Lectures on Partial Differential Equations

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June 3, 2004

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Chapter 1

The translation equation

1.1 The constant coefficient translation equation

One of the simplest partial differential equations is

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0, \tag{1.1}$$

where a is constant. Its solution is

$$u(x,t) = f(x - at). \tag{1.2}$$

Thus this equation describes the *translation* of a function at *velocity* given by a. This is a very simple example of a linear equation with constant coefficients. For a physical interpretation, think of u as the density of a substance being carried along in a fluid moving at constant velocity a.

The natural way of specifying a solution of this equation is by the *initial value problem* $u(x,0) = f(x)$. Notice that while for an ordinary differential equation the solution is determined up to an unknown constant, for a partial differential equation the solution is determined up to an unknown function.

We can check directly that the equation is satisfied by computing

$$f'(x-at)\frac{\partial(x-at)}{\partial t} + af'(x-at)\frac{\partial(x-at)}{\partial x} = -af'(x-at) + af'(x-at) = 0. \tag{1.3}$$

1.2 The variable coefficient translation equation

More interesting variants arise when we consider linear equations with variable coefficients. In the following examples we will have a velocity $a(x)$ that is a given function of position x.

For instance, there is the *forward translation equation*

$$\frac{\partial u}{\partial t} + \frac{\partial a(x)u}{\partial x} = 0. \tag{1.4}$$

An equation of this form with the derivative on the outside is also called a *conservation law*. For a physical interpretation, think of the u as the density of a substance being carried along in a fluid moving at a velocity v that varies as a function of position.

Another example is the *backward translation equation*

$$\frac{\partial u}{\partial t} - a(x)\frac{\partial u}{\partial x} = 0. \tag{1.5}$$

To solve the forward equation, consider the ordinary differential equation

$$\frac{dx}{dt} = a(x) \tag{1.6}$$

describing motion with the given velocity. Take the initial condition $x = x_0$ when $t = 0$. The ordinary differential equation has solution $x(t)$ with $x(0) = x_0$.

Now look at a solution $u(x, t)$ of the forward equation. Evaluate this on the solution curve, the *characteristic curve*. This gives a function $u = u(x(t), t)$ of time t. Its derivative is

$$\frac{du}{dt} = \frac{\partial u}{\partial t}\frac{dt}{dt} + \frac{\partial u}{\partial x}\frac{dx(t)}{dt}. \tag{1.7}$$

This follows from the chain rule for partial derivatives. However from the forward equation this is

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + a(x(t))\frac{\partial u}{\partial x} = -a'(x(t))u. \tag{1.8}$$

This is an ordinary differential equation for u as a function of t that can be solved explicitly. The solution is

$$u(t) = u(0)\exp(-\int_0^t a'(x(s))\,ds). \tag{1.9}$$

For each x and t we can try to find the x_0 such that the curve starting at x_0 at time 0 reaches x at time t. We know how u changes along such a curve. From this, we get the solution of the equation

$$u(x, t) = f(x_0)\exp(-\int_0^t a'(x(s))\,ds). \tag{1.10}$$

Example: Consider the forward equation

$$\frac{\partial u}{\partial t} + \frac{\partial xu}{\partial x} = 0. \tag{1.11}$$

The characteristic curve solving $dx/dt = x$ starting at x_0 is $x = x_0e^t$. Thus the solution of the equation is

$$u(x, t) = f(xe^{-t})e^{-t}. \tag{1.12}$$

Notice that the integral of $u(x,t)$ over all x is independent of time. The fact that the integral of $u(x,t)$ over all x is independent of time is a general fact about such conservation laws, and the factor in the solution is just what is needed to make this happen.

The backward equation may be solved in a similar way by integrating along the curves $dx/dt = -a(x)$. However in this case the calculation shows that the solutions are constant along these curves.

Example: Consider the backward equation

$$\frac{\partial u}{\partial t} - x\frac{\partial u}{\partial x} = 0. \tag{1.13}$$

The characteristic curve solving $dx/dt = -x$ starting at x_0 is $x = x_0 e^{-t}$. Thus the solution of the equation is

$$u(x,t) = f(xe^t). \tag{1.14}$$

1.3 The nonlinear translation equation

Consider the nonlinear conservation law

$$\frac{\partial u}{\partial t} + \frac{\partial g(u)}{\partial x} = 0. \tag{1.15}$$

This may also be written as

$$\frac{\partial u}{\partial t} + a(u)\frac{\partial u}{\partial x} = 0, \tag{1.16}$$

where $a(u) = g'(u)$. As a physical interpretation, think of a substance with density u being carried along at a velocity $g(u)/u$ that depends on the density of the substance. Then the amount of the flow of the substance is $g(u)$.

The solution of this nonlinear equation is more subtle. Consider the characteristic curve satisfying

$$\frac{dx}{dt} = a(u) \tag{1.17}$$

with $x = x_0$ when $t = 0$. The curve depends on the unknown solution. However, along any such curve

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{dx}{dt} = 0. \tag{1.18}$$

So for the nonlinear equation the solutions are constant along these characteristic curves.

The solution with initial function f can be obtained as follows. Since u at x, t is $f(x_0)$, and $x = x_0 + a(u)t$, we have the following formula for $u = u(x,t)$:

$$u = f(x - a(u)t). \tag{1.19}$$

We can try to solve this for u. We know that when $t = 0$ the solution is $u = f(x)$. So we might hope that when $t > 0$ we can solve this. When could this fail? To see when, compute

$$\frac{\partial u}{\partial t} = \frac{-f'(x - a(u))a(u)}{1 + f'(x - a(u)t)a'(u)t}. \tag{1.20}$$

From this we see that when $f'(x_0)a'(f(x_0)) > 0$, then $1 + f'(x_0)a'(f(x_0)) \neq 0$ and there should be no problem. However, when this is negative, there can be big trouble.

The problem is that two characteristic curves with different x_0 can meet at a common x and t. Thus $x = x_0 + a(f(x_0))t$ has more than one solution x_0. There is an ambiguity in the definition of the solution. This is known as the formation of a *shock*. Again, the symptom of a problem is when $\partial x_0/\partial x$ is singular, that is, when $\partial x/\partial x_0 = 1 + a'(f(x_0))f'(x_0)t = 0$.

