73
Laplacian models

... on aura donc $\Delta u = 0$; cette équation remarquable nous sera de la plus grande utilité .... (Laplace)

If one has to stick to this damned quantum jumping, then I regret ever having been involved in this thing. I don't like it (quantum mechanics), and I'm sorry I ever had anything to do with it. (Schrödinger)

73.1 Introduction

In this chapter, we present some basic models involving the Laplacian, including models for heat conduction, elasticity, electromagnetics, fluid mechanics, and gravitation. In deriving these models, we make use of the basics of Calculus in several dimensions including Gauss' and Stokes' theorems, and we get a quick and easy introduction to some of mysteries of the mechanics and physics of "continuous media". We also make connections to linear algebra when discretizing the Laplacian using the 5-point scheme and variants of "Svensson's formula".

73.2 Heat conduction

We first model *heat conduction* in a heat-conducting material occupying the volume Ω in $\mathbb{R}^3$ with boundary Γ, over a time interval $I = [0, T]$. We let $u(x,t)$ denote the *temperature* and $q(x,t)$ the *heat flux* at the point x at time t. The heat flux is a vector $q = (q_1, q_2, q_3)$, where q_i is the heat flux, or rate of heat flowing in the direction x_i. We let $f(x,t)$ denote the rate of heat (per unit of volume) supplied at (x,t) by a *heat source*.

We derive the model using a basic *conservation law* expressing *conservation of heat* in the following form: for any fixed domain V in Ω with boundary S, the rate of the total heat introduced in V by the external source is equal to the rate of the total heat accumulated in V plus the total heat flux through S. This is based on the conviction that the heat introduced in V by the external source can choose between two options only: (i) flow out of V or (ii) be accumulated in V. With S denoting the boundary of V and n denoting the outward unit normal to S, see Fig. 73.1, the conservation law can be expressed as

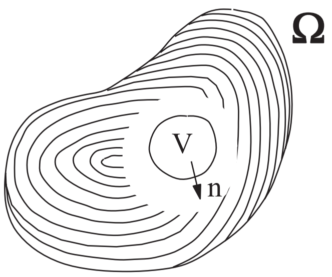

FIGURE 73.1. An arbitrary subset V of a heat conducting body Ω.

$$\int_V f\,dx = \frac{\partial}{\partial t}\int_V \lambda u\,dx + \int_S q\cdot n\,ds, \tag{73.1}$$

where $\lambda(x,t)$ is the *heat capacity coefficient* giving the amount heat per unit of volume needed to raise the temperature one unit, and all functions are evaluated at a specific time $t \in I$. By the Divergence theorem,

$$\int_S q\cdot n\,ds = \int_V \nabla\cdot q\,dx,$$

and combined with (73.1), this implies that

$$\int_V \left(\frac{\partial}{\partial t}(\lambda u) + \nabla\cdot q\right)\,dx = \int_V f\,dx,$$

where the time derivative could be moved under the integral sign because V does not depend on time t. Since V is arbitrary, assuming the integrands are Lipschitz continuous, it follows that

$$\frac{\partial}{\partial t}(\lambda u)(x,t) + \nabla\cdot q(x,t) = f(x,t) \quad \text{for all } x\in\Omega,\ 0<t\le T, \tag{73.2}$$

which is a differential equation describing *conservation of heat* involving two unknowns: the temperature $u(x,t)$ and the heat flux $q(x,t)$. We thus have one equation and two unknowns and we need yet another equation.

The second equation is a *constitutive equation* that couples the heat flux q to the temperature gradient ∇u. *Fourier's law* states that heat flows from warm to cold regions with the heat flux proportional to the temperature gradient:

$$q(x,t) = -a(x,t)\nabla u(x,t) \quad \text{for } x \in \Omega,\ 0 < t \le T \tag{73.3}$$

where the factor of proportionality $a(x,t)$ is the coefficient of heat conductivity. Note the minus sign indicating that the heat flows from warm to cold regions, and that the heat conductivity $a(x,t)$ is positive. Combining (73.2) and (73.3), we obtain the basic differential equation describing heat conduction:

$$\frac{\partial}{\partial t}(\lambda u) - \nabla \cdot (a\nabla u) = f \quad \text{in } \Omega \times (0,T], \tag{73.4}$$

where $a(x,t)$ and $\lambda(x,t)$ are given positive coefficients depending on (x,t) and $f(x,t)$ is a given heat source, and the unknown $u(x,t)$ represents the temperature.

To define the solution uniquely, the differential equation is complemented by initial and boundary conditions. The complete model with *Dirichlet boundary conditions* reads

$$\begin{cases} \frac{\partial}{\partial t}(\lambda u) - \nabla \cdot (a\nabla u) = f & \text{in } \Omega \times (0,T], \\ u = u_b & \text{on } \Gamma \times (0,T], \\ u(x,0) = u_0(x) & \text{for } x \in \Omega, \end{cases} \tag{73.5}$$

where u_0 is the initial temperature and u_b is the boundary temperature. The Dirichlet boundary condition corresponds to immersing the body Ω in a large reservoir with a specified temperature u_b and assuming that the boundary acts as a perfect thermal conductor so that the temperature of the body on the boundary is equal to the specified outside reservoir temperature u_b. Note that the given boundary temperature $u_b = u_b(x,t)$ may vary with (x,t).

Other commonly encountered boundary conditions are *Neumann* and *Robin* boundary conditions. A Neumann boundary condition corresponds to prescribing the heat flux $q \cdot n$ across (out of) the boundary:

$$q \cdot n = -a\nabla u \cdot n = -a\frac{\partial u}{\partial n} = -a\partial_n u = g \quad \text{on } \Gamma,$$

with g given. A *homogeneous Neumann boundary condition* with $g = 0$ corresponds to a perfectly insulating boundary with the heat flux across the boundary being zero. A homogenous Robin boundary condition is intermediate with the boundary neither being perfectly conducting nor perfectly insulated, with the heat flux through the boundary being proportional to the difference of the temperature u inside and a given temperature u_b outside Ω:

$$-a\partial_n u = \kappa(u - u_b)$$

with κ a positive coefficient representing the heat conductivity of the boundary.

Partitioning the boundary Γ into disjoint pieces Γ_1, Γ_2 and Γ_3 with different types of boundary conditions, the *general initial boundary value problem* IBVP for the heat equation has the form,

$$\begin{cases} \frac{\partial}{\partial t}(\lambda u) - \nabla \cdot (a\nabla u) = f & \text{in } \Omega \times (0,T], \\ u = u_b & \text{on } \Gamma_1 \times (0,T], \\ -a\partial_n u = g & \text{on } \Gamma_2 \times (0,T], \\ a\partial_n u + \kappa(u - u_b) = 0 & \text{on } \Gamma_3 \times (0,T], \\ u(x,0) = u_0(x) & \text{for } x \in \Omega, \end{cases} \tag{73.6}$$

where u_b represents a given "exterior" boundary temperature, and g represents a given outward normal heat flux on the boundary.

We note that in a stationary situation with $\frac{\partial}{\partial t}(\lambda u) = 0$ and with the heat source $f = 0$, the equation (73.2) expressing conservation of heat, takes the form

$$\nabla \cdot q = 0. \tag{73.7}$$

If heat is neither produced nor accumulated, then conservation of heat is expressed by the equation $\nabla \cdot q = 0$, that is, the heat flux q is *divergence-free*. Below we shall meet several other examples of divergence-free fields.

73.3 The heat equation

We refer to the special case of (73.6) with $\lambda = a = 1$ as the *heat equation*. In the case with homogeneous Dirichlet boundary conditions, we get the model

$$\begin{cases} \frac{\partial u}{\partial t} - \Delta u = f & \text{in } \Omega \times (0,T], \\ u = 0 & \text{on } \Gamma \times (0,T], \\ u(x,0) = u_0(x) & \text{for } x \in \Omega, \end{cases}$$

where u_0 is the initial temperature, and $\Delta u = \nabla \cdot (\nabla u)$ is the Laplacian. The heat equation serves as a basic prototype of a *parabolic problem*.

FIGURE 73.2. Poisson (1781-1840): "Life is good for only two things: to study mathematics and to teach it"

73.4 Stationary heat conduction: Poisson's equation

The stationary analog of (73.6) reads

$$\begin{cases} -\nabla \cdot (a\nabla u) = f & \text{in } \Omega, \\ u = u_b & \text{on } \Gamma_1, \\ -a\partial_n u = g & \text{on } \Gamma_2, \\ a\partial_n u + \kappa(u - u_b) = 0 & \text{on } \Gamma_3. \end{cases} \tag{73.8}$$

Choosing $a = 1$ leads to the *Poisson equation*:

$$\begin{cases} -\Delta u = f & \text{in } \Omega, \\ u = u_1 & \text{on } \Gamma_1, \\ -a\partial_n u = g_2 & \text{on } \Gamma_2, \\ a\partial_n u + \kappa(u - u_b) = g_3 & \text{on } \Gamma_3. \end{cases} \tag{73.9}$$

In the case of homogeneous Dirichlet boundary conditions on the whole of the boundary, the Poisson equation reads

$$\begin{cases} -\Delta u = f & \text{in } \Omega, \\ u = 0 & \text{on } \Gamma. \end{cases} \tag{73.10}$$

Poisson's equation serves as a basic model of an *elliptic* problem and has numerous applications in physics and mechanics. We present the basic applications below. Poisson's equation $-\Delta u = f$ with $f = 0$ is referred to as *Laplace's equation*: $\Delta u = 0$.

