\partial p}+q\frac{\partial F}{\partial q}.$$

In summary, we have the following system of ODEs for x, y, p, q and u, known as *Charpit's equations*:

$$\frac{\mathrm{d}x}{\mathrm{d}\tau}=\frac{\partial F}{\partial p}, \qquad \frac{\mathrm{d}y}{\mathrm{d}\tau}=\frac{\partial F}{\partial q},$$

$$\frac{\mathrm{d}p}{\mathrm{d}\tau}=-\frac{\partial F}{\partial x}-p\frac{\partial F}{\partial u}, \qquad \frac{\mathrm{d}q}{\mathrm{d}\tau}=-\frac{\partial F}{\partial y}-q\frac{\partial F}{\partial u}, \qquad \frac{\mathrm{d}u}{\mathrm{d}\tau}=p\frac{\partial F}{\partial p}+q\frac{\partial F}{\partial q}. \tag{3.5}$$

3.4.1 Boundary data

We now consider how to impose boundary conditions on a solution found by Charpit's method. We assume that the conditions are given as Cauchy data which specifies u along some curve Γ in the (x, y)-plane:

$$x = x_0(s), \quad y = y_0(s), \quad u = u_0(s), \tag{3.6}$$

for s in some (possibly infinite) interval. We also require initial conditions for p and q, say $p = p_0(s)$, $q = q_0(s)$, which are obtained by differentiating u_0 with respect to s and using the PDE (3.1):

$$\frac{\mathrm{d}u_0}{\mathrm{d}s} = p_0 \frac{\mathrm{d}x_0}{\mathrm{d}s} + q_0 \frac{\mathrm{d}y_0}{\mathrm{d}s}, \quad F\left(p_0, q_0, u_0, x_0, y_0\right) = 0. \tag{3.7}$$

The two equations (3.7) may be solved (in principle, if not explicitly) for p_0 and q_0 provided the condition

$$\frac{\mathrm{d}x_0}{\mathrm{d}s}\frac{\partial F}{\partial q_0} - \frac{\mathrm{d}y_0}{\mathrm{d}s}\frac{\partial F}{\partial p_0} \neq 0 \tag{3.8}$$

is satisfied. This is the same as insisting that Γ not be parallel to a ray.

Charpit's method consists of solving the ODEs (3.5) for (p, q, u, x, y), with (3.6) and (3.7) as initial data at $\tau = 0$. This gives (p, q, u, x, y) all as functions of s and τ and, in principle, allows us to reconstruct the solution surface $u = u(x, y)$.

Example 1. Sugar on a spoon
Consider sugar piled up on a spoon such that its height is given by $u(x, y)$. At criticality, just before the sugar would start to slide off the spoon, the sugar makes a constant angle (the "angle of repose") γ with the horizontal, that is

$$|\boldsymbol{\nabla} u|^2 = \left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2 = \tan^2\gamma.$$

After normalisation, (such as taking $u = \tan\gamma\ \bar{u}$) this can be written as the *Eikonal equation*

$$\left(\frac{\partial u}{\partial x}\right)^2 + \left(\frac{\partial u}{\partial y}\right)^2 = 1, \tag{3.9}$$

which is of the form (3.1) with

$$F(p, q) = \tfrac{1}{2}\left(p^2 + q^2 - 1\right).$$

Charpit's equations for this particular F are

$$\frac{\mathrm{d}x}{\mathrm{d}\tau} = p, \quad \frac{\mathrm{d}y}{\mathrm{d}\tau} = q, \quad \frac{\mathrm{d}p}{\mathrm{d}\tau} = 0, \quad \frac{\mathrm{d}q}{\mathrm{d}\tau} = 0, \quad \frac{\mathrm{d}u}{\mathrm{d}\tau} = p^2 + q^2 = 1.$$

Notice that p and q are constant along rays and, hence, given by their boundary values:

$$p = p_0(s), \quad q = q_0(s).$$

The remaining ODEs are then readily integrated to give

$$x = x_0(s) + p_0(s)\tau, \quad y = y_0(s) + q_0(s)\tau, \quad u = u_0(s) + \tau.$$

Notice that the slope of a ray is given by $q_0(s)/p_0(s)$ which is constant along each ray. Thus the rays are *straight lines*, along which u increases linearly with τ.

At the edge of the spoon, the height is zero, so $u_0(s) = 0$. Then we have the system

$$\frac{\mathrm{d}x_0}{\mathrm{d}s}p_0 + \frac{\mathrm{d}y_0}{\mathrm{d}s}q_0 = 0, \quad p_0^2 + q_0^2 = 1$$

for p_0 and q_0, whose solution is

$$p_0 = \frac{\mp y_0'}{\sqrt{(x_0')^2 + (y_0')^2}}, \quad q_0 = \frac{\pm x_0'}{\sqrt{(x_0')^2 + (y_0')^2}}, \tag{3.10}$$

where $'$ is used as shorthand for $d/\mathrm{d}s$. The vector (p_0, q_0) is the *unit normal* to the boundary Γ. Hence the rays are straight lines perpendicular to Γ and $u(x, y)$ is simply the *distance* of the point (x, y) from Γ.

Notice that there are two possible solutions corresponding to the $\pm$ in (3.10). The correct solution is chosen by ensuring that the rays propagate *into* the region of interest, not out of it. So, in (3.10), we have to choose (p_0, q_0) to be the *inward* pointing normal. Otherwise the solution corresponds to the sandpile outside a spoon-shaped hole in a table.

If the spoon is elliptical, then we can write

$$x_0(s) = a\cos(s), \quad y_0(s) = b\sin(s), \quad 0 \le s < 2\pi,$$

for some constants a and b, and the solution is given parametrically by

$$x = a\cos(s) - \frac{b\tau\cos(s)}{\sqrt{a^2\sin^2(s) + b^2\cos^2(s)}}, \quad y = b\sin(s) - \frac{a\tau\sin(s)}{\sqrt{a^2\sin^2(s) + b^2\cos^2(s)}}, \quad u = \tau.$$

The rays and solution surface are shown in Figure 3.1. Notice that a ridge line, across which p and q are discontinuous, forms along the x-axis, between the $x = -(a^2 - b^2)/a$ and $x = +(a^2 - b^2)/a$. In this figure $a = 2$ and $b = 1$; if $a < b$ then the ridge at the corresponding position along the y-axis.

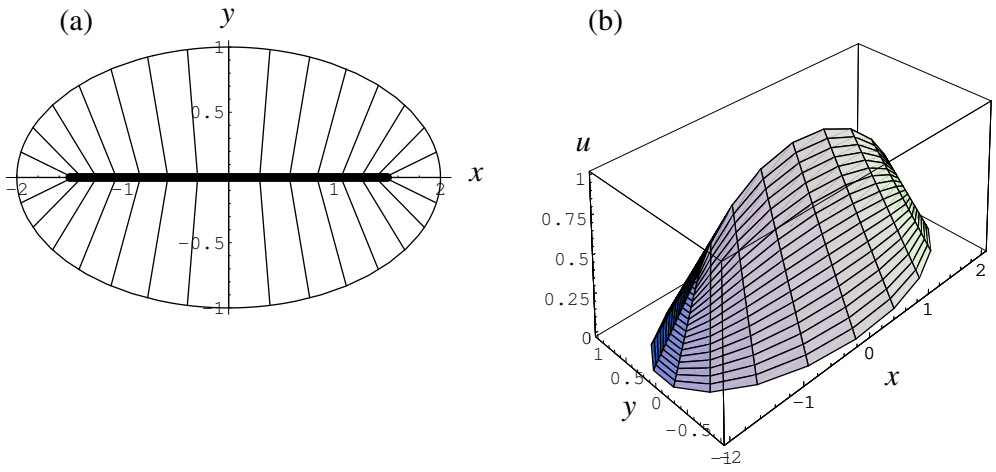

Figure 3.1: (a) Rays for a sugar heap on an elliptical spoon with $a = 2$ and $b = 1$; the bold line marks the ridge. (b) The corresponding pile height $u(x, y)$.

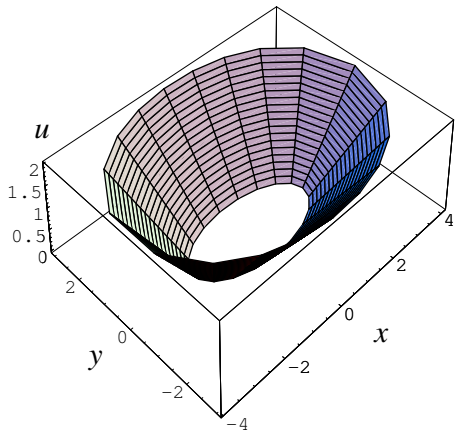

Figure 3.2: The height $u(x, y)$ of a sandpile outside an elliptical hole with $a = 2$ and $b = 1$.