Example: One very special example is when $a(u) = u$. This has the following interpretation. Let u be the velocity of a gas of particles moving freely with no viscosity. Then the rate of change du/dt along the curve $dx/dt = u$ describing the motion of a particle is zero. This says that

$$\frac{\partial u}{\partial t} + u\frac{\partial u}{\partial x} = 0. \tag{1.21}$$

In this case $a'(u) = 1$. As one might expect, faster particles move faster. Thus if the initial condition $f(x)$ satisfies $f'(x) < 0$, then there will be faster particles to the left and slower particles to the right. The fast particles will eventually catch up with the slow particles. An easy example to compute is $f(x) = -x$. The characteristic curves are $x = x_0(1 - t)$. The particles to the left of the origin are moving fast at velocity $-x_0$, and the particles at the origin are stationary. At $t = 1$ they are all at the same place. The equation for the solution is $u = tu - x$ which has solution

$$u = -\frac{x}{1 - t}. \tag{1.22}$$

At time $t = 1$ there is a bad singularity.

Example: Here is a model for traffic flow. There is a density u of cars on a highway. The velocity of the cars is $c(1 - u)$ for u between 0 and maximum density 1. Here $c > 0$ is the velocity at very low density. The flow of cars is thus $c(1 - u)u$, since it is also proportional to the number of cars. The conservation law is

$$\frac{\partial u}{\partial t} + \frac{\partial c(u - u^2)}{\partial x} = 0. \tag{1.23}$$

This can also be written as

$$\frac{\partial u}{\partial t} + c(1 - 2u)\frac{\partial u}{\partial x} = 0. \tag{1.24}$$

In this example $a(u) = c(1 - 2u)$. Notice that the characteristics can go backwards, even though the cars are going forward.

In the present example $a'(u) = -2c$. Since this is negative, we expect trouble when the initial condition $f'(x) > 0$. This says that there are more cars ahead than behind. In this case there will be a shock.

1.4 Problems

1. An equation that is a sort of average of the backward and forward equations is
$$\frac{\partial u}{\partial t} + \frac{1}{2}\left(\frac{\partial a(x)u}{\partial x} + a(x)\frac{\partial u}{\partial x}\right) = 0. \tag{1.25}$$
Solve the initial value problem for this equation in the case when $a(x) = x$. Thus, solve
$$\frac{\partial u}{\partial t} + x\frac{\partial u}{\partial x} + \frac{1}{2}u = 0 \tag{1.26}$$
with $u(x, 0) = f(x)$. Show that the space integral of the square of the solution is constant in time.

2. Consider the equation
$$\frac{\partial u}{\partial t} + u^2\frac{\partial u}{\partial x} = 0 \tag{1.27}$$
with initial condition $u = x$ when $t = 0$. Find the solution. Be careful about the sign in front of the square root. Use the initial condition to reject solutions that blow up at zero. Also, find where this solution becomes singular at later times.

3. Consider the traffic flow equation with initial condition $f(x) = x/L$ for $0 \le x \le L$ and 0 to the left and 1 to the right. Solve the equation, and describe shock formation. Recall that a shock occurs at a place where two or more characteristics meet.

Chapter 2

The wave equation

2.1 The first order system

Let $c > 0$ be a constant. The wave system consists of the two equations

$$\frac{\partial u}{\partial t} + \frac{\partial v}{\partial x} = 0 \tag{2.1}$$

and

$$\frac{\partial v}{\partial t} + c^2 \frac{\partial u}{\partial x} = 0. \tag{2.2}$$

These are the equations of *wave propagation*.

One physical interpretation is as an equation for sound waves in one dimension. Let ρ be the density and v be the velocity of the fluid. The equation of conservation of mass says that

$$\frac{\partial \rho}{\partial t} + \frac{\partial \rho v}{\partial x} = 0. \tag{2.3}$$

The equation of motion says that mass times acceleration is equal to force. This says that

$$\rho \left(\frac{\partial v}{\partial t} + v \frac{\partial v}{\partial x} \right) = -c(\rho)^2 \frac{\partial \rho}{\partial x}. \tag{2.4}$$

Here the pressure gradient that produces the force is assumed to be proportional to the density gradient. If ρ is close to an average value ρ_0 and if v is small, then these non-linear equation may be approximated by the linear equations

$$\frac{\partial \rho}{\partial t} + \rho_0 \frac{\partial v}{\partial x} = 0 \tag{2.5}$$

and

$$\rho_0 \frac{\partial v}{\partial t} = -c(\rho_0)^2 \frac{\partial \rho}{\partial x}. \tag{2.6}$$

Then if $u = \rho/\rho_0$ we get the wave system as written above.

Another physical interpretation of the wave equation is as an equation for a plane electromagnetic field. Consider a wave that travels in the x direction. It is polarized so that the electric field E is in the y direction and the magnetic field B is in the z direction. Then the equation is

$$\frac{\partial B}{\partial t} + \frac{\partial E}{\partial x} = 0 \tag{2.7}$$

and

$$\frac{\partial E}{\partial t} + c^2 \frac{\partial B}{\partial x} = 0. \tag{2.8}$$

In any case, the wave system is one of the most important of all partial differential equations. There are now two families of characteristic curves, given by

$$\frac{dx}{dt} = \pm c. \tag{2.9}$$

This says that in this approximation the influence travels at the *sound speed* (in the gas interpretation) or at the *speed of light* (in the electromagnetic interpretation).

We notice that along these curves $x = x_0 \pm ct$ we have

$$\frac{d(cu \pm v)}{dt} = 0. \tag{2.10}$$

Thus

$$cu(x,t) \pm v(x,t) = cu_0(x_0) \pm v_0(x_0) = cu_0(x \mp ct) + v_0(x \mp ct). \tag{2.11}$$

Thus

$$u(x,t) = \frac{1}{2}[u_0(x-ct) + u_0(x+ct)] + \frac{1}{2c}[v_0(x-ct) - v_0(x+ct)] \tag{2.12}$$

and

$$v(x,t) = \frac{c}{2}[u_0(x-ct) - u_0(x+ct)] + \frac{1}{2}[v_0(x-ct) + v_0(x+ct)]. \tag{2.13}$$

There is another approach that gives the same result. We can solve these equations by trying a general solution of the form

$$u = \frac{1}{2}[f(x-ct) + g(x+ct)]. \tag{2.14}$$

This represents a wave travelling toward the right plus a wave travelling toward the left. In order to match with the equation for v we need

$$v = \frac{1}{2}c[f(x-ct) - g(x+ct)]. \tag{2.15}$$

Notice that the velocity of the wave travelling toward the left enters with a minus sign. Say that we want to solve the wave equation with given initial values u_0 and v_0 at $t = 0$. Then we simply solve the equations $u_0 = (1/2)[f(x)+g(x)]$ and $v_0 = (1/2)c[(f(x) - g(x)]$ for $f(x)$ and $g(x)$. Then we have the solution given above. This represents waves that travel at velocities $\pm c$ in both directions.