We now give a couple of analytic solutions to the heat equation in simple situations:

EXAMPLE 73.1. The stationary temperature u in a heat conduction unit cube Q with heat production and conduction coefficient equal to one, zero boundary temperature for $x_1 = 0, 1$, and zero heat flux for $x_2, x_3 = 0, 1$, is given by

$$u(x) = \frac{1}{2}(x_1(1 - x_1).$$

We see that the temperature is maximal for $x_1 = 0.5$ and drops off quadratically towards the Dirichlet boundary, see Fig. 73.3 for a plot in the corresponding case in two dimension in the unit square.

EXAMPLE 73.2. Consider the homogenous heat equation in the unit square Q with $f = 0$ and homogenous Dirichlet boundary conditions: the function

$$u(x, t) = e^{-(n^2+m^2)t} \sin(nx_1) \sin(mx_2)$$

with $m, n = 1, 2, 3, ...$ is a solution of the homogenous heat equation $\frac{\partial u}{\partial t} - \Delta u = 0$ with initial value $u_0(x_1, x_2) = \sin(nx_1) \sin(mx_2)$, see Fig. 73.3. We see that the temperature $u(x, t)$ decays exponentially in time very quickly if n and/or m is only moderately large. This corresponds to the fact that a temperature oscillating in space, is quickly levelled out.

EXAMPLE 73.3. The stationary temperature $u(x)$ between the two planes $\{x_3 = 0\}$ and $\{x_3 = 1\}$ bounding a heat conducting layer with heat conductivity coefficient equal to one, zero heat source, and the temperature $u = 1$ on $\{x_3 = 1\}$ and $u = 0$ on $\{x_3 = 0\}$, is given by $u(x) = x_3$ displaying a linear variation of the temperature between the plates. No surprise of course.

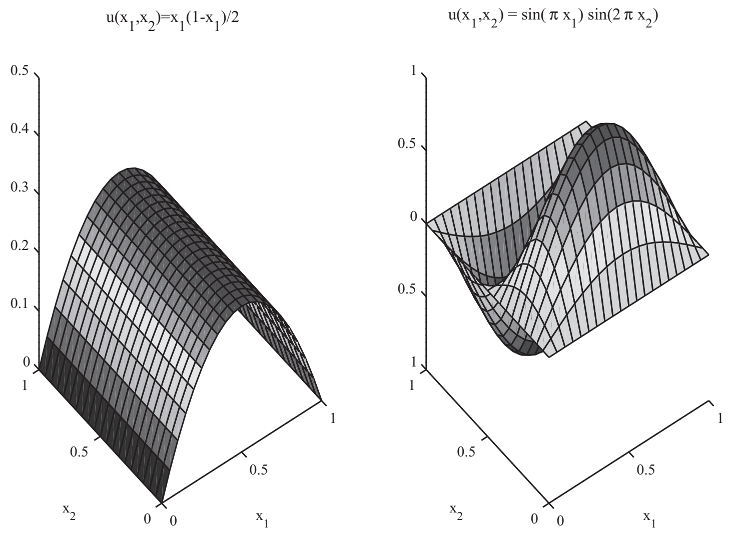

FIGURE 73.3. The functions $\frac{1}{2}(x_1(1-x_1)$ and $sin(\pi x_1) sin(2\pi x_2)$

73.5 Convection-diffusion-reaction

The heat equation models the physical phenomenon of *diffusion*, and we now extend this model to include the phenomena of *convection* and *reaction*. We obtain a scalar *convection-diffusion-reaction* equation, which is another basic model in science. We consider a typical case where u represents the concentration of a certain chemical species subject to convection in a given velocity field $\beta(x,t)$, diffusion with diffusion coefficient $\epsilon(x,t)$ and reaction with reaction rate $\alpha(x,t)$. For example, u may represent the concentration of a contaminant in a volume of water moving with the velocity $\beta(x,t)$.

The model results from a principle of conservation of mass together with a constitutive equation generalizing Fourier's law expressing the *flow rate* q of the chemical species in terms of ∇u and βu. Conservation of mass is expressed by

$$\dot{u} + \nabla \cdot q + \alpha u = f,$$

where f represents a source term, and the constitutive law takes the form

$$q = \beta u - \epsilon \nabla u.$$

which says that the total flow rate q is the sum of a convective rate βu and a diffusive rate $-\epsilon \nabla u$. The model thus takes the form:

$$\dot{u} + \nabla \cdot (\beta u) + \alpha u - \nabla \cdot (\epsilon \nabla u) = f \quad \text{in } \Omega \times (0, T], \qquad (73.11)$$

together with initial and boundary conditions, where Ω is domain in space and $[0, T]$ a given time interval. We shall meet this model and generalizations thereof in several different contexts below.

73.6 Elastic membrane

Consider a horizontal elastic net covering the unit square $Q = \{x \in \mathbb{R}^2 : 0 \le x_i \le 1, i = 1, 2\}$ formed by elastic strings tied together at nodes $a_{ij} \in \mathbb{R}^2$ in a uniform quadrilateral mesh with mesh size $h = 1/N$, so that $a_{ij} = (ih, jh)$, $i, j = 0, 1, ..., N$, where N is the number of cells in each coordinate direction. Assume that the net is stretched so that the tension in each string is equal to h, corresponding to the tension being equal to one per unit of length. Note the normalization introduced says that the tension in each string decreases as the number of strings increases. We refer to the situation in which all the nodes lie in the plane of the square and there is no external load on the net as the unloaded reference configuration of the net.

Suppose the net is subject to a set of downward vertical loads of size $f_{ij}h^2$ at the nodes a_{ij}. The net will deform under the loads and the nodes will be displaced from the initial unloaded reference configuration. Let the vertical displacement of node a_{ij} be denoted by $u_{i,j}$. If the displacements are small, then (recalling the Chapter String theory) the vertical upward force from the net on node a_{ij} is equal to

$$(u_{i,j} - u_{i-1,j}) + (u_{i,j} - u_{i+1,j}) + (u_{i,j} - u_{i,j-1}) + (u_{i,j} - u_{i,j+1}),$$

with contributions from the four pieces of string meeting at a_{ij}. This is because the vertical slope of the line between for example node (i, j) and $(i-1, j)$ is equal to $(u_{i,j} - u_{i-1,j})/h$ and the tension is h. We thus obtain the following vertical equilibrium equation for each node a_{ij}:

$$-\frac{u_{i-1,j} - 2u_{i,j} + u_{i+1,j}}{h^2} - \frac{u_{i,j-1} - 2u_{i,j} + u_{i,j+1}}{h^2} = f_{ij}.$$

Passing to the limit as h tends to zero, and recalling that Taylor's theorem implies

$$\lim_{h \to 0} \frac{v(x-h) - 2v(x) + v(x+h)}{h^2} = v''(x) = \frac{d^2v}{dx^2}(x)$$

if $v : \mathbb{R} \to \mathbb{R}$ is twice differentiable, we are led to the equation

$$-\Delta u(x) = f(x).$$

This equation expresses the equilibrium of a horizontal membrane made by an elastic fabric and carrying a vertical load of intensity (force per unit area) $f(x)$, where $u(x)$ is the vertical displacement of the membrane at x and we assume that the membrane in its unloaded plane reference configuration is prestressed to uniform tension in all directions.

We can generalize to a horizontal membrane covering a general domain Ω in $\mathbb{R}^2$. Assuming the membrane is fixed at the boundary Γ of Ω, so that the vertical displacement $u(x)$ is zero at Γ, we thus obtain Poisson's equation

$$-\Delta u = f \quad \text{in } \Omega, \; u = 0 \quad \text{on } \Gamma \tag{73.12}$$

as a model for the vertical deflection of a horizontal elastic membrane spanned over the boundary Γ of a domain Ω in $\mathbb{R}^2$, subject to a vertical load of intensity $f(x)$. This is a basic model of elasticity theory.

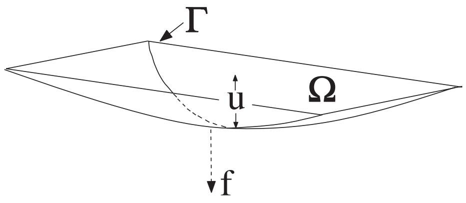

FIGURE 73.4. An elastic membrane under a load $f(x)$ and supported at Γ.