If the other root is taken for p and q, then the rays propagate *out* of the ellipse as τ is increased from zero, and the parametric solution is now

$$x = a\cos(s) + \frac{b\tau\cos(s)}{\sqrt{a^2\sin^2(s) + b^2\cos^2(s)}}, \quad y = b\sin(s) + \frac{a\tau\sin(s)}{\sqrt{a^2\sin^2(s) + b^2\cos^2(s)}}, \quad u = \tau.$$

This corresponds to a sandpile on a table with an elliptical hole, as shown in Figure 3.2.

3.4.2 Discontinuities

Example 1 illustrates that it is possible for rays to intersect. This happens first where the Jacobian J of the transformation for x, y first becomes zero. Note that this reproduces the criterion (3.8) for Cauchy data *not* to determine a unique solution on Γ. If rays are allowed to cross, then the solution becomes multi-valued, which is clearly unphysical for a pile of sugar. Instead, we must allow shocks to form across which the solution is discontinuous. Recall that, for nonlinear PDEs, shocks are different from characteristics. The conditions that must be applied across a shock depend on the physical situation being modelled. For the sugar heap problem, it is clear that u must be continuous everywhere, since a discontinuity in u (corresponding to a vertical "cliff") cannot be sustained. This forces the shock, *i.e.* the ridge line, to be along the x-axis as shown in Figure 3.1. In general, the region of validity of the solution obtained by Charpit's method is bounded by curves on which $J = 0$.

Example 2. Solve the PDE

$$\frac{\partial u}{\partial x} = \left(\frac{\partial u}{\partial y}\right)^2$$

subject to $u = u_0(y)$ on $x = 0$.

Set $F = p - q^2$ and parametrise the initial conditions via

$$x = 0,\ y = s,\ u = u_0(s),\ p = p_0(s),\ q = q_0(s),$$

where

$$q_0(s) = u_0'(s), \quad p_0(s) = q_0(s)^2 = \left(u_0'(s)\right)^2.$$

Charpit's equations are

$$\frac{\mathrm{d}x}{\mathrm{d}\tau} = 1, \quad \frac{\mathrm{d}y}{\mathrm{d}\tau} = -2q, \quad \frac{\mathrm{d}p}{\mathrm{d}\tau} = \frac{\mathrm{d}q}{\mathrm{d}\tau} = 0, \quad \frac{\mathrm{d}u}{\mathrm{d}\tau} = p - 2q^2 = -p,$$

and the solution is

$$x = t, \quad y = s - 2tu_0'(s), \quad p = \left(u_0'(s)\right)^2, \quad q = u_0'(s), \quad u = u_0(s) - t\left(u_0'(s)\right)^2.$$

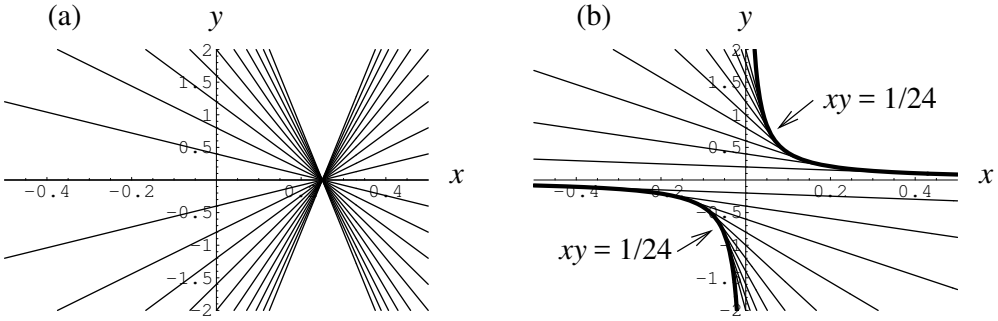

Figure 3.3: Rays for Example 2. (a) $u_0(s) = s^2$; (b) $u_0(s) = s^3$.

The rays are straight lines given by

$$y + 2xu_0'(s) - s = 0,$$

and their envelope is found parametrically by differentiating with respect to s:

$$x = \frac{1}{2u_0''(s)}, \quad y = s - \frac{u_0'(s)}{u_0''(s)}.$$

For example, if $u_0(s) = s^2$, then the solution in explicit form is

$$u = \frac{y^2}{1 - 4x}.$$

The rays in this case are given by $y = s(1 - 4x)$ so, as illustrated in Figure 3.3(a), they all pass through the point $(1/4, 0)$, and the solution is defined in $x < 1/4$.

If $u_0(s) = s^3$, then the solution is

$$u = s^3(1 - 9xs), \quad \text{where} \quad s = \frac{1 - \sqrt{1 - 24xy}}{12x}.$$

The rays are given by $y = s - 6s^2x$, and their envelope is the curve $24xy = 1$, as illustrated in Figure 3.3(b). The solution is therefore defined in the region $24xy < 1$ (which is where s is real).

3.5 High-frequency asymptotics

The study of waves has produced some very innovative mathematical ideas. One of the most commonly encountered of these relates to studying situations where the wave lengths of interest are much shorter than the variations in size of the

region of interest. Hence gravity waves in rivers. estuaries; electromagnetic waves from radar, illuminations; noise in rooms and from aircraft. Mathematically these situations can be explored by examining behaviour of a monochromatic wave using Helmholtz equations (either scalar or vector) in the limit of $k \to \infty$. Below we examine some of these ideas under the heading of geometrical optics.

3.5.1 Geometrical optics

The theory of *geometrical optics* arises from considering the limit $k \to \infty$ to analyse the behaviour of (2.5). Note that a naive approach to taking $k \to \infty$ simply neglects all the derivatives in the problem and gets nowhere.

The central idea to taking this limit is to recognise that the solution ϕ will vary on a very short length scale $(1/k)$ due to the wave structure. However we anticipate that although the waves will have this high frequency their amplitude may varying over a much longer scale. The approach we use it the so-called *WKBJ method*, which involves writing ϕ in the form

$$\phi(x, y) = A(x, y)\mathrm{e}^{\mathrm{i}ku(x,y)}, \tag{3.11}$$

where A and u represent the *amplitude* and *phase* respectively of the solution. Then (2.5) becomes

$$\nabla^2 A + \mathrm{i}k\left(A\nabla^2 u + 2\boldsymbol{\nabla} A \cdot \boldsymbol{\nabla} u\right) + k^2 A\left(1 - |\boldsymbol{\nabla} u|^2\right) = 0. \tag{3.12}$$

Having had this WKBJ assumption we now seek solutions in which A is asymptotic expansions of the form

$$A \sim A_0 + \frac{A_1}{k} + \frac{A_2}{k^2} + \ldots.$$

Note that we can simply allow u to be an order one function independent of ϵ as, if we did assume an asymptotic expansion for u, there would be ambiguity since such behaviour is already accounted for in the expansion of A.

Using these assumptions and considering the leading order problem for, (3.12) implies that u_0 satisfies the *Eikonal equation*

$$|\boldsymbol{\nabla} u|^2 = 1. \tag{3.13}$$

Then the successive terms in the amplitude expansion satisfy the *transport equations*

$$\begin{aligned} 2\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} A_0 + A_0 \nabla^2 u &= 0, \\ 2\boldsymbol{\nabla} u \cdot \boldsymbol{\nabla} A_n + A_n \nabla^2 u &= \mathrm{i}\nabla^2 A_{n-1}, \quad n \geq 1. \end{aligned}$$

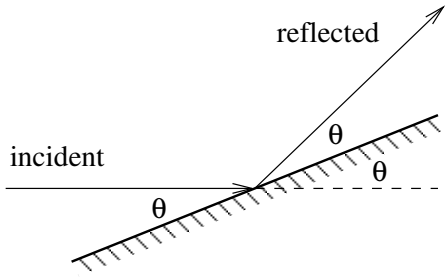

Figure 3.4: Illustration of Snell's law.

The Eikonal equation (3.13) may be solved exactly as in Example 1. The rays correspond to light rays and all the familiar properties of geometrical optics, for example that light travels in straight lines, follow from the solution of Charpit's equations.