Notice that both u and v satisfy the wave equation described in the next section.

2.2 The second order equation

The *wave equation* is a second order equation that describes motion in two directions. Let $c > 0$ be the speed of propagation. The wave equation is

$$(\frac{\partial}{\partial t} + c\frac{\partial}{\partial x})(\frac{\partial}{\partial t} - c\frac{\partial}{\partial x})u = 0. \tag{2.16}$$

Thus we expect waves moving at velocities $\pm c$. This equation may be written also as

$$\frac{\partial^2 u}{\partial t^2} - c^2\frac{\partial^2 u}{\partial x^2} = 0. \tag{2.17}$$

This equation is also sometimes thought of as the equation for the motion of a stretched string. The second derivative with respect to time is the acceleration. The force is proportional to the second derivative with respect to space.

When the wave equation describes motion in an infinite interval there is a fairly simple solution, the *d'Alembert solution*. The general solution is

$$u(x,t) = f(x-ct) + g(x+ct). \tag{2.18}$$

Say that we want the solution that satisfies the initial conditions $u = \phi(x)$ and $\partial u/\partial t = \psi(x)$ when $t = 0$. We obtain

$$f(x) + g(x) = \phi(x) \tag{2.19}$$

and

$$-cf'(x) + cg'(x) = \psi(x). \tag{2.20}$$

Integration of the second equation gives

$$f(x) - g(x) = -\frac{1}{c}\int_\alpha^x \psi(y)\,dy. \tag{2.21}$$

Theorem 2.1 *The d'Alembert solution of the initial value problem for the wave equation on an infinite space interval is*

$$u(x,t) = \frac{1}{2}[\phi(x-ct) + \phi(x+ct)] + \frac{1}{2c}\int_{x-ct}^{x+ct} \psi(y)\,dy. \tag{2.22}$$

If we let $M_{x,ct}(f)$ be the average over the interval of length $2ct$ centered at x, then this solution may also be written

$$u(x,t) = \frac{\partial}{\partial t}(tM_{x,ct}(\phi)) + tM_{x,ct}(\psi). \tag{2.23}$$

We now look at the case of a finite length space interval $a \le x \le b$. In the case it turns out that it is desirable to solve the problem with initial conditions at $t = 0$ and with boundary conditions at $x = a$ and $x = b$. The initial conditions are $u(x,0) = \phi(x)$ and $\partial u/\partial t(x,0) = \psi(x)$ as before. The boundary conditions are $u(a,t) = \alpha(t)$ and $u(b,t) = \beta(t)$. The solution in this case is fairly complicated. The following lemma is helpful.

Lemma 2.1 *For each $h, k > 0$ the solution of the wave equation satisfies the parallelogram identity*

$$u(x,t) = u(x-ch, t-h) + u(x+ck, t-k) - u(x-ch+ck, t-h-k). \quad (2.24)$$

This lemma can be checked easily for the solutions $f(x-ct)$ and for the solutions $g(x+ct)$ separately.

Theorem 2.2 *The solution of the initial-boundary problem for the wave equation is determined by the d'Alembert equation together with the parallelogram identity.*

Proof: Consider the triangular region where the d'Alembert solution determines the solution. The solution is determined outside of this region by the parallelogram identity. The parallelogram either has two point in the interior and one on the boundary, or it has all three points in the interior.

2.3 Three dimensions

The d'Alembert solution is all the more important because there is a closely related result for the three dimensional wave equation

$$\frac{\partial^2 u}{\partial t^2} = \nabla_{\mathbf{x}}^2 u. \quad (2.25)$$

Here $\mathbf{x} = (x, y, z)$ and

$$\nabla_{\mathbf{x}}^2 = \nabla_{\mathbf{x}} \cdot \nabla_{\mathbf{x}} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2} \quad (2.26)$$

is the Laplace operator.

One physical interpretation of the three-dimensional wave equation is in terms of sound propagation. Let u be the relative density. Let $\mathbf{v}$ the velocity. The equations of wave propagation in the linear approximation are

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{v} = 0 \quad (2.27)$$

and

$$\frac{\partial \mathbf{v}}{\partial t} + c^2 \nabla u = 0. \quad (2.28)$$

These equations represent conservation of mass and momentum. They lead immediately to the wave equation.

This operator may be written in spherical polar coordinates in the form

$$\nabla_{\mathbf{x}}^2 = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} + \frac{1}{r^2} L, \quad (2.29)$$

where L involves only angular differentiations. Explicitly,

$$L = \frac{1}{\sin\theta}\frac{\partial}{\partial\theta}\sin\theta\frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta}\frac{\partial^2}{\partial\phi}, \tag{2.30}$$

where θ is the co-latitude and ϕ the longitude.

It is worth remarking that if we make the change of variable $w = ru$, then the equation in spherical polar coordinates becomes

$$r\nabla^2_{\mathbf{x}}\frac{w}{r} = \left(\frac{\partial^2}{\partial r^2} + \frac{1}{r^2}L\right)w. \tag{2.31}$$

In other words, the radial part looks like the corresponding one-dimensional operator. This suggests that the solution in three dimensions should bear a kinship to the solution in one dimension. In fact, given a solution $w(r)$ of the one-dimensional wave equation, the solution $u(r) = w(r)/r$ is a spherically symmetric solution of the three-dimensional wave equation.