EXAMPLE 73.4. If $\Omega = \{x \in \mathbb{R}^2 : \|x\| < 1\}$ is the unit disc, and the load f is radially symmetric, then the deflection u will also be radially symmetric. Recalling the form of the Laplacian in polar coordinates from the Chapter The divergence, rotation and Laplacian, we can write (73.12) in the form

$$-\Delta u = -\frac{1}{r}\frac{\partial}{\partial r}(r\frac{\partial u}{\partial r}) = f(r) \quad \text{for } 0 < r < 1,\ u(1) = 0, \frac{\partial u}{\partial r}(0) = 0.$$

Note the boundary condition $\frac{\partial u}{\partial r}(0) = 0$, which has no counterpart in x-coordinates, says that $u(x)$ is differentiable at $x = 0$. If $\frac{\partial u}{\partial r}(0) \neq 0$, then $u(x)$ has a a conical "to" at $x = 0$ and thus is not differentiable at $x = 0$. If $f(r) = 1$, then the solution is given by

$$u(r) = \frac{1}{4}(1 - r^2) \quad \text{for } 0 \leq r \leq 1.$$

73.7 Solving the Poisson equation

Suppose we would like to numerically solve the Poisson equation

$$-\Delta u = f \quad \text{in } Q, \quad u = u_b \quad \text{on } \Gamma$$

where Q is the unit square with boundary Γ and $f(x)$ a given function on Q. Recalling the derivation of the model $-\Delta u = f$ from the previous section, we are led to computing approximations $U_{i,j}$ of $u(ih, jh)$ for $i, j = 0, 1, ..., N$, where $h = 1/N$, from the system of equations

$$-\frac{U_{i-1,j} - 2U_{i,j} + U_{i+1,j}}{h^2} - \frac{U_{i,j-1} - 2U_{i,j} + U_{i,j+1}}{h^2} = f(ih, jh),$$
$$i, j = 1, ..., N-1,$$

that is

$$4U_{i,j} - U_{i-1,j} - U_{i+1,j} - U_{i,j-1} - U_{i,j+1} = h^2 f(ih, jh),$$
$$i, j = 1, ..., N-1, \quad (73.13)$$

where $U_{i,j} = u_b(ih, jh)$ if i or j is equal to 0 or N. We see that this is an $m \times m$ system of equations with $m = (N-1)\times(N-1)$ in the unknowns $U_{i,j}$ where $i, j = 1, ..., N-1$. This is the famous *5-point scheme* for the Poisson's equation, where the unknown $U_{i,j}$ is coupled to its four neighbors $U_{i-1,j}$, $U_{i+1,j}$, $U_{i,j-1}$, $U_{i,j+1}$.

If $f = 0$, then the 5-point scheme takes the form ("Svensson's formula")

$$U_{i,j} = \frac{1}{4}(U_{i-1,j} + U_{i+1,j} + U_{i,j-1} + U_{i,j+1}),$$

stating that each value $U_{i,j}$ is the mean value of the neighboring values.

Note that (73.13) is a linear system of equations for the values of U that requires some work to solve. For example, we may try to solve (73.13) by fixed point iteration as follows with $k = 0, 1, ...$

$$U_{i,j}^{k+1} = U_{i,j}^k$$
$$- \alpha\big(4U_{i,j}^k - U_{i-1,j}^k - U_{i+1,j}^k - U_{i,j-1}^k - U_{i,j+1}^k - h^2 f(ih, jh)\big), \quad (73.14)$$

for $i, j = 1, ..., N-1$, with $U_{i,j}^{k+1} = u_b(ih, jh)$ if i or j is equal to 0 or N. Here, $U_{i,j}^k$ is an approximation of $U_{i,j}$ after k steps starting with an initial approximation U_{ij}^0 and α is a positive constant. It turns out that if α is sufficiently small, then the iteration converges, see Problem 73.9, although the convergence gets slower as the step size h decreases.

EXAMPLE 73.5. Assuming x_2 independence, we are led to the model

$$-u''(x) = f(x) \quad \text{for } 0 < x < 1, \quad u(0) = u_0,\ u(1) = u_1,$$

where $u'(x) = \frac{du}{dx}$. The corresponding discrete model takes the form

$$-(U_{i-1} - 2U_i + U_{i+1}) = h^2 f(ih),$$
$$i = 1, ..., N-1,\ U_0 = u_0,\ U_N = u_1, \quad (73.15)$$

with U_i representing an approximation of $u(ih)$. Assuming for simplicity $u_0 = u_1 = 0$, the discrete model can be written in the form

$$AU = b,$$

with $U = (U_1, ..., U_{N-1})$, $b = (b_1, ..., b_{N-1})$ with $b_i = h^2 f(ih)$, $A = (a_{ij})$ an $(N-1)\times(N-1)$ matrix with $a_{ii} = 2$, $a_{i,i-1} = a_{i-1,i} = -1$ and

$a_{ij} = 0$ if $|i - j| > 1$. The fixed point iteration described above can be written

$$U^{k+1} = U^k - \alpha(AU^k - b),$$

and the criterion of convergence is $\|I - \alpha A\| < 1$, which we prove in Problem 73.9 to be valid if $\alpha > 0$ is sufficiently small. Here, $\|I - \alpha A\|$ is the Euclidean norm of the matrix $I - \alpha A$ and the Spectral theorem implies

$$\|I - \alpha A\| = \max_i |1 - \alpha\lambda_i|,$$

where the λ_i are the eigenvalues of the symmetric matrix A.

73.8 The wave equation: vibrating elastic membrane

We now model the dynamic motion of the elastic membrane considered above in the static. We complement the given exterior force $f(x,t)$, which now may be dependent on time, by a dynamic force, which according to Newton's law, takes the form $m\ddot{u}$, with m representing mass per unit area and $\ddot{u}$ representing the acceleration of vertical displacement u. This to leads to the *wave equation*, modeling a vibrating membrane subject to an exterior load,

$$\begin{cases} \ddot{u} - \Delta u = f & \text{in } \Omega \times (0,T], \\ u = 0 & \text{on } \Gamma \times (0,T], \\ u(x,0) = u^0(x),\ \dot{u}(x,0) = \dot{u}^0(x) & \text{for } x \in \Omega, \end{cases} \tag{73.16}$$

where Ω denotes a domain in $\mathbb{R}^d$ with boundary Γ, u^0 is a given initial displacement, $\dot{u}^0$ is a given initial displacement velocity, and we assume homogeneous Dirichlet boundary conditions for simplicity. Other boundary conditions, notably periodic boundary conditions, are also relevant for this model.

73.9 Fluid mechanics

Fluid flow opens a rich field for mathematical modelling. We think of a fluid as a collection of many small "fluid particles" and we seek to describe the fluid flow resulting from the motion of all these fluid particles. We work under the assumption that the particles are so small and there are so many, that we can treat the fluid as a continuum. Usually, we use an *Eulerian* mode of description in which we describe the flow in terms of the *velocity* $u(x,t) \in \mathbb{R}^3$ of the fluid particles at position $x \in \mathbb{R}^3$ at time t, or simply the velocity of the fluid at (x,t). This corresponds to attaching an observer to each fixed point x for the purpose of observing the velocity $u(x,t)$ of the fluid particles that happen to be at position x at time t. The observer thus sits at position x and watches the fluid particles swirl by.

Alternatively, in a *Lagrangian* mode of description, an observer is attached to each fluid particle with the purpose of observing the change of velocity of the fluid particle with time. In this case, the observer follows the particle. The different modes of description are both useful and may also be used together, see the chapters on Convection-diffusion in CDE.

The equation of mass conservation

We consider the flow of a fluid within a certain volume $\Omega \in \mathbb{R}^3$ using an Eulerian description with $u(x,t)$ representing the velocity of the fluid at x at time t. The velocity u is a vector $u = (u_1, u_2, u_3)$.

Let $\rho(x,t)$ denote the *density* of a fluid at (x,t) measuring the mass of the fluid particles per unit of volume. Let V be a fixed volume with boundary S. The total mass of the fluid in V at time t is given by

$$\int_V \rho(x,t)\,dx.$$

The mass of fluid at time t passing out through the boundary S per unit of time is given by

$$\int_S \rho(x,t)u(x,t)\cdot n(x)\,ds(x) = \int_V \nabla\cdot(\rho u)(x,t)\,dx,$$

where we used the Divergence theorem. The rate of change of mass in V plus the rate of mass flow through the boundary must be zero if we assume that no fluid is added or removed, which leads to the following expression of *mass conservation*,

$$\frac{\partial}{\partial t}\int_V \rho(x,t)\,dx + \int_V \nabla\cdot(\rho u)(x,t)\,dx = 0.$$

If ρ varies smoothly, then $\frac{\partial}{\partial t}$ may be moved under the integral sign and since V was arbitrarily, we are led to the differential equation expressing *mass conservation*,

$$\frac{\partial \rho}{\partial t} + \nabla\cdot(\rho u) = 0, \tag{73.17}$$

Of course this is a basic equation of mathematical modelling. Performing the differentiation with respect to x, we can express mass conservation in the form

$$\frac{\partial \rho}{\partial t} + u\cdot\nabla\rho + \rho\nabla\cdot u = 0. \tag{73.18}$$

Particle paths and streamlines

Let the velocity of a fluid be given by the function $u(x,t)$. Consider the IVP

$$\frac{d}{dt}x(t) = u(x(t),t) \quad \text{for } t > 0,\, x(0) = x_0.$$

The solution $x(t)$ represents the curve, or path or trajectory, followed by a fluid particle that starts at position x_0 at time $t = 0$ and moves with velocity $u(x(t),t)$ for $t > 0$. If the velocity $u(x,t) = u(x)$ is independent of time t, then particle paths are also referred to as *streamlines*.

Incompressible flow

If the fluid velocity $u(x,t)$ satisfies

$$\nabla \cdot u(x,t) = \Big(\frac{\partial u_1}{\partial x_1} + \frac{\partial u_2}{\partial x_2} + \frac{\partial u_3}{\partial x_3}\Big)(x,t) = 0 \quad \text{for } x \in \Omega\, t > 0,$$

then the flow is said to be *incompressible* in Ω for $t > 0$.