Example 3. Reflecting plane waves

One obvious solution of (3.13) is $u = x$, which corresponds to a plane wave moving in the x-direction. Now we examine what happens if such a wave impinges on a reflecting wall given by a curve Γ in the (x, y)-plane. We decompose the state variable ϕ into an *incident* wave ϕ_I, namely a plane wave with constant amplitude a, and a *reflected* wave ϕ_R:

$$\phi = \phi_I + \phi_R, \quad \phi_I = a\mathrm{e}^{\mathrm{i}kx}.$$

Now we apply the WKBJ ansatz to ϕ_R:

$$\phi_R = A\mathrm{e}^{\mathrm{i}ku(x,y)}.$$

The boundary conditions depend on the physical situation being modelled and exactly what the state variable ϕ represents. The simplest case is to impose the Dirichlet condition $\phi = 0$ on Γ, which leads to

$$u = x, \quad A_0 = -a \quad \text{on } \Gamma. \tag{3.14}$$

Other possibilities are $\partial\phi/\partial n = 0$ or the "Robin condition" $\partial\phi/\partial n + \lambda\phi = 0$, but it is readily verified that the leading-order boundary conditions (3.14) are unchanged in either case.

The solution of Charpit's equations for the Eikonal equation was already obtained in Example 1:

$$p = p_0(s), \quad q = q_0(s), \quad x = x_0(s) + p_0(s)\tau, \quad y = y_0(s) + q_0(s)\tau, \quad u = u_0(s) + \tau.$$

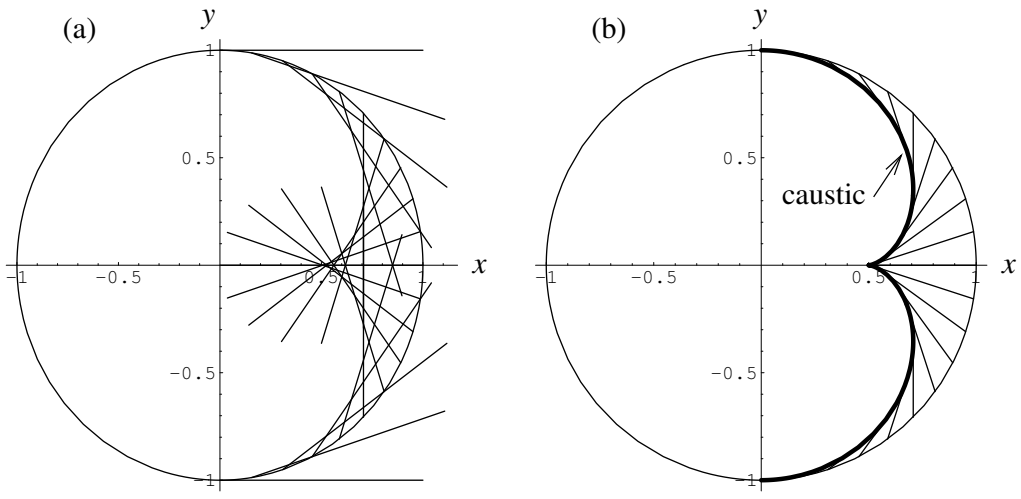

Figure 3.5: (a) Reflected rays for Example 4. (b) Rays truncated by a caustic on which $J = 0$.

For simplicity we suppose that s parametrises arc-length along Γ so we can write $x_0' = \cos\theta$, $y_0' = \sin\theta$ where θ is the angle between Γ and the x-axis. The boundary condition (3.14) implies that $u_0(s) = x_0(s)$, and then p_0 and q_0 are obtained from

$$x_0' p_0 + y_0' q_0 = x_0', \quad p_0^2 + q_0^2 = 1.$$

This system has two solutions, one of which is $p_0 = 1$, $q_0 = 0$, corresponding to the incident wave. The reflected wave is given by the other solution

$$p_0 = 1 - 2(y_0')^2 = \cos(2\theta), \quad q_0 = 2x_0' y_0' = \sin(2\theta).$$

Hence the reflected ray makes an angle of 2θ with the x-axis. This is *Snell's law*: as illustrated in Figure 3.4, it implies that the angle of incidence to the wall equals the angle of reflection from it.

Note that in analysing this problem we have not had to consider any shocks created by interaction of the waves. This is because the underlying physical problem is modelled by Helmholtz equation, which because it is linear, we could break the solution into an incident wave ϕ_I and a reflected wave π_R and the fact that these waves might simultaneously occur at the same position and time is physically acceptable.

Example 4. The caustic in a teacup
As a special case of Example 3, we now consider the case where Γ is the unit circle, parametrised (say) by $x_0(s) = \cos(s)$, $y_0(s) = \sin(s)$. The rays reflected from the

circle are given parametrically by

$$x = \cos(s) - \tau\cos(2s), \quad y = \sin(s) - \tau\sin(2s).$$

and the phase is then given by $u = \cos(s) + t$.

As shown in Figure 3.5(a), the reflected waves start to cross a finite distance from the circle. The envelope of the rays is where the Jacobian

$$J = \frac{\partial x}{\partial s}\frac{\partial F}{\partial q} - \frac{\partial y}{\partial s}\frac{\partial F}{\partial p} = 0,$$

which may be solved to give

$$\tau = \tfrac{1}{2}\cos(s).$$

Thus $J = 0$ on the curve given parametrically by

$$x = \cos(s)\left(1 - \tfrac{1}{2}\cos(2s)\right), \quad y = \sin(s) - \tfrac{1}{2}\cos(s)\sin(2s) = \sin^3(s), \qquad (3.15)$$

and such a curve is called a *caustic*. A single-valued solution may be obtained by truncating the rays when they reach the caustic, as shown in Figure 3.5(b). A caustic similar to this may often be observed if a bright light is shone on a cup of coffee.

An alternative way to find the caustic is to note that the rays are given by

$$F(x, y; s) = x\sin(2s) - y\cos(2s) - \sin(s) = 0.$$

Their envelope may therefore be found by solving

$$F = \frac{\partial F}{\partial \lambda} = 0,$$

that is

$$x\sin(2s) - y\cos(2s) - \sin(s) = 2x\cos(2s) + 2y\sin(2s) - \cos(s) = 0,$$

whose simultaneous solution reproduces (3.15).

Example 4 illustrates that a single-valued ray solution may be obtained by truncating rays at any caustic where the Jacobian is zero. It may be shown that the asymptotic ansatz (3.11) breaks down, with $A \to \infty$ as the caustic is approached. The method of matched asymptotic expansions yields the appropriate correction in the neighbourhood of a caustic and allows the behaviour in the dark zone beyond the caustic (corresponding to *complex rays*) to be found.

3.5.2 Kelvin Ship waves

Suppose we have a ship (or a duck) travelling at constant speed V on deep water, which we take to occupy the region $z < 0$. To model the behaviour we use the ideas of Stokes waves that were discussed earlier. For inviscid, incompressible, irrotational flow the velocity potential ϕ satisfies

$$\nabla^2\phi = 0 \qquad \text{in } z < 0,$$

with

$$|\nabla\phi| \to 0 \qquad \text{as } x^2 + y^2 + z^2 \to \infty.$$

On the free surface the linearised kinematic and Bernoulli conditions are

$$\frac{\partial\phi}{\partial z} = \frac{\partial h}{\partial t}, \qquad \frac{\partial\phi}{\partial t} + gh = 0 \qquad \text{on } z = 0,$$

away from the ship, where h is the free-surface elevation, which can be eliminated to give the single condition

$$\frac{\partial^2\phi}{\partial t^2} + g\frac{\partial\phi}{\partial z} = 0 \qquad \text{on } z = 0.$$

Let us consider steady waves in a frame moving with the ship by writing

$$x - Vt = \frac{X}{\epsilon}, \quad y = \frac{Y}{\epsilon}, \quad t = \frac{T}{\epsilon}.$$

Here ϵ is an artificial small parameter—the limit $\epsilon \to 0$ corresponds to looking in the far-field, a long distance from the ship. Writing $\phi(x - Vt, y, z, t) = \Phi(X, Y, z)$ we find

$$\epsilon^2\left(\frac{\partial^2\Phi}{\partial X^2} + \frac{\partial^2\Phi}{\partial Y^2}\right) + \frac{\partial^2\Phi}{\partial z^2} = 0 \qquad \text{in } z < 0, \tag{3.16}$$

with

$$\epsilon^2 V^2\frac{\partial^2\Phi}{\partial X^2} + g\frac{\partial\phi}{\partial z} = 0 \qquad \text{on } z = 0. \tag{3.17}$$

We look for a WKBJ solution

$$\Phi = A\mathrm{e}^{\mathrm{i}u/\epsilon}.$$

At leading order in (3.16) this gives

$$\frac{\partial u}{\partial z} = 0,$$

so that the phase u is independent of z at leading order. The next order in (3.16) then gives

$$-\left(\left(\frac{\partial u}{\partial X}\right)^2 + \left(\frac{\partial u}{\partial Y}\right)^2\right)A + \frac{\partial^2 A}{\partial z^2} = 0.$$

Since u is independent of z this equation can be solved to give

$$A = a(X, Y)\mathrm{e}^{z(p^2+q^2)^{1/2}},$$

where we have written

$$p = \frac{\partial u}{\partial X}, \qquad q = \frac{\partial u}{\partial Y}.$$

Now substituting into (3.17) gives, at leading order

$$-V^2p^2 + g(p^2 + q^2)^{1/2} = 0,$$

or, on squaring,

$$V^4p^4 = g^2(p^2 + q^2). \tag{3.18}$$

This equation can be solved by Charpit's method. The rays are straight lines.