The way to get the general relation between three dimensions and one dimensions is to average over spheres. Consider a function $f(\mathbf{x}+\mathbf{x}')$. Then it is clear that

$$\nabla^2_{\mathbf{x}} f(\mathbf{x}+\mathbf{x}') = \nabla^2_{\mathbf{x}'} f(\mathbf{x}+\mathbf{x}'). \tag{2.32}$$

Now take an average of this equation as $\mathbf{x}'$ varies over a sphere centered at 0. Thus let $M_{\mathbf{x},r}(f)$ be the average of f over the spherical surface centered at $\mathbf{x}$ with radius r. Temporarily take spherical polar coordinates centered at $\mathbf{x}$. Average over the angles with respect to the angular measure $\sin\theta\, d\theta\, d\phi/(4\pi)$. An integration by parts shows that the contribution from the angular part of the Laplacian is zero. Thus we have the following remarkable identity.

$$\nabla^2_{\mathbf{x}} M_{\mathbf{x},r}(f) = \frac{1}{r^2}\frac{\partial}{\partial r}r^2\frac{\partial}{\partial r}M_{\mathbf{x},r}(f). \tag{2.33}$$

If we replace $M_{\mathbf{x},r}$ by $rM_{\mathbf{x},r}$, then we get

$$\nabla^2_{\mathbf{x}} rM_{\mathbf{x},ct}(f) = \frac{\partial^2}{\partial r^2}rM_{\mathbf{x},r}(f). \tag{2.34}$$

Thus $ctM_{\mathbf{x},ct}(f)$ satisfies the three-dimensional wave equation. This kind of solution may be used to obtain the following *Kirchoff* solution of the initial value problem.

Theorem 2.3 *The solution of the initial value problem for the three-dimensional wave equation in infinite space is*

$$u(\mathbf{x},t) = \frac{\partial}{\partial t}(tM_{\mathbf{x},ct}(\phi)) + tM_{\mathbf{x},ct}(\psi), \tag{2.35}$$

where in the three-dimensional case $M_{\mathbf{x},ct}(f)$ is the average of f over the spherical surface centered at $\mathbf{x}$ with radius ct.

Note that if instead of taking the average over the sphere, we take the integral $I_{\mathbf{x},ct}$ over the sphere, then the solution is

$$u(\mathbf{x},t) = \frac{\partial}{\partial t}(\frac{1}{4\pi c^2 t}I_{\mathbf{x},ct}(\phi)) + \frac{1}{4\pi c^2 t}I_{\mathbf{x},ct}(\psi). \tag{2.36}$$

2.4 Conservation of mass and momentum

In this section we look at the physics of conservation laws. The most important ones, of course, are conservation of mass, of momentum, and of energy.

A *conservation law* is an equation of the form

$$\frac{\partial u}{\partial t} + \frac{\partial J}{\partial x} = 0. \tag{2.37}$$

When the *current* J is specified, this gives an equation for u.

The interpretation of this equation is most easily seen in its integrated form. This is

$$\frac{d}{dt}\int_a^b u\,dx + J|_{x=b} - J|_{x=a} = 0. \tag{2.38}$$

This says that the change in the quantity is given by the amount of current flowing in at the left minus the amount of current flowing out at the right.

The simplest example is the equation of *conservation of mass*. In this case the dependent variable ρ is the *density*. The current is $J = v\rho$, where v is the *velocity*. This says that the transport of mass across a fixed point depends on how much is there and how fast it is moving. Thus the equation is

$$\frac{\partial \rho}{\partial t} + \frac{\partial v\rho}{\partial x} = 0. \tag{2.39}$$

The velocity might be a given function of time t and displacement x. The task is then to solve for the density as a function of x and t. Or the velocity may result from solving another equation. Then we would have to solve a system.

A much more complicated example is the equation of *conservation of momentum*. Here the quantity of interest is the momentum density $v\rho$. The convective current is then $v\rho v$, which says that momentum $v\rho$ is being swept along at velocity v. There is also a term due to the force arising from change in pressure p. (We assume for simplicity that there are no viscous forces.) The equation is

$$\frac{\partial \rho v}{\partial t} + \frac{\partial v\rho v}{\partial x} + \frac{\partial p}{\partial x} = 0. \tag{2.40}$$

We can use the equation of conservation of mass to write this in a somewhat different form:

$$\rho[\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x}] = -\frac{\partial p}{\partial x} = -c^2\frac{\partial \rho}{\partial x}. \tag{2.41}$$

Here we have defined

$$c^2 = \frac{\partial p}{\partial \rho}. \tag{2.42}$$

It will turn out that c is the *speed of sound*.

In general the pressure is a function of the density and the temperature. However suppose for the moment that it can be taken to be a function of the density alone. Then the mass and momentum equations together give a rather complicated system, the equations of *gas dynamics*. However they take a simple

form in the *linear approximation*. This is when we assume that v is small and ρ is close to a constant ρ_0. Then we can write the equation of conservation of mass in the approximate form

$$\frac{\partial \rho}{\partial t} + \rho_0 \frac{\partial v}{\partial x} = 0 \tag{2.43}$$

and the equation of conservation of momentum in the approximate form

$$\rho_0 \frac{\partial v}{\partial t} + c^2 \frac{\partial \rho}{\partial x} = 0. \tag{2.44}$$

Make the change of variables $u = \rho/\rho_0$. Then the two equations have the simple form

$$\frac{\partial u}{\partial t} + \frac{\partial v}{\partial x} = 0 \tag{2.45}$$

and

$$\frac{\partial v}{\partial t} + c^2 \frac{\partial u}{\partial x} = 0. \tag{2.46}$$

These are the equations of *linear wave propagation*. We have seen that these may be solved by the method of characteristics.

It is possible to do a similar analysis with the non-linear system consisting of

$$\frac{\partial \rho}{\partial t} + \frac{\partial v\rho}{\partial x} = 0 \tag{2.47}$$

and

$$\rho[\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x}] + c^2 \frac{\partial \rho}{\partial x} = 0. \tag{2.48}$$

Here c is a function of ρ.

We can write these equations in an equivalent form as

$$\frac{\partial \rho}{\partial t} + v\frac{\partial \rho}{\partial x} + \rho \frac{\partial v}{\partial x} = 0. \tag{2.49}$$

and

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} + \frac{c^2}{\rho}\frac{\partial \rho}{\partial x} = 0. \tag{2.50}$$

The characteristic curves are $dx/dt = v \pm c$. For the non-linear equation the characteristic velocity is the sum of the fluid velocity plus or minus the sound speed. We can evaluate the change of ρ and v along these curves. We get

$$\frac{d\rho}{dt} = \pm c\frac{\partial \rho}{\partial x} - \rho\frac{\partial v}{\partial x}, \tag{2.51}$$

and

$$\frac{dv}{dt} = -\frac{c^2}{\rho}\frac{\partial \rho}{\partial x} \pm c\frac{\partial v}{\partial x}. \tag{2.52}$$

In order to make these match up, we multiply the first equation by c/ρ. If we let ℓ be a function with $\rho d\ell/d\rho = c$, then we get

$$\frac{d\ell}{dt} = \pm\frac{c^2}{\rho}\frac{\partial \rho}{\partial x} - c\frac{\partial v}{\partial x}. \tag{2.53}$$

From this we see that

$$\frac{d(\ell \pm v)}{dt} = 0. \tag{2.54}$$

Thus we have quantities that are constant along the two characteristic curves. Since the curves themselves depend on the solutions, this does not immediately solve the problem. However it gives at least a starting point for an analysis of these equations.