If the flow is incompressible, the equation (73.18) of mass conservation takes the form

$$\frac{\partial \rho}{\partial t} + u \cdot \nabla \rho = 0. \tag{73.19}$$

Since $\frac{dx}{dt} = u$ for a $x(t)$ particle path, the Chain rule implies

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

This says that the density is constant along particle paths, or in other words the volume occupied by a certain set of fluid particles is constant. So, the fluid cannot be compressed. It is common to assume that the density of an incompressible fluid is constant.

Water is very nearly incompressible; it is very difficult to change the total volume of a bucket of water. Air is compressible; the air tank of a diver contains a huge volume of air at normal pressure compressed and stored in a small volume at high pressure. But to get the air into the tank consumes energy.

Incompressible potential flow

In so-called *stationary flow*, the velocity $u(x,t)$ is independent of time and thus the fluid velocity $u(x)$ is a function of $x \in \Omega$. Note that in a stationary flow the fluid particles at x are moving if $u(x) \neq 0$, but the velocity of the fluid particles at x does not change with time.

The velocity field $u(x)$ of *rotation-free* fluid flow satisfies $\nabla \times u = 0$, which implies $u = \nabla\varphi$ for a scalar *velocity potential* φ under appropriate convexity assumptions. If the fluid is *incompressible*, then $\nabla \cdot u = 0$, and we obtain the Laplace equation $\Delta\varphi = 0$ for the potential of a rotation-free incompressible flow. At a solid boundary, through which the fluid cannot penetrate, the normal velocity of the fluid is zero, which translates into a homogeneous Neumann boundary condition $\partial_n\varphi = 0$ for the potential φ.

We now give some basic examples of incompressible potential flow. For simplicity, we consider situations in which the velocity $u(x)$ is independent of the x_3-coordinate.

EXAMPLE 73.6. The potential

$$\varphi(x_1, x_2) = x_1^2 - x_2^2$$

satisfies $\Delta\varphi = 0$ and the corresponding flow velocity $u = \nabla\varphi$ is given by

$$u(x) = (2x_1, -2x_2).$$

This represents stationary flow in a corner, see Fig. 73.5. A streamline $x(t)$ satisfies $\frac{dx}{dt} = (2x_1, -2x_2)$, which is a separable equation with solutions satisfying

$$x_1(t)x_2(t) = c,$$

where c is a constant, see Fig. 73.5. We check by computing $\frac{d}{dt}x_1x_2 = \dot{x}_1x_2 + x_1\dot{x}_2 = 2x_1x_2 - 2x_1 2x_2 = 0$.

EXAMPLE 73.7. The potential

$$\varphi(x) = \log(\|x\|)$$

satisfies $\Delta\varphi(x) = 0$ for $x \neq 0$, and the corresponding flow velocity $u = \nabla\varphi$ is given by $u(x) = \frac{x}{\|x\|^2}$, see Fig. 73.5.

EXAMPLE 73.8. We consider incompressible potential flow around an infinite circular cylinder along the x_3-axis with cross-section $\Omega = \{x = (x_1, x_2) \in \mathbb{R}^2 : \|x\| < 1\}$ from left to right, see Fig. 73.5. The potential φ is given in polar coordinates $x = r(\cos(\theta), \sin(\theta))$ by

$$\varphi(x) = \varphi(r, \theta) = (r + \frac{1}{r})\cos(\theta),$$

corresponding to a flow from right to left sweeping around Ω and approaching $u(x) = (1, 0)$ for $\|x_1\|$ large and x_2 bounded. We note that $\Delta\varphi = 0$ for $r \neq 0$, and that $\frac{\partial\varphi}{\partial r} = 1 - 1/r^2 = 0$ for $r = 1$ and thus the flow is tangential to the boundary of Ω.

Note that fluid flow is rarely rotation-free in the whole region occupied by the fluid. In particular, if the fluid is viscous then rotation is generated at solid boundaries.

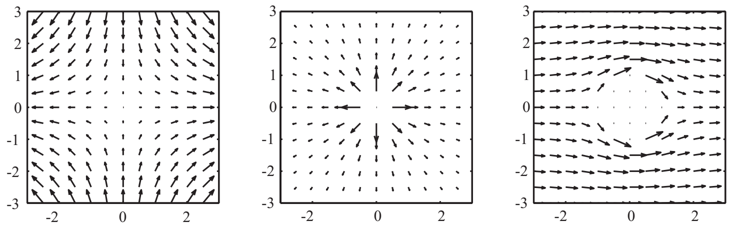

FIGURE 73.5. Examples of incompressible potential flow

Incompressible flow with rotation

We now consider basic examples of incompressible flow in two dimensions with non-zero rotation. We assume $u(x) = (u_1(x), u_2(x))$ satisfies $\nabla \cdot u = 0$, where $x = (x_1, x_2)$. Defining $v = (-u_2, u_1)$ this equation reads $\nabla \times v = 0$ and under appropriate convexity assumptions, there is a potential φ with $v = \nabla\varphi$. Thus,

$$u = (v_2, -v_1) = (\frac{\partial\varphi}{\partial x_2}, -\frac{\partial\varphi}{\partial x_1}) = \nabla \times \varphi.$$

With the rotation $\nabla \times u = f$ given, we are led to the Poisson equation for φ,

$$f = \nabla \times u = \nabla \times (\nabla \times \varphi) = -\Delta\varphi.$$

EXAMPLE 73.9. Given $f = 4$ we find the corresponding solution $\varphi(x) = -\|x\|^2$ with $u(x_1, x_2) = (-2x_2, 2x_1)$, see Fig. 73.6. Choosing $\varphi(x) = \log(\|x\|)$ corresponds to $f(x) = 0$ for $x \neq 0$, and the corresponding velocity $u(x_1, x_2) = \|x\|^{-2}(x_2, -x_1)$, see Fig. 73.6.

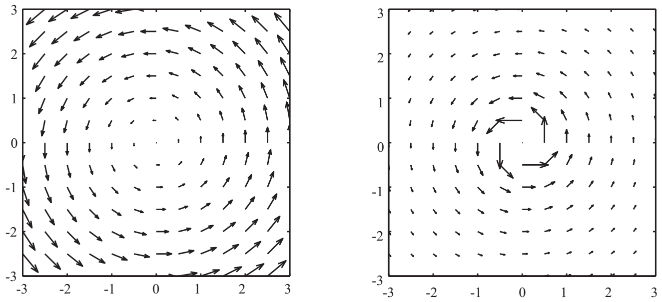

FIGURE 73.6. Incompressible flow with rotation

The Euler and Navier-Stokes equations

The *Euler equations* for an incompressible *inviscid* fluid with constant density equal to one, take the form

$$\frac{\partial u}{\partial t} + (u \cdot \nabla)u + \nabla p = f, \quad \nabla \cdot u = 0, \tag{73.20}$$

where $u(x,t)$ is the velocity and $p(x,t)$ the *pressure* of the fluid at the point x at time t, and f is an applied volume force like a gravitational force. In an inviscid fluid, the *viscosity* is zero and the only interior force acting between the fluid particles is the pressure force that is equal in all directions and acts normal to any surface. The equation $\nabla \cdot u = 0$ expresses the incompressibility of the flow. The first equation expresses Newton's law stating that the acceleration $\frac{d}{dt}u(x(t),t)$, where $x(t)$ is the trajectory followed by a fluid particle satisfying $\frac{dx}{dt} = u(x(t),t)$, is equal to the force $-\nabla p + f$, consisting of the pressure force $-\nabla p$ and the applied force f. We see this by computing with the the Chain rule and the equation $\frac{dx}{dt} = u(x(t),t)$ to get

$$\frac{d}{dt}u_i(x(t),t) = \frac{\partial u_i}{\partial t} + \frac{dx}{dt} \cdot \nabla u_i = \frac{\partial u_i}{\partial t} + (u \cdot \nabla)u_i,$$

which leads to the vector form (73.20). The *Navier-Stokes equations* are modifications of the Euler equations with an additional viscous force term $-\nu\Delta u$, where ν is the viscosity coefficient. In a fluid with non-zero viscosity, there are also tangential (shear) forces acting on a surface.

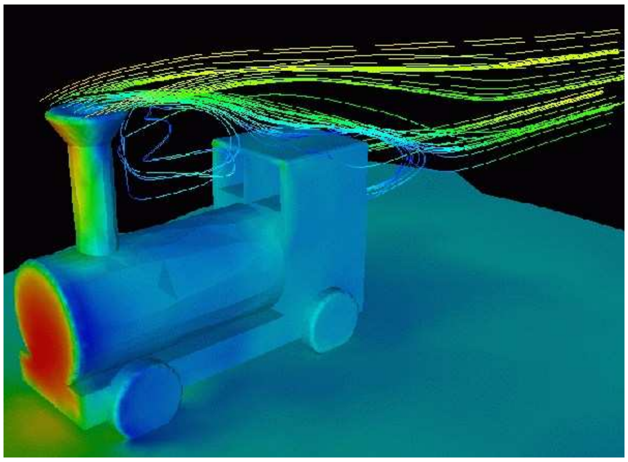

FIGURE 73.7. Flow of air and pressure around a toy train

73.10 Maxwell's equations

The interaction between electric and magnetic fields are described by *Maxwell's equations*:

$$\begin{cases} \dfrac{\partial B}{\partial t} + \nabla \times E = 0, \\ -\dfrac{\partial D}{\partial t} + \nabla \times H = J, \\ \nabla \cdot B = 0, \quad \nabla \cdot D = \rho, \\ B = \mu H, \quad D = \epsilon E, \quad J = \sigma E, \end{cases} \tag{73.21}$$

where E is the *electric field*, H is the *magnetic field* , D is the *electric displacement*, B is the *magnetic flux* , J is the *electric current*, ρ is the *charge*, μ is the *magnetic permeability*, ϵ is the *dielectric constant* of *electric permittivity*, and σ is the *electric conductivity*. The first equation is referred to as *Faraday's law*, the second is *Ampère's law*, $\nabla \cdot D = \rho$ is *Coulomb's law*, *Gauss law* $\nabla \cdot B = 0$ expresses the absence of "magnetic charge", and $J = \sigma E$ is *Ohm's law*. Maxwell included the term $\partial D/\partial t$ for purely mathematical reasons and then used Calculus to predict the existence of electromagnetic waves before these had been observed experimentally.