4 Energy Minimization

4.1 Introduction

In this section we will focus on two key techniques that can be exploited in problems where a minimisation is necessary such as energy minimisation. The two methods are i) the calculus of variations and ii) Lagrange multipliers to explore various problems. By combining these two, we can tackle many problems that would not be possible using conventional techniques. In particular, these are very powerful when we wish to minimise integrals under certain fixed constraints

4.2 The calculus of variations

The calculus of variations came about due to a mathematical challenge in 1697. During those days it was customary to try and flush out your mathematical rivals by setting challenging problems for them to solve. Johann Bernouilli, one of the Bernouilli mathematics clan, posed the *Brachristochrone* problem:

Given two points A and B, with B below A, what is the curve of fastest descent? i.e. what path will carry a frictionless body from A to B in the smallest amount of time?

To solve this problem, we first need to write down an expression for the total amount of time it takes to get from A to B along a given path. From conservation of energy:

$$\frac{1}{2}mv^2 = mgh \tag{4.1}$$

so the velocity v of the particle at a height h is given by:

$$v = \sqrt{2gh}. \tag{4.2}$$

Consider a curve $y(x)$ between A and B, as shown in figure **??**. The local angle from horizontal of the curve is θ. Then

$$\frac{dx}{dt} = v\cos\theta, \quad \frac{dy}{dx} = -\tan\theta. \tag{4.3}$$

The total travel time is given by

$$T = \int_{x_A}^{x_B} \frac{dx}{v\cos\theta} = \int_{x_A}^{x_B} \frac{\sqrt{1+y'^2}}{\sqrt{2gy}} dx \tag{4.4}$$

where x_A and x_B are the x-coordinates of the points A,B, and we have used the results of equation (4.3) to obtain the second equality.

Thus we have reduced the original question to the problem of: What is the path $y(x)$ that minimises the integral $T = \int f(x, y, y')dx$?

4.2.1 The 1d Euler-Lagrange equation

We solve this problem by deriving the Euler-Lagrange equations. In calculus, you learn that you find a minimum of a function $f(x)$ by solving the equation $df/dx = 0$. We can generalise this to minimising integrals: If we make a small perturbation to the path $y(x) \to y + \delta y$, we find the minimum by requiring that the resulting change $\delta T = 0$:

$$T + \delta T = \int_{x_A}^{x_B} f(x, y + \delta y, y' + \delta y')dx \tag{4.5}$$

Thus

$$\delta T = \int_{x_A}^{x_B} \left[f(x, y + \delta y, y' + \delta y') - f(x, y, y')\right] dx = 0 \tag{4.6}$$

and from Taylor expanding f,

$$\delta T = \int_{x_A}^{x_B} \left[\frac{\partial f}{\partial y}\delta y + \frac{\partial f}{\partial y'}\delta y'\right] dx = 0. \tag{4.7}$$

We integrate by parts (noticing that $\delta y' = d(\delta y)/dx$) to obtain:

$$\left[\delta y \frac{\partial f}{\partial y'}\right]_{x_A}^{x_B} + \int_{x_A}^{x_B} \delta y \left[\frac{\partial f}{\partial y} - \frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right)\right] dx = 0. \tag{4.8}$$

If the path is fixed at $y(x_A)$, and $y(x_B)$, then $\delta y(x_A) = \delta y(x_B) = 0$, and we can throw away the first term. Then provided f is sufficiently smooth, the only way that the integral can always be 0 is if

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\left(\frac{\partial f}{\partial y'}\right) = 0. \tag{4.9}$$

This is the well-known Euler-Lagrange equation that you will probably have encountered before. WARNING: it is not always the case that we can throw away the first term in equation 4.8. We will come across some examples later where we need to worry about the extra term.

In your first problem sheet, you'll use the Euler-Lagrange equation to prove the Beltrami identity: When $\partial f/\partial x = 0$,

$$f - y'\frac{\partial f}{\partial y'} = C, \tag{4.10}$$

where C is a constant.

We can use this result in the brachristochrone time equation (4.4) to obtain

$$\frac{1}{\sqrt{1+y'^2}\sqrt{2gy}} = C \tag{4.11}$$

or

$$\frac{dy}{dx} = \sqrt{\frac{c_0 - y}{y}}. \tag{4.12}$$

We can solve this numerically to find the final solution - an inverted cycloid generated by a circle of diameter c_0.

4.2.2 Higher order Euler-Lagrange equations

You can also derive Euler-Lagrange equations for higher order problems. In the first problem sheet, you'll also prove that if we minimise:

$$\int_{x_A}^{x_B} f(x, y, y', y'')dx \tag{4.13}$$

then

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} + \frac{d^2}{dx^2}\frac{\partial f}{\partial y''} = 0, \tag{4.14}$$

provided certain boundary conditions are met (which you should state).

Later, we will also return to derive Euler-Lagrange equations for the case when we need to minimise volume or area integrals rather than line integrals like those above.

4.3 Lagrange multipliers

The second important technique that we will use is the Lagrange multipliers. This is a useful way to find minima or maxima of functions subject to a constraint. For example:

Minimise $f(x, y)$ subject to the constraint $g(x, y) = c$.

The solution technique is illustrated in Figure **??**. $g(x, y)$ gives some curve in the (x, y) plane. If we plot $f(x, y)$ as we move along this curve, there will be a minimum at some point, (x_0, y_0). Here, f does not change in the direction tangent to the curve $g(x, y) = c$ so ∇f must point in the normal direction $\mathbf{n}$, so $\nabla f \propto \mathbf{n}$. Note that

$$\mathbf{n} \propto \nabla(g(x, y) - c), \tag{4.15}$$

so $\nabla f \propto \nabla(g(x, y) - c)$, or

$$\nabla f - \lambda \nabla(g - c) = 0, \tag{4.16}$$

where λ is the Lagrange multiplier.

Interestingly, we shall see that the Lagrange multiplier often turns out to be an important variable. For instance, when we calculate the shape of a droplet on a flat surface, the Lagrange multiplier will give the pressure inside of the droplet.

4.3.1 Quick example

What shape should a rectangular box be in order to minimise its surface area for a given volume ratio?

Let x, y, z be the lengths of the sides of the box. Then we have the volume constraint $V = xyz$. We want to minimise the surface area $A = 2(xy + yz + xz)$, so from the equation (4.16)

$$\frac{\partial}{\partial x}\left[2(xy + yz + xz) - \lambda(xyz - V)\right] = 0 \tag{4.17}$$

$$\frac{\partial}{\partial y}\left[2(xy + yz + xz) - \lambda(xyz - V)\right] = 0 \tag{4.18}$$

$$\frac{\partial}{\partial z}\left[2(xy + yz + xz) - \lambda(xyz - V)\right] = 0 \tag{4.19}$$

and we find

$$2(y + z) - \lambda yz = 0, \quad 2(x + z) - \lambda xz = 0, \quad 2(x + y) - \lambda xy = 0. \tag{4.20}$$

From symmetry, we guess that there is a solution $x = y = z$ and find that $\lambda = 4/x$. Finally, we also need to check that this is a minimum solution - I leave this to you to satisfy yourself.

4.4 Combining Lagrange multipliers with the Calculus of Variations

The power of Lagrange multipliers and the Calculus of Variations can really be seen when we combine the two techniques together. Often (especially when minimising energy problems), we need to find the minimum of an integral subject to a constraint. For example, we wish to minimise

$$E = \int_a^b f(x, y, y')dx \tag{4.21}$$

subject to

$$\int_a^b g(x, y, y')dx = C. \tag{4.22}$$

Using the natural extension of equation (4.16), this problem is equivalent to minimising

$$\int_a^b (f(x, y, y') - \lambda g(x, y, y'))dx. \tag{4.23}$$

Where λ is a Lagrange multiplier. This can be solved using the Euler-Lagrange equations,

4.5 Energy minimisation

The principle of minimum total potential energy is one of the fundamental laws governing the physical behaviour of everything in the world around us. It is a consequence of the 2nd law of thermodynamics, and essentially says that any body or structure will deform or move to a position that minimises its total potential energy. The lost energy will be dissipated as heat.