2.5 Problems

1. Let u_0 and v_0 be functions that vanish outside of a bounded interval of space. Consider the solution of the wave system for the density u and velocity v with these initial conditions. Find the behavior of the solution $u(x,t)$ for fixed x and t large.

2. Let ϕ and ψ be positive functions that each vanish outside of a bounded interval. Consider the wave equation with the initial conditions $u = \phi$ and $\partial u/\partial t = \psi$ at $t = 0$. Find the behavior of the solution $u(x,t)$ for fixed x and t large.

3. Show that if u is a solution of the wave equation, then u satisfies the identity

   $$u(x+ch,t+k)+u(x-ch,t-k) = u(x+ck,t+h)+u(x-ck,t-h). \tag{2.55}$$

   Hint: The general solution is the sum of $f(x-ct)$ and $g(x+ct)$.

4. Show that if u satisfies the identity in the last problem, then u must be a solution of the wave equation. Hint: Let $k = 0$.

5. Show that the Kirchoff solution of the three-dimensional wave equation satisfies the appropriate initial conditions.

6. Let ϕ and ψ be positive functions that each vanish outside of a bounded region. Consider the three-dimensional wave equation with the initial conditions $u = \phi$ and $\partial u/\partial t = \psi$ at $t = 0$. Find the behavior of the solution $u(\mathbf{x},t)$ for fixed $\mathbf{x}$ and t large.

7. Show that the two forms (2.40) and (2.41) of the law of conservation of momentum are equivalent.

8. We expect that for fixed temperature, an increase in density is accompanied by an increase in pressure. What would go wrong mathematically with the linear wave system for sound propagation if $\partial p/\partial \rho$ were negative?

Chapter 3

The diffusion equation

3.1 Random characteristics

The next equation to be considered is called the *diffusion equation* or the *heat equation*. In the diffusion form it arises as a conservation law as follows. We assume that there is some conserved substance that is a kind of impurity. Random thermal motion makes it diffuse. The diffusion current is given by *Fick's law*:

$$J = -\frac{\sigma^2}{2}\frac{\partial \rho}{\partial x}. \tag{3.1}$$

The conservation law

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0 \tag{3.2}$$

gives rise to the diffusion equation

$$\frac{\partial \rho}{\partial t} = \frac{\sigma^2}{2}\frac{\partial^2 \rho}{\partial x^2}. \tag{3.3}$$

One can think of the solution as describing the probability that a single particle has diffused to the vicinity of a given point after a certain time. Or one can think many impurity particles, in which case one can think of the solution as describing the density of the particles as a function of time.

This equation can be also be solved by characteristics, but they are random. Let $\Delta t > 0$ and $\Delta x > 0$ and let $t = 2n\Delta t$. (We take the number of steps to be even only for convenience.) Then the random characteristic is defined by

$$x = \sum_{i=1}^{2n} \pm \Delta x \tag{3.4}$$

where

$$\Delta x = \sigma\sqrt{\Delta t}. \tag{3.5}$$

The plus and minus signs are determined by $2n$ coin tosses. Thus this is an inefficient way of moving. However when Δt and Δx are small, the Δx is much

larger than the Δt. So this is a very irregular motion, but it is effective in moving the particle. This model with discrete steps is called the *random walk* model of diffusion.

It is possible to give a detailed analysis of the probability that the diffusing particle arrives at a given point. The only mathematical fact that we need is an identity for binomial coefficients. Recall that $\binom{n}{r}$ is the number of subsets of an n element set that have exactly r elements. The identity is

$$\binom{n}{r} r = \binom{n}{r-1}(n-r+1). \tag{3.6}$$

The reason this is true is because for each way of choosing an r element subset and then an element of the subset there is a corresponding way of choosing an $r-1$ element subset and then an element in its complement.

The probability that the particle gets to $x = 2k\Delta x$ in time $t = 2n\Delta t$ is the probability that the number of plus signs minus the number of minus signs is $2k$. Thus it is necessary to get $(n+k)$ plus signs and $n-k$ minus signs.

Each pattern of $2n$ plus signs and minus signs has probability $1/2^{2n}$. The number of patterns that give $n+k$ plus signs is given by the number of ways of choosing $n+k$ time intervals out of the total $2n$. This is of course a binomial coefficient. So the probability of being at x at time t is

$$\rho(x,t)\, 2\Delta x = \binom{2n}{n+k}\frac{1}{2^{2n}}. \tag{3.7}$$

Now we can use the identity

$$\binom{2n}{n+k} = \binom{2n}{n+k-1}\frac{n-k+1}{n+k} = \binom{2n}{n+k-1}\frac{1-\frac{k-1}{n}}{1+\frac{k}{n}}. \tag{3.8}$$

If we use the approximation $\exp(z) \approx 1+z$ valid for small z, this gives

$$\binom{2n}{n+k} \approx \binom{2n}{n+k-1}\exp(-\frac{2k-1}{n}). \tag{3.9}$$

If we use this repeatedly, we get

$$\binom{2n}{n+k} \approx \binom{2n}{n}\exp(-\frac{1+3+5+\cdots+2k-1}{n}). \tag{3.10}$$

One of the pleasures of mathematics is evaluating such a sum. The result is

$$\binom{2n}{n+k} \approx \binom{2n}{n}\exp(-\frac{k^2}{n}). \tag{3.11}$$

Let

$$c(n) = \binom{2n}{n}\frac{1}{2^{2n}}. \tag{3.12}$$

Then

$$\rho(x,t)\,2\Delta x \approx c(n)\exp(-\frac{k^2}{n}). \tag{3.13}$$

If we convert back into x and t, we get that the probability of being at x at time t is given by the *Gaussian* law of probability

$$\rho(x,t)\,2\Delta x \approx c(\frac{\sigma^2 t}{2(\Delta x)^2})\exp(-\frac{x^2}{2\sigma^2 t}). \tag{3.14}$$