FIGURE 73.8. Maxwell (1831-1879), inventor of the mathematical theory of electromagnetism: "We can scarcely avoid the conclusion that light consists in the transverse undulations of the same medium which is the cause of electric and magnetic phenomena".

Typical boundary conditions include various combinations of $E \cdot n$ (perfect insulator), $E \times n$ (perfect conductor), $H \cdot n$ and $H \times n$.

Maxwell's equations describe the whole world of electromagnetic phenomena with an astounding economy of notation and accuracy of modelling. Our modern information society builds on electromagnetic waves. We shall now pick out a couple of Laplace equation models from Maxwell's equations by considering some basic particular cases.

Electrostatics

A basic problem in *electrostatics* is to describe the stationary electric field $E(x)$ in a volume Ω in $\mathbb{R}^3$ containing *charges* of density $\rho(x)$ and enclosed by a perfectly conducting surface Γ. Faraday's law states that

$$\nabla \times E = 0 \quad \text{in } \Omega,$$

since we assume that $\frac{\partial B}{\partial t} = 0$. Recalling Chapter Potential fields, it follows that the electric field E is the gradient of a scalar *electric potential* φ, i.e. $E = \nabla\varphi$. Coulomb's law says

$$\nabla \cdot E = \rho \quad \text{in } \Omega,$$

so we are led to the Poisson equation for the potential φ,

$$\Delta\varphi = \nabla \cdot \nabla\varphi = \rho \quad \text{in } \Omega.$$

The boundary condition $E \times n = 0$ on the boundary Γ of Ω with n denoting the outward unit normal, says that the tangential component of E vanishes on the boundary. This models a perfectly conducting boundary in which differences in the electric field are leveled out. This means that $E = \nabla\varphi$ is normal to the boundary, so the boundary is a level surface of φ and the potential φ is constant on the boundary. Since φ is undetermined up to a constant, we may assume that $\varphi = 0$ on the boundary and we arrive at Poisson's equation $-\Delta\varphi = f$ with $f = -\rho$ in Ω with homogenous Dirichlet boundary conditions $\varphi = 0$ on Γ.

The potential $\varphi(x)$ of a point charge at the origin is given by

$$\varphi(x) = \frac{c}{\|x\|}$$

with the corresponding electric field

$$E(x) = -\frac{cx}{\|x\|^3}$$

and c a suitable constant. We shall return to this solution below.

EXAMPLE 73.10. Let $\Omega = \{x \in \mathbb{R}^2 : \|x\| < 1, x_1 < 0 \,\text{or}\, x_2 > 0\}$ be a circular disc with a piece cut out and a *reentrant* corner of angle $\omega = \frac{3\pi}{2}$, see Fig. 73.9. By a direct computation we can verify that the function

$$\varphi(x) = r^\alpha \sin(\alpha\theta)$$

expressed in polar coordinates $x = r(\cos(\theta), \sin(\theta))$, where $\alpha = \frac{\pi}{\omega} = \frac{2}{3}$, satisfies the Laplace equation $\Delta\varphi = 0$ in Ω and the boundary condition $\varphi = 0$ in the straight parts of the boundary meeting at the origin. Letting φ represent an electric potential, the corresponding electric field $E(x) = \nabla\varphi(x)$ satisfies

$$\frac{\partial E}{\partial r} = \alpha r^{\alpha-1} \sin(\alpha\theta)$$

and thus since $\alpha < 1$, is singular (infinite) at the corner where $r = 0$. This means that the electric field is very strong close to the corner, and the sharper the corner (α smaller) the stronger is the field. This may support the observation that an electric lightening is more likely to hit the pointed tower of church than a smooth hill, or the design of an electronic scanner where electrons pop out of the pin of a sharp needle.

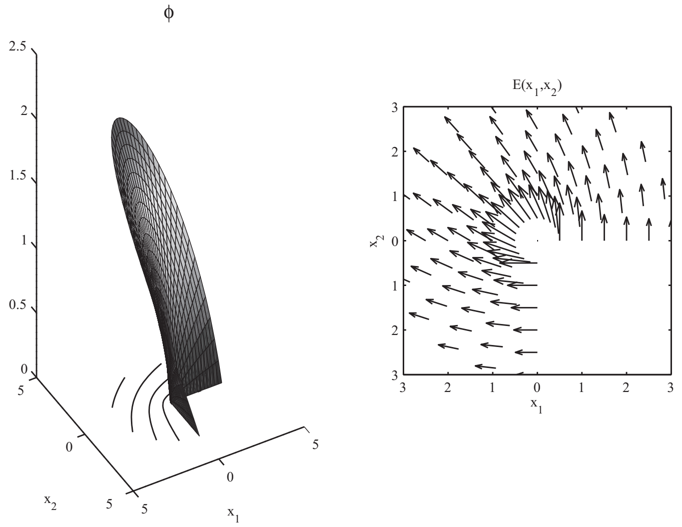

FIGURE 73.9. A potential with singular electric field

EXAMPLE 73.11. The potential φ of the electric field between two concentric spheres $S_1 = \{x \in \mathbb{R}^3 : \|x\| < r_1\}$ and $S_2 = \{x \in \mathbb{R}^3 : \|x\| < r_2\}$ with $r_2 > r_1$, is given by

$$\varphi(x) = \frac{1}{\|x\|}$$

if we assume that $\varphi = 1/r_i$ on S_i, $i = 1, 2$.

EXAMPLE 73.12. The function

$$\varphi(x_1, x_2)) = \arctan(\frac{x_2}{x_1})$$

defined for $x_1 > 0$ satisfies $\Delta\varphi(x) = 0$ for $x_1 > 0$, and is constant $= \arctan(c)$ on rays $x_2 = cx_1$ through the origin of slope c. The corresponding electric field $E(x) = \nabla\varphi(x)$ given by

$$E(x) = \frac{(-x_2, x_1)}{\|x\|^2}.$$

We see that $E(x)$ is singular at $x = 0$.

Magnetostatics

The basic problem in *magnetostatics* arises by combining Gauss' law $\nabla \cdot H = 0$, assuming μ constant and guaranteeing that $H = \nabla \times \varphi$ for some vector potential ψ satisfying $\nabla \cdot \psi = 0$, with Faraday's law $\nabla \times H = J$ to give

$$\nabla \times (\nabla \times \psi) = -\Delta\psi = J,$$

where we use the facts that $\nabla \times (\nabla \times \psi) = -\Delta\psi + \nabla(\nabla \cdot \psi)$ and that $\nabla \cdot \varphi = 0$.

The magnetic field around a unit current J in the x_3-direction is given by

$$H(x) = \frac{1}{2\pi} \frac{(-x_2, x_1, 0)}{\|x\|^2},$$

which can be verified by direct computation showing that $\nabla \cdot H(x) = 0$ and $\nabla \times H(x) = 0$ for $(x_1, x_2) \neq 0$. The presence of the factor $\frac{1}{2\pi}$ makes $\int_\Gamma H \cdot ds = 1$ for any counter-clockwise oriented circle in the x_1x_2-plane, from which by Stokes theorem follows that $\nabla \times H = J$, see the next section on Gravitation and delta functions.

Time-dependent magnetics

In low frequency applications, the term $\frac{\partial D}{\partial t}$ so cleverly introduced by Maxwell, plays a minor role and can be discarded. Let's see where this leads. Since $\nabla \cdot B = 0$, we can write B as $B = \nabla \times \psi$, where ψ is a magnetic vector potential. Inserting this into Faraday's law gives

$$\nabla \times \left(\frac{\partial\psi}{\partial t} + E \right) = 0,$$

from which it follows that

$$\frac{\partial\psi}{\partial t} + E = \nabla\varphi,$$

for some scalar potential φ. Multiplying by σ and using the laws of Ohm and Ampère, we obtain a vector equation for the magnetic potential ψ:

$$\sigma\frac{\partial\psi}{\partial t} + \nabla\times\left(\mu^{-1}\nabla\times\psi\right) = \sigma\nabla\varphi.$$

This system reduces to a scalar equation in two variables if we assume that $B = (B_1, B_2, 0)$ is independent of x_3. It then follows that ψ has the form $\psi = (0, 0, u)$ for some scalar function u that depends only on x_1 and x_2, so that $B_1 = \partial u/\partial x_2$ and $B_2 = -\partial u/\partial x_1$. We end up with a scalar equation for the scalar magnetic potential u in the form

$$\sigma\frac{\partial u}{\partial t} - \nabla\cdot\left(\mu^{-1}\nabla u\right) = f, \tag{73.22}$$

for some function $f(x_1, x_2)$. Choosing $\sigma = \mu = 1$ leads to the heat equation,

$$\begin{cases} \frac{\partial}{\partial t}u(x,t) - \Delta u(x,t) = f(x,t) & \text{for } x\in\Omega,\ 0 < t \leq T,\\ u(x,t) = 0 & \text{for } x\in\Gamma,\ 0 < t \leq T,\\ u(x,0) = u_0(x) & \text{for } x\in\Omega, \end{cases} \tag{73.23}$$

where $\Omega\subset\mathbb{R}^2$ with boundary Γ, and we posed homogeneous Dirichlet boundary conditions. In the stationary case, we again obtain Poisson's equation with Dirichlet boundary conditions.