For example, if you stand on a tightrope, it will stretch to lower your gravitational potential energy. This simultaneously increases the rope's stored elastic energy. The principle of minimum total potential energy then says that the final position is the point where the elastic energy + gravitational potential energy is minimised. Obviously if you fall off you will minimise your potential energy even more.

This principle is very useful for deriving the governing equations of complex (and simple) systems. You will be used to deriving equations of systems in equilibrium by considering force balance at points, but we shall see that we cannot use this approach for some systems. In fact, even in simple situations, it is more rigorous to derive the governing equations from minimising energy; analytical mechanicians will not consider equations valid unless they can be derived in this way (and this can cause strife).

4.5.1 Example: Mass on a spring

As a simple example, consider putting a mass M on a linear spring of stiffness k, as shown in figure **??**. If the initial length of the spring is x_0, and it stretches to a length x then its elastic energy is $\frac{1}{2}k(x-x_0)^2$. The gravitational potential energy of the mass is Mgz, where z is its height.

We hang the mass on the spring. Then the total potential energy is

$$E = Mgz + \frac{1}{2}k(z-z_0)^2 \tag{4.24}$$

where z_0 is the initial position of the end of the spring before the mass is placed on it.

We minimise E by setting $dE/dz = 0$ to find $Mg + k(z-z_0) = 0$. This is the usual force-balance equation that you would normally write down straight away. Note that in this case, a big advantage is that we do not have to do the usual head scratching about getting the signs right.

The case above was for a simple, linear-elastic spring, but in real life springs are not always linear elastic! A material like rubber needs to be treated using a special model. This means that it has a more complex strain energy function, and we cannot just write down the simple force balance. The strain energy of a Neo-Hookean solid (a good model for rubber) that is stretched uniaxially is:

$$E_{el} = C\left[\left(\frac{l}{l_0}\right)^2 + 2\frac{l_0}{l}\right], \tag{4.25}$$

where l is the length of the rubber spring, and l_0 and C are constants.

We can find the equilibrium length of the spring by minimising the elastic potential energy E_{el} to find that $l = l_0$ when there is no force on the spring. Then you can hang a weight on the spring to obtain its equilibrium position. First we

write down the energy

$$E = C\left[\left(\frac{z}{l_0}\right)^2 + 2\frac{l_0}{z}\right] + Mg(h-z). \tag{4.26}$$

(note we have flipped z to point downwards here for simplicity, as shown in figure **??**). Then we minimise to obtain the equilibrium equation:

$$2C\left(\frac{z}{l_0^2} - \frac{l_0}{z^2}\right) = Mg. \tag{4.27}$$

We can analyse this expression asymptotically to see that rubber initially behaves like a linear spring which gets softer for large deformation.

4.5.2 Surface tension and capillary statics

In this lecture we'll look at phenomena in liquids when surface tension is important. Surface tension is important in a wide variety of situations, in particular at lengthscales below the capillary length $l_c = \sqrt{\gamma/\rho g}$, where γ is surface tension and ρ is the density of the liquid (for water, $l_c \sim 3$mm). Here, we'll concentrate on capillary statics - i.e. the shape of liquids in equilibrium.

What is surface tension?

(Modified from the Topics in Fluid Mechanics notes)

Liquids consist of molecules tightly packed together and interacting with one another through an attractive force (this is why gases condense to form liquids when the molecules are slowed down by cooling). A molecule in the bulk of a liquid is therefore happy in the sense that it feels these attractive interactions from all directions. A molecule at the liquid surface, however, is unhappy because it has attractive interactions with only half as many neighbours as the bulk molecule. This unhappiness corresponds to an excess potential energy of the liquid that is proportional to the surface area, A:

$$E_{cap} = \gamma A. \tag{4.28}$$

γ represents the excess potential energy per unit area of surface, and is known as either the *surface energy* or the *surface tension*. The value of γ depends on the liquid, but for most pure liquids, $\gamma \sim 2 \times 10^{-2}\mathrm{J/m^2}$. This is because in liquids, the thermal energy of a molecule must be comparable in size to the attractive energy with its neighbours. If the thermal energy is much greater, then molecules will easily escape from the liquid and become a gas. If the thermal energy is too small,

molecules will get locked into place and form a crystal lattice. The thermal energy of a molecule is $k_BT = 4 \times 10^{-21}$J at room temperature. The attractive interaction $\sim \gamma a^2$. Thus $\gamma \sim k_BT/a^2$. Most molecules are of a similar size ($a \sim 0.5$nm), hence why surface tension is always roughly the same magnitude. Liquid metals are an exception with surface tensions about 20 times higher than usual.

Force vs energy interpretation

A common source of confusion is: should we think about surface tension as a force or an energy? Let's do a simple thought experiment. We consider a bath of water that has constant volume, and ignore gravity effects. Originally the surface area is vanishingly small, and we apply a constant force F to pull open a larger area. If we extend the surface area to be $A = xt$, where t is the thickness of the bath in the y-direction, then the total surface energy is $E_{cap} = \gamma A$. The work done by the force (which you can think of as reducing the potential energy of the system) is $E_F = -Fx$. Thus the total potential energy of the system is

$$E_{cap} + E_F = \gamma xt - Fx \tag{4.29}$$

minimising this with respect to x, we find that $\gamma = F/t$. i.e. there is a force of size γ per unit length of the contact line that is trying to pull back along the surface.

Thus for a liquid, surface tension can equivalently be thought of as a force per unit length, or an excess potential energy per unit area.

The shape of a small droplet on a surface

Firstly, let's consider the shape of a small droplet on a flat surface, as shown in figure **??**. For the moment we'll ignore gravity, and use our experience which tells us that small droplets always want to form spherical caps (you can prove this rigorously using energy minimisation if you would like!). There are three separate interfaces: the solid/liquid, solid/vapour and liquid/vapour interfaces, and each of these has a surface energy. Let's call these $\gamma_{sl}, \gamma_{sv}, \gamma_{lv}$ respectively.

We assume that the droplet forms a spherical cap of height h, contact radius a and radius of curvature r. Then, from wikipedia, we have that the curved area of the spherical cap is $\pi(a^2 + h^2)$ and its volume is $V = \frac{\pi h}{6}(3a^2 + h^2)$. Thus the total potential energy of the system is

$$E = \pi(a^2 + h^2)\gamma_{lv} + \pi a^2(\gamma_{sl} - \gamma_{sv}) + E_0, \tag{4.30}$$

where E_0 is a constant equal to the total area of the flat, bare surface multiplied by γ_{sv}.

We need to minimise this subject to a constant total volume of the droplet, so

we minimise

$$U = \pi(a^2 + h^2)\gamma_{lv} + \pi a^2(\gamma_{sl} - \gamma_{sv}) - \lambda\left(\frac{\pi h}{6}(3a^2 + h^2) - V\right). \tag{4.31}$$

First, $\partial U/\partial a$ gives

$$\gamma_{lv} + \gamma_{sl} - \gamma_{sv} = \frac{\lambda h}{2}. \tag{4.32}$$

Then $\partial U/\partial h$ gives (after some manipulation)

$$\frac{2h^2\gamma_{lv}}{a^2 + h^2} = \frac{\lambda h}{2}. \tag{4.33}$$

Combining these, and noting that $2h^2/(a^2 + h^2) = (1 - \cos\theta)$, where θ is the contact angle of the droplet, we obtain Young's law:

$$\gamma_{lv}\cos\theta + \gamma_{sl} - \gamma_{sv} = 0. \tag{4.34}$$

This is illustrated in figure **??**. Amazingly, it says that the contact angle of a droplet is independent of the droplet size. We have proven Young's law for the simple case of a droplet on a flat surface. However, this result also applies to more general surfaces: in equilibrium the contact angle of a droplet always takes the value given by equation (4.34).

If you recall, we mentioned earlier that the Lagrange multiplier often takes an important value. I leave it as a challenge to you to show that here $\lambda = 2\gamma_{lv}/R$, the Laplace pressure inside the droplet (R is the radius of curvature of the spherical cap).

The meniscus equation

Now let's consider the shape of a liquid in a tank with a wall at $x = 0$, as shown in figure **??**. We want to be able to predict what is the shape of the meniscus against the tank wall.

The energy can be split into three parts: the gravitational potential energy of the liquid, the surface energy of the free surface, and the surface energy of the walls. We first calculate the gravitational potential energy.