Theorem 3.1 *In the limit of $\Delta t \to 0$, the probability that the random walk with step $\pm\Delta x = \pm\sigma\sqrt{\Delta t}$ in time interval Δt is in an interval $a < x \leq b$ at time t is*

$$\int_a^b \rho(x,t)\,dx = \frac{1}{\sqrt{2\pi\sigma^2 t}}\int_a^b \exp(-\frac{x^2}{2\sigma^2 t})\,dx. \tag{3.15}$$

This limit of the random walk model as Δt and Δx approach zero with $\Delta x = \sigma\sqrt{\Delta t}$ is called the *Wiener process* model of diffusion. As noted in the theorem, this gives the exact Gaussian solution of the diffusion equation. This limit is also sometimes called the limit of *Brownian motion*, but this terminology runs the risk of confusing the mathematical description with the physical effect.

The factor $1/\sqrt{2\pi\sigma^2 t}$ in front is precisely the factor that is needed to make the total probability equal to one. By using this and working backward, it is not difficult to see that $c(n) \approx 1/\sqrt{\pi n}$.

3.2 Einstein

The ultimate mechanism for diffusion is random molecular motion, and the amount of such motion depends on temperature. The possible states of a system in equilibrium may be considered as random. The probability distribution depends on the temperature. The fundamental principle of thermal equilibrium says that this probability is given by the *Boltzmann factor*. This is

$$\text{prob} \sim \exp(-\frac{\text{energy}}{kT}). \tag{3.16}$$

Here T is the *absolute temperature* and k is the Boltzmann constant. The product kT represents the energy equivalent of the temperature T.

Albert Einstein found a remarkable formula for the diffusion coefficient. The formula says that

$$\frac{1}{2}\sigma^2 = \frac{kT}{\gamma}. \tag{3.17}$$

The parameter $\gamma > 0$ is the *friction coefficient*. This formula says that diffusion is encouraged by high temperature and small friction.

This formula is amazing because formulas in physics usually involve the notion of acceleration. However the paths of the diffusing particles do not even have well-defined velocities. This is because $\Delta x = \pm\sigma\sqrt{\Delta t}$ implies $\Delta x/\Delta t = \pm\sigma/\sqrt{\Delta t}$. In the limit of $\Delta t = 0$ this is $\pm\infty$.

One way to deal with this problem would be to try a more complicated and realistic model of motion in which the particles do have velocities. But Einstein was much more clever than this. His idea was to imagine that in addition to diffusion there is a constant *force* f acting on the particles. For example, one could think of the force f as being the force of gravity. (If we measure x upward, then f is negative.) It is known that the density of particles in such a force field is an exponential function of the height. This is because the energy is $-fx$. So the expression for the probability density as a function of height is given by the Boltzmann factor

$$\rho(x) = C \exp(\frac{fx}{kT}). \tag{3.18}$$

This says that the chance of finding a particle at a particular height is less as one moves higher. This chance depends on the ratio of the potential energy $-fx$ of a particle to its thermal energy kT.

The next task was to correlate this with the diffusive motion. Consider a particle with velocity v moving in a fluid with friction force $-\gamma v$ and with external force f. The equation of motion is

$$m\frac{dv}{dt} = -\gamma v + f + \text{ noise } . \tag{3.19}$$

If the average acceleration is zero, then the particle has reached an average *terminal velocity* a given by $\gamma a = f$. This suggests that the proper equation should be

$$\frac{\partial \rho}{\partial t} + \frac{\partial a\rho}{\partial x} = \frac{\sigma^2}{2}\frac{\partial^2 \rho}{\partial x^2}. \tag{3.20}$$

This equation describes the combined effect of translational motion at the terminal velocity and diffusion.

Einstein noted that if $a\rho = (\sigma^2/2)\partial\rho/\partial x$, then ρ is an equilibrium solution of the equation. This says that

$$\rho(x) = C \exp(\frac{2ax}{\sigma^2}). \tag{3.21}$$

If we match the two exponential factors, we get $\sigma^2/(2a) = kT/f$. This in turn gives $\gamma\sigma^2/(2f) = kT/f$. Since $f \neq 0$, we can cancel the $1/f$ factors and get the Einstein relation $\gamma\sigma^2/2 = kT$. The value of f is not important, all that matters is that it is not zero.

Ornstein and Uhlenbeck gave another derivation of the Einstein formula for the diffusion coefficient. The idea is that the particles do have a velocity, but it is random. In equilibrium the velocity distribution for a component of velocity is given by the Boltzmann factor

$$\rho(v) = \frac{1}{\sqrt{2\pi kT/m}} \exp(-\frac{mv^2}{2kT}). \tag{3.22}$$

Then the expected energy of this component is

$$\frac{1}{2}m(\Delta v)^2 = \int_{-\infty}^{\infty} \frac{1}{2}mv^2 \rho(v)\, dv = \frac{1}{2}kT. \tag{3.23}$$

Here kT is the energy corresponding to absolute temperature T. So for a particle of small mass these velocities satisfy $(\Delta v)^2 = kT/m$. On the average they are very large, but finite.

The second idea is that the velocity maintains itself only for a short time, the *relaxation time* Δt. This comes from the supposition that the velocity satisfies the equation

$$m\frac{dv}{dt} = -\gamma v + \text{ noise } . \tag{3.24}$$

From this we see that the relaxation rate is γ/m and so the relaxation time is

$$\Delta t = 2m/\gamma. \tag{3.25}$$

The factor of two turns out to give a more accurate description of the time scale on which motion persists. In any case, for a particle of small mass m this is a very small number.

Ornstein and Uhlenbeck gave a sophisticated treatment of how the velocity varies with time, and this is considered later in this chapter. However a crude derivation of the diffusion coefficient results by using these values of Δv and Δt in the random walk model of diffusion. Then the distance $\pm\Delta x$ traveled in each interval of length Δt is given by $\pm\Delta x = \pm\Delta v\,\Delta t$. This is explicitly $(\Delta x)^2 = (kT/m)(2m/\gamma)^2 = 4mkT/\gamma^2$. That is,

$$(\Delta x)^2 = (2kT/\gamma)\Delta t. \tag{3.26}$$

Again the diffusion coefficient is given by the Einstein relation. Since the Ornstein-Uhlenbeck process explicitly involves the mass and the random velocity, it gives a more detailed physical picture of diffusion than the description given by Einstein. The clever thing about Einstein's derivation is that it work in the limit of zero mass and infinite random velocity.