73.11 Gravitation

In his famous treatise *Mécanique Céleste* in five volumes published during 1799-1825, Laplace extended Newton's theory of gravitation and in particular developed a theory for describing gravitational fields based on using gravitational potentials that satisfy Laplace's equation, or more generally Poisson's equation.

We consider a gravitational field in $\mathbb{R}^3$ with gravitational force $F(x)$ at position x, generated by a distribution of mass of density $\rho(x)$. We recall that the work of a unit mass, moving along a curve Γ is given by

$$\int_\Gamma F\cdot ds,$$

If the curve Γ is closed, then the total work performed by the gravitational forces should be zero. Stokes' theorem implies that a gravitational field F should satisfy $\nabla\times F = 0$. Using the basic result of the Chapter Potential fields, we conclude that F is the gradient of a scalar potential φ, i.e.

$$F(x) = \nabla\varphi(x). \tag{73.24}$$

Laplace proposed the following relation between the gravitational field F and the mass distribution ρ,

$$-\nabla \cdot F(x) = \rho(x), \tag{73.25}$$

assuming the gravitational constant is normalized to one. This is analogous to Coulomb's law $\nabla \cdot E = \rho$ in electrostatics and also to the energy balance equation $\nabla \cdot q = f$ for stationary heat conduction, where q is the heat flux and f a heat source. In particular, (73.25) states that $\nabla \cdot F(x) = 0$ at points x where there is no mass so that $\rho(x) = 0$. Combining (73.24) and (73.25), we obtain Poisson's equation $-\Delta\varphi = \rho$ for the gravitational potential φ.

Since the origin and property of gravitation of "acting at a distance" is still lacking a convincing physical explication, the equation $-\nabla \cdot F(x) = \rho(x)$ including $\nabla \cdot F = 0$ in empty space, should be viewed as a basic postulate on the nature of a gravitational field. Of course it seems very difficult to motivate that $\nabla \cdot F$ should be something different from zero in empty space, but a real a "proof" that $\nabla \cdot F$ must be zero in empty space seems to be missing.

Newton considered gravitational fields generated by *point masses*. Mathematically, a unit point mass at a point $z \in \mathbb{R}^3$ is represented by the so-called *delta function* δ_z at z, defined by the property that for any smooth function v,

$$\int_{\mathbb{R}^3} \delta_z \, v \, dx = v(z), \tag{73.26}$$

where the integration is to be interpreted in a generalized sense. We could think of a δ_z as a limit of positive functions $\varphi_h(x)$ such that $\varphi_h(x) = 0$ if $\|x - z\| > h$ and

$$\int_{\mathbb{R}^3} \varphi_h(x) \, dx = 1,$$

as h tends to zero. For example we may choose

$$\varphi_h(x) = \frac{3}{4\pi h^3} \quad \text{if } \|x - z\| < h$$

and $\varphi_h(x) = 0$ elsewhere. If $v(x)$ is Lipschitz continuous at z, then

$$lim_{h\to 0} \int_{\mathbb{R}^3} \varphi_h(x) v(x) \, dx = v(z),$$

which gives (73.26) its meaning. The function $\varphi_h(x)$ represents a very tall and narrow "hump" around z with volume one.

We expect that the gravitational potential $\Phi(x)$ corresponding to a unit point mass at the origin, to satisfy

$$-\Delta\Phi = \delta_0 \quad \text{in } \mathbb{R}^3, \tag{73.27}$$

assuming the gravitational constant to be equal to one. To give a precise meaning to this equation involving the somewhat mysterious delta function δ_0 at 0, we first formally multiply by a smooth *test function* v vanishing outside a bounded set to get

$$-\int_{\mathbb{R}^3} \Delta\Phi(x)v(x)\,dx = v(0). \tag{73.28}$$

Next, we integrate the left-hand side by parts formally using Green's formula to move the Laplacian from E to v, noting that the boundary terms disappear since v vanishes outside a bounded set. We may thus reformulate (73.27) as seeking a potential $E(x)$ satisfying

$$-\int_{\mathbb{R}^3} \Phi(x)\Delta v(x)\,dx = v(0), \tag{73.29}$$

for all smooth functions $v(x)$ vanishing outside a bounded set. We may view this as the concrete interpretation of (73.27), which is perfectly well defined since now the Laplacian acts on the smooth function $v(x)$ and the potential Φ is assumed to be integrable. We also require the potential $\Phi(x)$ to decay to zero as $\|x\|$ tends to infinity, which corresponds to a "zero Dirichlet boundary condition at infinity".

In the Chapter The divergence, rotation and Laplacian, we showed that the function $1/\|x\|$ satisfies Laplace's equation $\Delta u(x) = 0$ for $0 \neq x \in \mathbb{R}^3$, while it is singular at $x = 0$. We shall prove that the following scaled version of this function satisfies (73.29):

$$\Phi(x) = \frac{1}{4\pi}\frac{1}{\|x\|}. \tag{73.30}$$

We refer to this function as the *fundamental solution* of $-\Delta$ in $\mathbb{R}^3$. We conclude in particular that the gravitational field in $\mathbb{R}^3$ created by a unit point mass at the origin is given by

$$F(x) = \nabla\Phi(x) = -\frac{1}{4\pi}\frac{x}{\|x\|^3},$$

which is precisely Newton's inverse square law of gravitation. Laplace thus gives a motivation why the exponent should be two, which Newton did not (and therefore was criticized by Leibniz). Of course, it still remains to motivate (73.25). In the context of heat conduction, the fundamental solution $E(x)$ represents the stationary temperature in a homogeneous body with heat conductivity equal to one filling the whole of $\mathbb{R}^3$, subject to a concentrated heat source of strength one at the origin and with the temperature tending to zero as $\|x\|$ tends to infinity.

We now prove that the function $\Phi(x)$ defined by (73.30) satisfies (73.29). We first note that since Δv is smooth and vanishes outside a bounded set and $\Phi(x)$ is integrable over bounded domains,

$$\int_{\mathbb{R}^3} \Phi \Delta v \, dx = \lim_{a \to 0^+} \int_{D_a} \Phi \Delta v \, dx, \tag{73.31}$$

where $D_a = \{x \in \mathbb{R}^3 : a < \|x\| < a^{-1}\}$, with a small positive, is a bounded region obtained from $\mathbb{R}^3$ by removing a little sphere of radius a with boundary surface S_a and also points further away from the origin than a^{-1}, see Fig. 73.10. We now use Green's formula on D_a with $w = \Phi$. Since

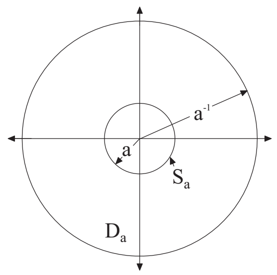

FIGURE 73.10. A cross-section of the domain D_a.

v is zero for $\|x\|$ large, the integrals over the outside boundary vanish when a is sufficiently small. Using the fact that $\Delta\Phi = 0$ in D_a, $\Phi = 1/(4\pi a)$ on S_a and $\partial\Phi/\partial n = 1/(4\pi a^2)$ on S_a with the normal pointing in the direction of the origin, we obtain

$$-\int_{D_a} \Phi \Delta v \, dx = \int_{S_a} \frac{1}{4\pi a^2} v \, ds - \int_{S_a} \frac{1}{4\pi a} \frac{\partial v}{\partial n} \, ds = I_1(a) + I_2(a),$$

with the obvious definitions of $I_1(a)$ and $I_2(a)$. Now, $\lim_{a\to 0} I_1(a) = v(0)$ because $v(x)$ is continuous at $x = 0$ and the surface area of S_a is equal to $4\pi a^2$, while $\lim_{a\to 0} I_2(a) = 0$. The desired equality (73.29) now follows recalling (73.31).

The corresponding fundamental solution of $-\Delta$ in $\mathbb{R}^2$ is given by

$$\Phi(x) = \frac{1}{2\pi} \log(\frac{1}{\|x\|}). \tag{73.32}$$

In this case the fundamental solution is not zero at infinity.

Replacing 0 by an arbitrary point $z \in \mathbb{R}^3$, (73.29) becomes

$$-\int_{\mathbb{R}^3} \Phi(z - x) \Delta v(x) \, dx = v(z), \tag{73.33}$$

which leads to a solution formula for Poisson's equation in $\mathbb{R}^3$. For example, if u satisfies the Poisson equation $-\Delta u = f$ in $\mathbb{R}^3$ and $|u(x)| = O(\|x\|^{-1})$ as

$\|x\| \to \infty$, then u may be represented in terms of the fundamental solution Φ and the right-hand side f as follows:

$$u(z) = \int_{\mathbb{R}^3} \Phi(z-x) f(x)\, dx = \frac{1}{4\pi} \int_{\mathbb{R}^3} \frac{f(x)}{\|z-x\|}\, dx. \tag{73.34}$$

We see that $u(z)$ is a mean value of f centered around z weighted so that the influence of the values of $f(x)$ is inversely proportional to the distance from z.