Consider a parcel of fluid at height z, as shown in figure **??**. Its energy is $mg = (\rho dxdz)gz$. Thus if the height of the free surface is $h(x)$

$$E_g = \int_0^X \int_0^{h(x)} \rho g z dz dx = \int_0^X \rho g \frac{h^2}{2} dx \tag{4.35}$$

The surface energy of the free surface is

$$E_{\gamma_{lv}} = \gamma_{lv} \int_0^X \sqrt{1 + h'^2} dx, \tag{4.36}$$

while the free energy of the wall at $x = 0$ is

$$E_{wall} = (\gamma_{sl} - \gamma_{sv})h(0) + E_0 \tag{4.37}$$

Thus we need to minimise the total potential energy

$$E = \int_0^X \left[\rho g \frac{h^2}{2} + \gamma_{lv} \sqrt{1 + h'^2} \right] dx + (\gamma_{sl} - \gamma_{sv})h(0) + E_0 \tag{4.38}$$

The last term poses a small problem, as if $h(0)$ is not fixed, we can no longer immediately use the Euler-Lagrange technique as before. However, we can still solve this by making use of the extra term in equation (4.8) that we normally ignore.

Let $h \to h + \delta h$, as usual, and write the integrand as $f(x, h, h')$. Then from equation (4.8)

$$\delta E = \left[\delta h \frac{\partial f}{\partial h'} \right]_0^X + \int_0^X \delta h \left[\frac{\partial f}{\partial h} - \frac{d}{dx} \left(\frac{\partial f}{\partial h'} \right) \right] dx + (\gamma_{sl} - \gamma_{sv}) \delta h(0) = 0. \tag{4.39}$$

The only way we can ensure that the energy is minimised for all δh is if we have two conditions: firstly the standard Euler-Lagrange result:

$$\frac{\partial f}{\partial h} - \frac{d}{dx} \left(\frac{\partial f}{\partial h'} \right) = 0 \tag{4.40}$$

and secondly (assuming that $\delta h(X) = 0$) the boundary condition

$$-\frac{\partial f}{\partial h'}(0) + (\gamma_{sl} - \gamma_{sv}) = 0. \tag{4.41}$$

In the problems, you'll show that the equation for the free surface reduces to

$$\frac{\rho g h^2}{2} + \frac{\gamma_{lv}}{\sqrt{1 + h'^2}} = \gamma_{lv} \tag{4.42}$$

while the boundary condition means that the contact angle of the liquid must satisfy Young's law.

4.6 Elasticity

In this lecture we're going to look at how we can work out how elastic solids behave using energy minimisation. The key idea is that we can calculate the total elastic energy of a body by integrating its strain energy density W. W the strain energy per unit volume, and only depends upon the local strain of the solid: $W = W(\epsilon_{ij})$. Thus the total elastic energy of a solid body V is

$$E_{el} = \int_V W(\epsilon_{ij}) dV. \tag{4.43}$$

A key component of finite elasticity is selecting a suitable W to match the observed behaviour of the material that you are modelling. Neo-Hookean, and Mooney-Rivlin solids (that you saw examples of earlier) are specific examples of different models for W.

4.6.1 Elastic beams

Let's start by looking at the deformation of a thin elastic beam, that is initially flat, but which we bend to $y = h(x)$ by applying vertical forces. We assume that there is no stretching of the beam.

We need an expression for the strain energy density of the beam (i.e. the elastic energy per unit length). We will guess this by a bit of logical deduction. We know that the strain energy density depends on the strain, so it must be a function of h or its derivatives. First we notice that W cannot be a function of h, as otherwise the beam could increase its energy just by displacing it upwards or downwards. Second, we notice that W cannot be a function of h' otherwise a straight beam that was angled upwards at a constant angle would have a different elastic energy to a flat beam. Thus the lowest derivative that the energy can depend on is h''. However, the energy must depend on h''^2 so that the energy does not depend on whether the beam curves up or down.

Thus the simplest possible model for the strain energy density of a beam is $W = \frac{B}{2}h''^2$. This turns out to be exactly correct for a linear-elastic beam!

Let's now consider the problem where we put weights on a beam suspended between two points. Both ends of the beam are fixed with $h = h' = 0$. There is a distributed load $q(x)$ pushing upwards on the beam. Then the total energy consists of the elastic energy and the gravitational potential energy:

$$E = \int_0^L \frac{B}{2}(h'')^2 dx - \int_0^L q(x)h(x)dx. \tag{4.44}$$

We need to use the higher-dimensional Euler-Lagrange equation that you derived earlier (4.14), to minimise this expression:

$$\frac{\partial f}{\partial y} - \frac{d}{dx}\frac{\partial f}{\partial y'} + \frac{d^2}{dx^2}\frac{\partial f}{\partial y''} = 0. \tag{4.45}$$

Using this, we obtain

$$Bh'''' = q, \tag{4.46}$$

which is the static Euler-Lagrange beam equation.

For example, we can consider the case where the beam has an evenly distributed, constant pressure $q(x) = p$ pushing upwards along its surface. Solving the beam equation, we find

$$h = p\frac{x^2(L-x)^2}{24B}. \tag{4.47}$$

4.6.2 Stretching vs bending energy

We have just seen that the bending energy density of a thin sheet is $W_b = Bh''^2/2$. This is energy per unit length and width of the sheet and thus has units of $\mathrm{J/m^2}$. B can only depend on Young's modulus of the material, E (units of pressure), and the thickness of the beam t. From dimensional analysis we find that:

$$\frac{\mathrm{J}}{\mathrm{m}^2} \sim \frac{[B]}{\mathrm{m}^2}, \tag{4.48}$$

and so B has units of energy, and we must have $B \propto Et^3$. We can also consider the stretching energy density of a thin sheet. By analogy with a linear spring, $W_s = k\epsilon^2/2$, where ϵ is the local extensional strain. This time, from dimensional analysis, we find that $k \propto Et$. Thus we see that the energy to stretch (or compress) a sheet is proportional to t, but the energy to bend a sheet is proportional to t^3.

This is an important result. As t becomes small, bending energy will always be much smaller than stretching energy. Thus if you compress a sheet, it will prefer to bend rather than compress, as this results in a much lower stored energy. You can see this by putting a piece of paper on a table, and sliding the two ends towards each other. The paper does not compress, but instead rapidly buckles out of plane. Another example is what happens when you crumple up a ball of paper. In this case, there is no configuration the paper can take which only involves bending. It has to do a little bit of stretching, but it minimises this by confining the stretching to ridges and points. In between these, the paper bends as expected. This gives a scrunched up ball of paper its characteristic shape.

4.6.3 The elastica

The idea that an elastic sheet will bend and not stretch is the key principle of Euler's elastica. We have already seen that linear-elastic beams have a strain energy density of $W_b = Bh''^2/2$. In fact Euler showed that for large deformations, this can be generalised to $W_b = B\mathcal{K}^2/2$, where $\mathcal{K}$ is the local curvature of the beam.

$\mathcal{K}$ can be calculated from the normal vector to the beam from $\mathcal{K} = \nabla.\mathbf{n}$. If the position of the beam is $y = h(x)$, $\mathbf{n} = \nabla(y - h(x))/|\nabla(y - h(x))|$, so

$$\mathbf{n} = \frac{(-h', 1, 0)}{\sqrt{1 + h'^2}} \tag{4.49}$$

and

$$\mathcal{K} = \frac{-h''}{(1 + h'^2)^{3/2}}. \tag{4.50}$$

Alternatively, if s is arclength and θ is the angle from horizontal, then

$$\mathcal{K} = \frac{d\theta}{ds} \tag{4.51}$$

Let's use this to calculate the shape of a "ruck in a rug". We lay an elastic of length L on a flat surface, and bring the ends together with a force F, so that they are now a distance $L - \Delta L$ apart. The ends are clamped with $h = h' = 0$. What is the final shape?

In this case, the energy consists of three parts: the bending energy, the gravitational potential energy, and the energy done in compressing the ends together:

$$E = \int_0^L \frac{B}{2}\frac{d\theta}{ds}^2 ds + \int_0^L (\rho g t) h ds - F\Delta L \tag{4.52}$$

We note

$$\Delta L = L - \int_0^L \frac{dx}{ds} ds = \int_0^L (1 - \cos\theta) ds, \tag{4.53}$$

and that by integrating by parts,

$$\int_0^L (\rho g t) h ds = [\rho g t s h]_0^L - \int_0^L \rho g t s h_s ds = -\int_0^L \rho g t s \sin\theta ds \tag{4.54}$$

Thus

$$E = \int_0^L \left(\frac{B}{2}\frac{d\theta}{ds}^2 - \rho g t s \sin\theta - F(1 - \cos\theta) \right) ds \tag{4.55}$$

Using the Euler-Lagrange equation, we finally obtain the heavy elastica equation:

$$B\theta'' = -\rho g t s \cos\theta - F \sin\theta. \tag{4.56}$$

This is a surprisingly simple equation, given that we have to deal with curvatures, which normally bring in many nasty derivatives. It can be solved numerically, as you'll see in the Problems.