3.3 Energy

Now we turn to another interpretation for the same equation. This time the solution will represent temperature. The relevant conservation law is the law of *conservation of energy*. The energy density of a fluid is a sum of a kinetic energy part and an internal energy part. It is $\rho e = (1/2)\rho v^2 + \rho u$. Here e is the energy per mass. The u is the internal energy per mass, a function of the density and temperature. The current J has three parts. The first is just $\rho e v$, which describes how the energy density is transported at velocity v. The second is pv, which describes the work on the system. Finally the third is the heat flow J_q. This is given by

$$J_q = -\lambda\frac{\partial T}{\partial x}, \tag{3.27}$$

a quantity proportional to the temperature gradient. The fact that a temperature gradient produces heat flow in this way is called *Fourier's law*. Again we

neglect effects of viscosity. The conservation law takes the form

$$\frac{\partial \rho e}{\partial t} + \frac{\partial v \rho e}{\partial x} + \frac{\partial J_q}{\partial x} + \frac{\partial p v}{\partial x} = 0. \tag{3.28}$$

By using the laws of conservation of mass and momentum, this can be written in the alternate form

$$\rho[\frac{\partial u}{\partial t} + v\frac{\partial u}{\partial x}] + \frac{\partial J_q}{\partial x} + p\frac{\partial v}{\partial x} = 0. \tag{3.29}$$

This is a complicated equation. However in the case when $v = 0$ it takes the simple form

$$\rho\frac{\partial u}{\partial t} + \frac{\partial J_q}{\partial x} = 0. \tag{3.30}$$

Furthermore, we may write

$$\frac{\partial u}{\partial t} = \frac{\partial u}{\partial \rho}\frac{\partial \rho}{\partial t} + \frac{\partial u}{\partial T}\frac{\partial T}{\partial t}. \tag{3.31}$$

If the velocity is zero, then the first term on the right is zero. Let $c = \partial u/\partial T$. Then the equation for zero velocity becomes the *heat equation*

$$\rho c\frac{\partial T}{\partial t} + \frac{\partial J_q}{\partial x} = 0, \tag{3.32}$$

where J_q is given by Fourier's law. It says that in a motionless fluid the change in internal energy is given entirely by the heat flow.

3.4 Approximate delta functions

In the following we shall need the concept of *approximate delta functions*. This refers to functions δ_t depending on a parameter $t > 0$. The functions become more and more peaked near zero as t tends to zero. The standard example is the Gaussian $1/\sqrt{2\pi t}\exp(-x^2/(2\pi t))$.

Here are the properties that we require:

1. Positivity: For each $t > 0$ the function is positive:

$$\delta_t(x) \geq 0. \tag{3.33}$$

2. Integral: For each $t > 0$ the integral

$$\int_{-\infty}^{\infty} \delta_t(x)\, dx = 1. \tag{3.34}$$

3. Concentration: For each $c > 0$ the limit

$$\lim_{t\to 0} \int_{|x|\geq c} \delta_t(x)\, dx = 0. \tag{3.35}$$

The main theorem is the following.

Theorem 3.2 *Consider a family of approximate delta functions δ_t for $t > 0$. Let ϕ be a continuous bounded function. Then*

$$\lim_{t\to 0} \int_{-\infty}^{\infty} \delta_t(x-a)\phi(x)\,dx = \phi(a). \tag{3.36}$$

Proof: Let

$$u(a,t) = \int_{-\infty}^{\infty} \delta_t(x-a)\phi(x)\,dx. \tag{3.37}$$

Use the Integral property to write

$$u(a,t) - \phi(a) = \int_{-\infty}^{\infty} \delta_t(x-a)[\phi(x) - \phi(a)]\,dx. \tag{3.38}$$

Let $\epsilon > 0$. Since ϕ is continuous at a, there is a $c > 0$ such that for all x, $|x-a| < c$ implies $|\phi(x) - \phi(a)| < \epsilon$. Use the Positivity property to write

$$|u(a,t) - \phi(a)| \le \int_{-\infty}^{\infty} \delta_t(x-a)|\phi(x) - \phi(a)|\,dx, \tag{3.39}$$

and break up the integration into the parts where $|x-a| < c$ and where $|x-a| \ge c$. By the Integral property the contribution from the first part is less than ϵ. However since ϕ is bounded the contribution from the second part tends to zero as t tends to zero. Thus if we take t sufficiently small, then this is less than ϵ. This argument shows that for every $\epsilon > 0$ there is a t' such that $0 < t < t'$ implies $|u(a,t) - \phi(a)| < 2\epsilon$. This shows that $u(a,t) \to \phi(a)$ as $t \to 0$.

In the following we shall make use of many approximate delta functions. Here are some of the most useful.

Step The step function is the easiest case to understand geometrically.

$$\delta_t(x) = \frac{1}{2t} \text{ for } |x| \le t \tag{3.40}$$

and is zero elsewhere.

Triangle The triangle function has the advantage that it is continuous.

$$\delta_t(x) = \frac{1}{t}(1 - \frac{|x|}{t}) \text{ for } |x| \le t \tag{3.41}$$

and is zero elsewhere.

Gaussian The Gaussian is the natural function to use in the context of probability.

$$\delta_t(x) = \frac{1}{\sqrt{2\pi t^2}} \exp(-\frac{x^2}{2t^2}). \tag{3.42}$$

Exponential The exponential function is another convenient choice.

$$\delta_t(x) = \frac{1}{2t} \exp(-|x|/t). \tag{3.43}$$

Cauchy The Cauchy function has the advantage of being a rational function.

$$\delta_t(x) = \frac{1}{\pi} \frac{t}{t^2 + x^2}. \tag{3.44}$$

In all these examples except for the Gaussian it is easy to prove the Integral property. The concentration property takes a bit more thought. Here is a lemma that can help. In particular, it applies to all the above examples.