Similarly, the potential u resulting from a distribution of mass of density $\rho(x)$ on a (bounded) surface Γ in $\mathbb{R}^3$ is given by

$$u(z) = \frac{1}{4\pi} \int_{\Gamma} \frac{\rho(x)}{\|z-x\|}\, ds(x). \tag{73.35}$$

Formally, we obtain this formula by simply adding the potentials from all the different pieces of mass on Γ. One can show that the potential u defined by (73.35) is continuous in $\mathbb{R}^3$ if ρ is bounded on Γ, and of course u satisfies Laplace's equation away from Γ. Suppose now that we would like to determine the distribution of mass ρ on Γ so that the corresponding potential u defined by (73.35) is equal to a given potential u_0 on Γ, that is we seek in particular a function u solving the boundary value problem $\Delta u = 0$ in Ω and $u = u_0$ on Γ, where Ω is the volume enclosed by Γ. This leads to the following *integral equation*: given u_0 on Γ find the function ρ on Γ such that

$$\frac{1}{4\pi} \int_{\Gamma} \frac{\rho(y)}{\|x-y\|}\, ds(y) = u_0(x) \quad \text{for } x \in \Gamma. \tag{73.36}$$

This is a *Fredholm integral equation of the first kind*, named after the Swedish mathematician Ivar Fredholm (1866-1927). In the beginning of the 20th century, Fredholm and Hilbert were competing to prove the existence of solutions of the basic boundary value problems of mechanics and physics using integral equation methods. The integral equation (73.36) is an alternative way of formulating the boundary value problem of finding u such that $\Delta u = 0$ in Ω, and $u = u_0$ on Γ. Integral equations may also be solved using Galerkin methods.

73.12 The drum or the eigenvalue problem for the Laplacian

The *eigenvalue problem* for the Laplace operator with Dirichlet boundary conditions on a domain Ω in $\mathbb{R}^d$ with boundary Γ takes the form: Find nonzero *eigen-functions* $\varphi(x)$ with corresponding *eigenvalues* λ such that

$$\begin{cases} -\Delta\varphi = \lambda\varphi & \text{in } \Omega, \\ \varphi = 0 & \text{on } \Gamma. \end{cases} \tag{73.37}$$

In the one-dimensional case with $\Omega = (0, \pi)$, the eigenfunctions are (modulo normalization) $\varphi_n(x) = \sin(nx)$ with corresponding eigenvalues $\lambda_n = n^2$, $n = 1, 2, ...$ For a two-dimensional square $\Omega = (0, \pi) \times (0, \pi)$, the eigenfunctions are $\varphi_{nm}(x_1, x_2) = \sin(nx_1)\sin(mx_2)$, $n, m = 1, 2, ...$, with eigenvalues $\lambda_{nm} = n^2 + m^2$. It follows by multiplication by φ and integration by parts, that all eigenvalues λ are positive. More precisely, there is an increasing sequence of eigenvalues tending to infinity, and eigenfunctions corresponding to different eigenvalues are orthogonal with respect to the scalar product $(v, w) = \int_\Omega vw\,dx$.

If $\varphi(x)$ is an eigenfunction with corresponding eigenvalue λ, then the (real part of the) function $u(x, t) = \exp(it\sqrt{\lambda})\varphi(x)$ solves the homogeneous wave equation

$$\ddot{u} - \Delta u = 0 \text{ in } \Omega \times \mathbb{R}$$

corresponding to a vibrating elastic membrane (drum head) if $d = 2$ (string if $d = 1$). The smallest eigenvalue corresponds to the basic tone of the drum head.

In Fig. 73.11, we show contour plots for the first four eigenfunctions, corresponding to $\lambda_1 \approx 38.6$, $\lambda_2 \approx 83.2$, $\lambda_3 \approx 111.$, and $\lambda_4 \approx 122.$, in a case where Ω corresponds to the lid of a guitar with Dirichlet boundary conditions on the outer boundary, described as an ellipse, and Neumann boundary conditions at the hole in the lid,

Often the smaller eigenvalues are the most important in considerations of design. This is the case for example in designing suspension bridges, which must be built so that the lower eigenvalues of vibrations in the bridge are not close to possible wind-induced frequencies. This was not well understood in the early days of suspension bridges which caused the famous collapse of the Tacoma bridge in 1940.

The smallest eigenvalue is equal to the minimum value of the *Rayleigh quotient*

$$\frac{(\nabla\psi, \nabla\psi)}{(\psi, \psi)},$$

when varying over functions ψ satisfying the boundary conditions. More, generally, the eigenvalues corresponds to stationary values of the Rayleigh quotient.

73.13 Quantum Mechanics

The two most revolutionary achievements of physics during the 20th century was the development of of the *Theory of General Relativity* for Gravitation on astronomic scales by Einstein, and *Quantum Mechanics* for atomic scales by Schrödinger (1887-1961, Nobel Prize in Physics 1933). Einstein never fully accepted Quantum Mechanics, and the *Grand Unified Theory*

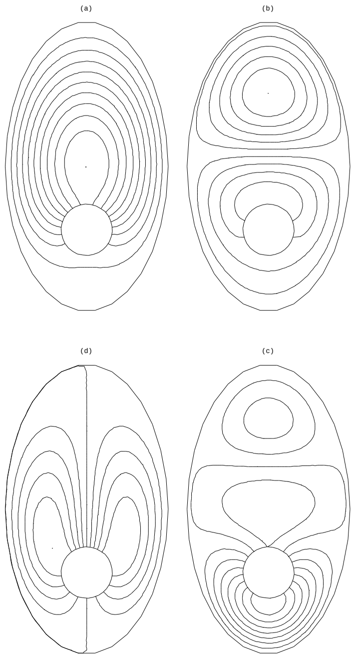

FIGURE 73.11. Contour plots of the first four eigenfunctions of the guitar lid corresponding to (a) $\lambda_1 \approx 38.6$, (b) $\lambda_2 \approx 83.2$, (c) $\lambda_3 \approx 111.$, and (d) $\lambda_4 \approx 122.$. These were computed with Femlab with a fixed mesh size of diameter .02.

connecting Gravitation and Quantum Mechanics is still missing, with *String Theory* being a recent attempt to fill the gap.

The basic equation of Quantum Mechanics is the *Schrödinger equation*, which for a system of N electrons (with the Born-Oppenheimer approximation) takes the following normalized form:

$$i\frac{\partial \varphi}{\partial t} = H\varphi = \big(-\frac{1}{2}\sum_j \Delta_j + V(r_1, ..., r_N)\big)\varphi, \qquad (73.38)$$

where $\varphi = \varphi(r_1, ..., r_N, t)$ is a *wave function* depending on the set of space coordinates $(r_1, ..., r_N)$ with each r_j varying over $\mathbb{R}^3$, together with time t, Δ_j denotes the Laplacian with respect to the coordinate $r_j \in \mathbb{R}^3$, and $V(r_1, ..., r_N)$ denotes a *potential* depending on $(r_1, ..., r_N)$ representing repulsive Coulomb forces between the electrons and attractive Coulomb forces between the electrons and the (fixed) nuclei of the system, $H = -\frac{1}{2}\sum_j \Delta_j + V$ is the *Hamiltonian* representing a sum of kinetic and potential energies, and i denotes the imaginary unit. The wave function is complex-valued and the square of its modulus represents an electron probability density.

The Schrödinger equation appears to give a very good description of phenomena on atomistic scales, but unfortunately it is not easy to deal with because of the large number of spatial dimensions involved: For a system with 100 electrons, which is still very small, the number of space dimensions is equal to 300, and standard techniques for either analytical or numerical solution fall very short. So, although the Schrödinger equation admittedly is a very beautiful equation which gives a surprisingly concise description of atomistic physics, it is certainly impossible to solve exactly analytically, and approximate solution becomes a key issue. The 1998 Nobel Prize in Chemistry was awarded Robert Kohn for his method for approximate solution of the Schrödinger equation based on using a single *electron density function* with the space dependence restricted to $\mathbb{R}^3$, independent of the number of electrons, and corresponding approximate potentials. Such simplified Schrödinger equations, referred to as *Kohn-Sham equations*, are today used extensively in computational chemistry.

The Hydrogen atom

The Hydrogen atom consisting of one electron and one neutron is the only case in which analytical solution of the Schrödinger equation is feasible: In this case the Schrödinger equation takes the following (normalized) form assuming the neutron is positioned at the origin: Find the wave function $\varphi(x,t)$ with $x \in \mathbb{R}^3$, such that for $t > 0$

$$i\frac{\partial\varphi}{\partial t} = (-\frac{1}{2}\Delta + V)\varphi \quad \text{in } \mathbb{R}^3, \tag{73.39}$$

where Δ is the usual Laplacian with respect to x, $V(x) = -\frac{1}{|x|}$ is the Coulomb potential of the proton, with the normalization that

$$\int_{\mathbb{R}^3} |\varphi(x,t)|^2\, dx = 1 \quad \text{for } t > 0.$$

For a domain $\Omega \in \mathbb{R}^3$, the integral

$$\int_{\Omega} |\varphi(x,t)|^2\, dx$$

represents the probability to find the electron in the domain Ω at time t. Formally, $-\frac{1}{2}\Delta$ corresponds to the kinetic energy $\frac{p^2}{2m}$ with p the momentum and m the mass, replacing p by $-i\nabla$ and setting $m = 1$.