4.7 General elastic equations

Finally, let's derive the general elastostatic equations for a given strain energy density function. Suppose that we prescribe the stresses over the surface of an elastic body.

In this case, the elastic energy of the body is

$$E_{el} = \int_V W(\epsilon_{ij}) dV - \int_S \mathbf{u}.\sigma.\mathbf{n} dS \tag{4.57}$$

where $\mathbf{n}$ is the normal to the body, S is the surface of the body, and $\mathbf{u}$ is the displacement at its surface. Recall that the strain is given by

$$\epsilon_{ij} = \frac{1}{2}\left(\frac{\partial u_i}{\partial x_j} + \frac{\partial u_j}{\partial x_i}\right) \tag{4.58}$$

We minimise the energy by letting $u \to u + \delta u$. Then

$$\delta E = \int_V \frac{\partial W}{\partial \epsilon_{ij}} \delta\epsilon_{ij} dV - \int_S \delta\mathbf{u}.\sigma.\mathbf{n} dS \tag{4.59}$$

and using equation (4.58)

$$\delta E = \frac{1}{2}\int_V \frac{\partial W}{\partial \epsilon_{ij}}\left(\frac{\partial \delta u_i}{\partial x_j} + \frac{\partial \delta u_i}{\partial x_j}\right) dV - \int_S \delta\mathbf{u}.\sigma.\mathbf{n} dS \tag{4.60}$$

ϵ_{ij} is symmetric, which gives

$$\delta E = \int_V \frac{\partial W}{\partial \epsilon_{ij}} \frac{\partial \delta u_i}{\partial x_j} dV - \int_S \delta\mathbf{u}.\sigma.\mathbf{n} dS \tag{4.61}$$

and we can rewrite this as

$$\delta E = \int_V \left[\frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial \epsilon_{ij}}\delta u_i\right) - \delta u_i \frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial \epsilon_{ij}}\right)\right] dV - \int_S \delta\mathbf{u}.\sigma.\mathbf{n} dS. \tag{4.62}$$

Using the divergence theorem, we obtain

$$\delta E = -\int_V \delta u_i \frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial \epsilon_{ij}}\right) dV + \int_S \left[\delta u_i \frac{\partial W}{\partial \epsilon_{ij}} n_j - \delta u_i \sigma_{ij} n_j\right] dS. \tag{4.63}$$

The only way that this can always be minimised is if

$$\frac{\partial}{\partial x_j}\left(\frac{\partial W}{\partial \epsilon_{ij}}\right) = 0 \tag{4.64}$$

in the bulk of the solid, while

$$\frac{\partial W}{\partial \epsilon_{ij}} = \sigma_{ij} \tag{4.65}$$

on the boundaries. If we compare equation (4.64) to the elastostatic equation $\nabla.\sigma = 0$, we see that these equations are satisfied if $\partial W/\partial \epsilon_{ij} = \sigma_{ij}$ everywhere. This demonstrates the importance of the choice of the strain energy density function W: it contains all the information to give us both the strains and the stresses in an elastic body.

Although this section is a little abstract, the other main point is to show you how we can generalise the Calculus of Variations to higher dimensions. In this case, we have to use the divergence theorem instead of integrating by parts. However otherwise, the procedure is completely analogous. Note also, that as before we cannot throw away automatically throw away surface terms - here they add an extra boundary constraint.

4.8 Liquid Crystals

Liquid crystals are an important tool that have found use in the majority of modern visual technologies. Most computer and TV screens incorporate liquid crystals, as does everything from your digital watch to a calculator screen. As you will be aware, in each of these cases, liquid crystals are use to alter the opacity of a small pixel on the screen, allowing the screen to display complex pictures. Liquid crystals are often found in many other places - the tobacco mosaic virus is a famous virus that shows liquid crystalline properties.

So what is a liquid crystal? The key is that the molecules or particles that make up the liquid crystal have some sort of directionality to them - these could be rod-like, disk-like, or more asymmetric. In certain temperature regimes, this directionality will make the molecules want to line up in a certain orientation. The temperature is important: when the temperature is too low, the molecules will form a rigid crystal lattice (see figure **??**). When the temperature is too high,

the molecules have so much thermal energy that they align themselves randomly. However, in between these two phases, the molecules want to align themselves, but have too much energy to form a crystal lattice. This means they have long-ranged *directional order*, but no long-ranged *positional order*.

We will focus our attention from hereon on a specific type of liquid crystal - the nematic liquid crystal. These consist of rod-like molecules or particles that want to line up parallel to each other (I'll refer to them as rods from now onwards). You can think of them as long, thin cylinders floating in a liquid phase. As we shall see, these have useful properties that make them ideal for liquid-crystal devices.

4.8.1 The potential energy density of a liquid crystal

As with the elasticity results that we derived in the previous lecture, we will model liquid crystals by defining a local potential energy density of the liquid crystal that depends on some local property of the individual particles. As mentioned above, the rods preferentially line up parallel to each other, so therefore the energy should be minimal when the particles are locally aligned. On the other hand, if the rods fan out from each other at a point, then the energy should be increased locally.

In fact we can separate the different ways that energy can be locally increased into three different categories: *Splay, twist*, and *bend*. Splay can be thought of as the rods all fanning out from a point in a plane. Twist is like a helix, with the rods twisting around as you move downwards through a sample. Bend is where the rods circle around a point.

The most natural way of characterising the local energy density is by using the local *director*, $\mathbf{n}$, of the rods. This is the unit vector that points along the long axis of the rod. Then

$$\nabla.\mathbf{n} \neq 0 \tag{4.66}$$

corresponds to splay.

$$\mathbf{n}.(\nabla \wedge \mathbf{n}) \neq 0 \tag{4.67}$$

corresponds to twist, and

$$\mathbf{n} \wedge (\nabla \wedge \mathbf{n}) \neq 0 \tag{4.68}$$

corresponds to bend.

The simplest model describing liquid crystal behaviour is given by the Frank distortion energy density:

$$W(\mathbf{n}) = \frac{K_1}{2}|\nabla.\mathbf{n}|^2 + \frac{K_2}{2}|\mathbf{n}.(\nabla \wedge \mathbf{n})|^2 + \frac{K_3}{2}|\mathbf{n} \wedge (\nabla \wedge \mathbf{n})|^2 \tag{4.69}$$

4.8.2 2D liquid crystals

Let's start by considering a 2D liquid crystal, as this will significantly simplify the energy density. To do this, we assume that

$$\mathbf{n} = (\cos\theta, \sin\theta, 0), \tag{4.70}$$

with $\theta = \theta(x, y)$. Then we find

$$\nabla.\mathbf{n} = -\sin\theta\frac{\partial\theta}{\partial x} + \cos\theta\frac{\partial\theta}{\partial y}, \tag{4.71}$$

$$\nabla \wedge \mathbf{n} = \left(\cos\theta\frac{\partial\theta}{\partial x} + \sin\theta\frac{\partial\theta}{\partial y}\right)\mathbf{k} \tag{4.72}$$

where $\mathbf{k}$ is the unit vector in the z direction. From this, we see that $\mathbf{n}.(\nabla \wedge \mathbf{n}) = 0$, and there is no twist.

If we continue to churn the handle, we eventually obtain that the distortion energy density reduces to:

$$W = \frac{K_1}{2}(\theta_x^2\sin^2\theta - 2\theta_x\theta_y\sin\theta\cos\theta + \theta_y^2\cos^2\theta) + \frac{K_3}{2}(\theta_x^2\cos^2\theta + 2\theta_x\theta_y\sin\theta\cos\theta + \theta_y^2\sin^2\theta). \tag{4.73}$$

This is still rather messy, but if we make the simplifying assumption that $K_1 = K_3 = K$, we find

$$W = \frac{K}{2}(\theta_x^2 + \theta_y^2) = \frac{K}{2}|\nabla\theta|^2. \tag{4.74}$$

So the local potential energy density only depends on the change in the angle of the rods in the liquid crystal. The assumption that $K_1 = K_3 = K$ is known as the one-constant approximation.

Strong anchoring

As you can imagine, rod-like liquid crystals will also have a preferential orientation when they meet a flat boundary. This can be controlled very specifically. For instance if you rub a piece of glass, the electrostatic charge will make the rods line up along the rubbing direction, parallel to the glass. The rods can also be force to line up perpendicular to, or at a fixed angle to the wall.

If the interaction is sufficiently strong that the rods take a fixed orientation at a boundary, then we can use this as a fixed boundary condition. For example, let's consider the case where the liquid crystal is placed between two walls: one at $y = 0$, and one at $y = d$. At the bottom wall, $\theta = 0$ (rods parallel to the wall), while at the top wall, $\theta = \pi/2$ (rods perpendicular to the wall).

θ is only a function of y, so the total distortion energy of the sample per unit length in the x direction is

$$\int_0^d \frac{K}{2}\theta_y^2 dy, \tag{4.75}$$

and from the Euler-Lagrange equation, we find that $\theta_{yy} = 0$, so we find the solution

$$\theta = \frac{\pi y}{2d}. \tag{4.76}$$

Note the subtlety that $\theta = -\frac{\pi y}{2d}$ is also a valid solution - the rods are assumed symmetrical, and so this will also satisfy the boundary conditions. The difference is that in the first solution, the rods rotate anticlockwise by a quarter turn as they move upwards towards the top boundary. In the second solution, the rods rotate clockwise by a quarter turn.

4.8.3 Weak anchoring

If the rods are not strongly anchored onto the wall, then we need to use a surface energy term to describe the energy of the interaction of the rod with the wall. The most well known of these is the Rapini-Papoular expression for the surface energy density:

$$w_s = \mathcal{W}\sin^2(\theta - \theta_p), \tag{4.77}$$

where θ_p is the preferred binding angle at the wall.

Let's return to the previous example (see Figure **??**), and assume that the preferred binding angle at the bottom is θ_b, and the preferred binding angle at the top is θ_t. Then the energy per unit length in the x direction becomes

$$E = \int_0^d \frac{K}{2}\theta_y^2 dy + \mathcal{W}\sin^2[\theta(0) - \theta_b] + \mathcal{W}\sin^2[\theta(d) - \theta_t], \tag{4.78}$$

then from equation (4.8), we have that

$$\delta E = \left[\delta\theta\frac{\partial f}{\partial \theta'}\right]_0^d + \int_0^d \delta\theta\left[-\frac{d}{dx}\left(\frac{\partial f}{\partial \theta'}\right)\right]dx + \mathcal{W}\sin^2[\theta(0) + \delta\theta(0) - \theta_b] + \mathcal{W}\sin^2[\theta(d) + \delta\theta(d) - \theta_t]$$
$$-\mathcal{W}\sin^2[\theta(0) - \theta_b] - \mathcal{W}\sin^2[\theta(d) - \theta_t] = 0 \tag{4.79}$$

We Taylor expand the last four terms to find

$$\left[\delta\theta K\frac{\partial\theta}{\partial y}\right]_0^d - \int_0^d \delta\theta K\theta_{yy}dy + \frac{\mathcal{W}\delta\theta(0)}{2}\sin[2(\theta(0)-\theta_b)] + \frac{\mathcal{W}\delta\theta(d)}{2}\sin[2(\theta(d)-\theta_t)] = 0. \tag{4.80}$$

Finally we see that the only way that this can always be zero is if

$$\theta_{yy} = 0 \tag{4.81}$$

in the bulk, while we have boundary conditions

$$K\theta_y(0) + \frac{\mathcal{W}}{2}\sin[2(\theta(0) - \theta_b)] \tag{4.82}$$

$$K\theta_y(d) + \frac{\mathcal{W}}{2}\sin[2(\theta(d) - \theta_t)]. \tag{4.83}$$

You can solve these. Here, I will just mention that there is a natural lengthscale in the equations $K/\mathcal{W}$. When the gap thickness d is much larger than this lengthscale, the anchoring is strong enough that it rotates all the rods to be at their preferred orientation at both boundaries. When $d \ll K/\mathcal{W}$, the anchoring is not strong enough to rotate the rods. Then all the rods will be at a constant, intermediate angle.

4.8.4 Electric and magnetic fields

The most useful property of liquid crystals stems from their ability to align with electric and magnetic fields ($\mathbf{E}$ and $\mathbf{B}$ respectively). For the case of an electric field, we can see that it's natural to construct a potential energy that depends on $\mathbf{E}.\mathbf{n}$. In fact the potential energy of a liquid crystal in an electric field is given by

$$E_{\text{elec}} = -\int_V \frac{1}{2}\epsilon_0 \Delta\epsilon (\mathbf{E}.\mathbf{n})^2 dV, \tag{4.84}$$

where ϵ_0 is the vacuum permittivity and $\Delta\epsilon$ is the electric dipole moment of the rods. Similarly the potential energy of a liquid crystal in an magnetic field is given by

$$E_{\text{mag}} = -\int_V \frac{1}{2}\mu_0^{-1} \Delta\chi (\mathbf{B}.\mathbf{n})^2 dV, \tag{4.85}$$

where μ_0 is the magnetic permeability of vacuum, and $\Delta\chi$ is the diamagnetic anisotropy of the rods.

4.8.5 Fréedericksz transitions

We can use these expressions to study a very useful property of liquid crystals: the fact that they will suddenly jump between orientations when an electric or magnetic field is applied that is above a certain strength. Depending on their

orientation, the rods will either block, or allow polarised light to pass. Thus we can use these fields to control the brightness of a liquid crystal pixel on a screen very accurately and quickly.

Let's go back to the strong anchoring geometry, but now assume that $\theta(0) = \theta(d) = 0$. i.e. the rods are constrained to lie parallel to the bottom and top plates. However, now we add an electric field that points in the y direction. In this case, $\mathbf{E} = (0, E, 0)$ and $\mathbf{n} = (\cos\theta, \sin\theta, 0)$ so that $\mathbf{E}.\mathbf{n} = E\sin\theta$.

Again we utilise the one-constant approximation, so that the total potential energy is:

$$\int_0^d \left[\frac{K}{2}\theta_y^2 - \frac{1}{2}\epsilon_0\Delta\epsilon E^2\sin^2\theta\right] dy. \tag{4.86}$$

We can use the Euler-Lagrange equation to then establish that

$$\epsilon_0\Delta\epsilon E^2\sin\theta\cos\theta + K\theta_{yy} = 0. \tag{4.87}$$

This has an obvious solution $\theta = 0$. However we want to know what the non-zero solution is when the electric field is strong enough to distort the rods. Multiply by θ_y and integrate once to obtain

$$K\theta_y^2 + \epsilon_0\Delta\epsilon E^2\sin^2\theta = c. \tag{4.88}$$

To determine the constant, note that the solution is expected to be symmetric about $y = d/2$. Therefore $\theta_y(d/2) = 0$, and $\theta(d/2) = \theta_m$, so

$$K\theta_y^2 + \epsilon_0\Delta\epsilon E^2(\sin^2\theta - \sin^2\theta_m) = 0. \tag{4.89}$$

We nondimensionalise by setting $d\hat{y} = y$, and $\xi_d = \sqrt{K/(\epsilon_0\Delta\epsilon E^2 d^2)}$ to obtain

$$\xi_d^2\theta_{\hat{y}}^2 + (\sin^2\theta - \sin^2\theta_m) = 0, \tag{4.90}$$

which we wish to solve with boundary conditions $\theta(0) = 0$ and $\theta(1/2) = \theta_m$.

Now let $k = \sin\theta_m$ and $t = \sin\theta/\sin\theta_m$ and after some rearrangement this becomes

$$\frac{\partial t}{\partial\hat{y}} = \frac{1}{\xi_d}\sqrt{1-t^2}\sqrt{1-k^2t^2}. \tag{4.91}$$

Separate and integrate from $\hat{y} = 0$ to $1/2$ (which corresponds to integrating t from 0 to 1):

$$\int_0^1 \frac{dt}{\sqrt{1-t^2}\sqrt{1-k^2t^2}} = \int_0^{1/2}\frac{d\hat{y}}{\xi_d} = \frac{1}{2\xi_d} = \frac{1}{2}\sqrt{\frac{\epsilon_0\Delta\epsilon E^2 d^2}{K}}. \tag{4.92}$$

The left hand side is the complete elliptic integral of the first kind $K(k)$. It has its smallest value when $k = 0$, where $K(0) = \pi/2$. Thus there is only a non-zero solution when

$$\sqrt{\frac{\epsilon_0 \Delta\epsilon E^2 d^2}{K}} > \pi. \tag{4.93}$$

In other words, the electric field has to exceed the critical strength

$$E_c = \frac{\pi}{d}\sqrt{\frac{K}{\epsilon_0 \Delta\epsilon}}, \tag{4.94}$$

and then the liquid crystal rods will start to rotate. Note that, from measuring E_c, we have a technique for measuring K.