In the time-harmonic case with a time-dependence of the form $exp(-i\omega t)$ with frequency ω, this leads to the eigenvalue problem: Find $\varphi(x) \neq 0$ and $\omega \in \mathbb{R}$ such that

$$H\varphi = \omega\varphi, \tag{73.40}$$

FIGURE 73.12. Schrödinger (1887-1961) at age 13: "I was a good student in all subjects, loved mathematics and physics, but also the strict logic of the ancient grammars, hated only memorising incidental dates and facts. Of the German poets, I loved especially the dramatists, but hated the pedantic dissection of this works"

with $H = -\frac{1}{2}\Delta + V$ the Hamiltonian and the eigenvalue ω representing an energy level. The eigenvalues are real and the (real) eigenfunction corresponding to the smallest eigenvalue (smallest energy) is referred to as the *ground state* and the eigenfunctions correspponding to larger eigenvalues as *bound states*.

Assuming spherical symmetry (73.40) takes the following form in spherical coordinates with r the radius: Find $\varphi(r)$ such that

$$-\frac{1}{2}\frac{d^2\varphi}{dr^2} - \frac{1}{r}\frac{d\varphi}{dr} - \frac{1}{r}\varphi = \omega\varphi \quad \text{for } r > 0,$$

with the side condition that $\varphi(0)$ is finite and $\varphi(x)$ is square integrable over $\mathbb{R}^3$. The ground state is given by the eigenfunction $\varphi(r) = \exp(-r)$ corresponding to the eigenvalue $\omega = -\frac{1}{2}$.

Chapter 73 Problems

73.1. Interpret the fixed point iteration for Poisson's equation as an explicit time stepping scheme for the heat equation $\frac{du}{dt} - \Delta u = f$ with time step αh^2 with the starting value given by the initial approximation U^0. Explain why the convergence is slow if h is small.

73.2. Consider a horizontal elastic membrane spanned over a circular ring with constant tension H in all directions in unloaded configuration. Discuss under what conditions the membrane can carry a non-zero volume of water and try to compute the volume.

73.3. Prove that (73.32) is a fundamental solution of $-\Delta$ in $\mathbb{R}^2$.

73.4. Because the presented mathematical models of heat flow and gravitation, namely Poisson's equation, are the same, it opens the possibility of thinking of a gravitational potential as "temperature" and a gravitational field as "heat flux". Can you "understand" something about gravitation using this analogy?

73.5. Present the integral equation corresponding to (73.36) in the case $d = 2$.

73.6. What equation is obtained if $\partial D/\partial t$ is not neglected in the setting of time-dependent magnetics, but the x_3 independence is kept?

73.7. Derive the heat equation describing the heat conduction in a thin piece of wire of length one whose ends are kept at a fixed temperature (i.e., derive the heat equation in one dimension):

$$\begin{cases} \dot{u} - u'' = f & \text{in } (0,1) \times (0,T], \\ u(0,t) = u(1,t) = 0 & \text{for } t \in (0,T], \\ u(x,0) = u_0(x) & \text{for } x \in (0,1). \end{cases} \tag{73.41}$$

73.8. Let $F(x)$ be the gravitational field generated by a homogeneous ball of mass m occupying the volume $\{x \in \mathbb{R}^3 : \|x\| \leq r\}$, satisfying $\nabla F(x) = \rho$ for $\|x\| < r$ and $\nabla F(x) = 0$ for $\|x\| > r$, where ρ is the density of the sphere. Argue that by symmetry $F(x) = f(\|x\|)\frac{-x}{\|x\|}$ for $\|x\| > r$ for some function $f : (0, \infty) \to \mathbb{R}$. Use the Divergence theorem to see that if $R > r$ then

$$\int_{S_R} F(x) \cdot n dS = 4\pi R^2 f(R) = \int_{B_R} \nabla F(x)\, dx = m,$$

where S_R is the boundary of the ball $B_R = \{x \in \mathbb{R}^3 : \|x\| \leq R\}$. Conclude that $f(R) = \frac{m}{4\pi R^2}$, and thus that $F(x) = \frac{m}{4\pi}\frac{-x}{\|x\|^3}$ for $\|x\| > r$. This gives an alternative way of handling of Newton's nightmare. Note the change of normalization with the factor $1/4\pi$ appearing here.

73.9. To analyze the convergence of the fixed point iteration for the system of equations (73.15), we need to show that $\|I - \alpha A\| < 1$, where $A = (a_{ij})$ is the $(N-1) \times (N-1)$ matrix with $a_{ii} = 2$, $a_{i,i-1} = a_{i-1,i} = -1$ and $a_{ij} = 0$ if

$|i-j| > 1$. Since A is symmetric, we have recalling the Chapter The Spectral Theorem:

$$\|I - \alpha A\| = \max_i |1 - \alpha\lambda_i|,$$

where λ_i, $i = 1, ..., N-1$, are the eigenvalues of A. To see this, diagonalize. Prove that for all nonzero $V \in \mathbb{R}^{N-1}$

$$AV \cdot V = \sum_{i,j=1}^{N-1} a_{ij} V_i V_j > 0,$$

and conclude that $\lambda_i > 0$ for all i (Hint: complete squares!). Show similarly that for all $V \in \mathbb{R}^{N-1}$

$$(I - \alpha A)V \cdot V \geq 0$$

if $\alpha \leq \frac{1}{4}$ (Hint: same as before!). Conclude that Fixed point iteration converges if $0 < \alpha \leq \frac{1}{4}$. Can you prove convergence if $\alpha < \frac{1}{2}$? What about convergence if $\alpha < 0$? Hint: Use that if A is a symmetric $m \times m$ matrix with eigenvalues $\lambda_1 \leq \lambda_2 \leq ... \leq \lambda_m$, then $\lambda_1 = \min_{V \in \mathbb{R}^m}(AV \cdot V)/(V \cdot V)$ and $\lambda_m = \max_{V \in \mathbb{R}^m}(AV \cdot V)/(V \cdot V)$, where $V \neq 0$.

73.10. Extend the above analysis to the 5-point scheme for the Laplacian and show that fixed point iteration converges if $0 < \alpha < \frac{1}{8}$ (or better $\alpha < \frac{1}{4}$).

73.11. Gather some friends and arrange them in a square regular grid, and ask them to keep updating their own value according to a Svensson's formula as the mean value of their neighbors (starting with zero), and assigning certain given values to the people at the boundary. Collect the values obtained after convergence. You have solved Laplace equation on a square with Dirichlet boundary values numerically. What value of α in fixed point iteration did you effectively use?

73.12. Prove Bernoulli's theorem stating that in stationary Euler flow satisfying $(u \cdot \nabla)u + \nabla p = 0$ the quantity $\frac{1}{2}\|u\|^2 + p$ is constant along streamlines.

73.13. Explain the *Magnus effect* causing a top-spin tennis ball curve downwards (see also Chapter *Analytic functions*).

73.14. Prove that the hydrogen atom is stable in the sense that the *Rayleigh quotient*

$$RQ(\psi) = \frac{\frac{1}{2}\int_\Omega |\nabla\psi|^2\,dx - \int_\Omega \psi^2/r\,dx}{\int_\Omega \psi^2\,dx},$$

satisfies

$$\min_{\psi \in V} RQ(\psi) \geq -2,$$

showing that the electron does not fall into the proton. Hint: estimate $\int_\Omega \psi \frac{\psi}{r}$ using Cauchy's inequality and the following Poincaré inequality for functions $\psi \in V$:

$$\int_\Omega \frac{\psi^2}{r^2}\,dx \leq 4\int_\Omega |\nabla\psi|^2\,dx. \qquad (73.42)$$

This shows that the potential energy cannot outpower the kinetic energy in the Rayleigh quotient. To prove the last inequality, use the representation

$$\int_\Omega \frac{\psi^2}{r^2}\,dx = -\int_\Omega 2\psi\nabla\psi\cdot\nabla\ln(|x|)\,dx.$$

resulting from Green's formula, together with Cauchy's inequality.

73.15. (a) Show that the eigenvalue problem for the hydrogen atom for eigenfunctions with radial dependence only, may be formulated as the following one-dimensional problem

$$-\frac{1}{2}\varphi_{rr}-\frac{1}{r}\varphi_r-\frac{1}{r}\varphi=\lambda\varphi,\quad r>0,\quad \varphi(0)\text{ finite},\quad \int_{\mathbb{R}}\varphi^2r^2\,dr<\infty,\qquad (73.43)$$

where $\varphi_r=\dfrac{d\varphi}{dr}$. (b) Show that $\psi(r)=\exp(-r)$ is an eigenfunction corresponding to the eigenvalue $\lambda=-\frac{1}{2}$. (b) Is this the smallest eigenvalue? (c) Determine λ_2 and the corresponding eigenfunction by using a change of variables of the form $\varphi(r)=v(r)\exp(-\frac{r}{2})$. (d) Solve (73.43) numerically.

> The idea of the continuum seems simple to us. We have somehow lost sight of the difficulties it implies ... We are told such a number as the square root of 2 worried Pythagoras and his school almost to exhaustion. Being used to such queer numbers from early childhood, we must be careful not to form a low idea of the mathematical intuition of these ancient sages; their worry was highly credible. (Schrödinger)