Lemma 3.1 *Suppose that δ_t satisfies the Positivity and Integral properties and the scaling property $\delta_t(x) = (1/t)\delta_1(x/t) \geq 0$. Then δ_t satisfies the Concentration property and hence is an approximate delta function.*

Proof: This follows from the fact that

$$\int_{|x|\geq c} \delta_t(x)\, dx = \int_{|x|\geq c} \delta_1(x/t)\, dx/t = \int_{|z|\geq c/t} \delta_1(z)\, dz \to 0 \tag{3.45}$$

as $t \to \infty$.

It is the custom to write the limit of an integral involving an approximate delta function as if it were an integral of a function. Thus one defines, for each continuous function f that vanishes outside of a bounded interval,

$$\int_{-\infty}^{\infty} \delta(x-a) f(x)\, dx = f(a). \tag{3.46}$$

The $\delta(x-a)$ is supposed to be a positive function that is zero when $x \neq a$, infinite at a, with total integral one. There is no such function. However working with such expressions is convenient, since it reminds one of various useful properties. In the end, the expression on the left hand side is just a convenient abbreviation for the expression on the right hand side.

Here is an example. Let $H(x)$ be the Heaviside function defines by $H(x) = 1$ for $x > 0$ and $H(x) = 0$ for $x < 0$. (The value of $H(0)$ is not important for present purposes.) This function is not differentiable. Nevertheless, we want to define integrals involving the derivative of this function, and we do this by assuming that we can do integration by parts. Thus we write

$$\int_{-\infty}^{\infty} H'(x-a) f(x)\, dx = -\int_{-\infty}^{\infty} H(x-a) f'(x)\, dx. \tag{3.47}$$

The left hand side is defined by the right hand side. From this it is not hard to see that

$$\int_{-\infty}^{\infty} H'(x-a) f(x)\, dx = -\int_{a}^{\infty} f'(x)\, dx = f(a). \tag{3.48}$$

This says that $H'(x-a) = \delta(x-a)$, in the sense that they give the same result in an integral.

In order to understand this, one can take approximate delta functions $\delta_t(x)$ and define approximate Heaviside functions $H_t(x) = \int_{-\infty}^{x} \delta_t(y)\, dy$. Then the entire calculation makes sense as a calculation involving functions. However when only the result as $t \to 0$ is of interest, then it is convenient to use above abbreviations.

3.5 The linear diffusion equation

Now we can return to the mathematics of the diffusion or heat equation. This equation is different because it describes random motion rather than steady motion. The equation has the form

$$\frac{\partial u}{\partial t} = \frac{1}{2}\sigma^2 \frac{\partial^2 u}{\partial x^2}. \tag{3.49}$$

The natural problem is to specify the initial condition $u(x,0) = \phi(x)$ and try to find the solution for $t > 0$.

This equation can be thought of as the equation for the random diffusion of particles. The rate of diffusion is proportional to the second derivative of the concentration with respect to the space variable. It can also be thought of as an equation for temperature.

Since this equation describes random motion, it seems plausible that its solution would involve the Gaussian distribution. Furthermore, the distribution should get more spread out as time goes on. Thus it is natural to look at a Gaussian distribution with variance parameter proportional to time. If the mean is zero and the variance is $\sigma^2 t$ for $t > 0$, then the Gaussian curve

$$g_t(x) = \frac{1}{\sqrt{2\pi\sigma^2 t}} e^{-\frac{x^2}{2\sigma^2 t}}. \tag{3.50}$$

The properties of this are

$$\int_{-\infty}^{\infty} g_t(x)\, dx = 1 \tag{3.51}$$

and

$$\int_{-\infty}^{\infty} x g_t(x)\, dx = 0 \tag{3.52}$$

and

$$\int_{-\infty}^{\infty} x^2 g_t(x)\, dx = \sigma^2 t. \tag{3.53}$$

It is not difficult to check that the function $g_t(x)$ satisfies the heat equation. We consider the initial value problem where the initial condition ϕ is bounded and continuous.

Theorem 3.3 *The solution for $t > 0$ of the heat equation on an infinite interval with bounded continuous initial condition $u(x, 0) = \phi(x)$ is*

$$u(x,t) = \int_{-\infty}^{\infty} g_t(x-y)\phi(y)\,dy. \tag{3.54}$$

Proof: It is easy to see that this is a solution of the heat equation by differentiating under the integral sign. The initial condition is satisfied since $g_t(x)$ is an approximate delta function.

It is not difficult to extend this result to the situation when there is also constant drift. For instance, consider the problem of finding the distribution $\rho(y,t)$ of a substance that is subject to both diffusion and a steady drift at velocity a. The equation is

$$\frac{\partial \rho}{\partial t} + \frac{\partial a\rho}{\partial y} = \frac{1}{2}\sigma^2 \frac{\partial^2 \rho}{\partial y^2}. \tag{3.55}$$

The solution is

$$\rho(y,t) = \int_{-\infty}^{\infty} g_t(y-at-x)\rho_0(x)\,dx. \tag{3.56}$$

The nice thing about this is that it is a simple combination of the solutions for steady translational motion and symmetric diffusion. Of course the situation is much more complicated when the diffusion coefficient $\sigma^2/2$ and drift coefficient a depend on the space variable y. The discussion of this topic will follow later in this chapter.

3.6 Diffusion and transport

There is a remarkable connection between the heat equation and one of the non-linear transport equations. This is known as the Cole-Hopf transformation. This can be seen by writing the solution of the heat equation in the form

$$u = \exp(-W/\sigma^2). \tag{3.57}$$

Then the heat equation is equivalent to

$$\frac{\partial W}{\partial t} + \frac{1}{2}\left(\frac{\partial W}{\partial x}\right)^2 = \frac{1}{2}\sigma^2 \frac{\partial^2 W}{\partial x^2}. \tag{3.58}$$

If we let

$$w = \frac{\partial W}{\partial x}, \tag{3.59}$$

then this gives

$$\frac{\partial w}{\partial t} + w\frac{\partial w}{\partial x} = \frac{1}{2}\sigma^2 \frac{\partial^2 w}{\partial x^2}. \tag{3.60}$$

This is the equation for the velocity of a gas moving freely except for the influence of viscosity. It is called the Burgers equation.

Say that we want to solve this equation with the initial condition $w(x,0) = h(x)$. Let H be the integral of h. Then this is the same as solving the heat equation with $u(x,0) = \exp(-H(x)/\sigma^2)$. This we can do without any problem. Then we can get the corresponding solution for $w(x,t)$ by using

$$w = -\sigma^2 \frac{1}{u}\frac{\partial u}{\partial x}. \tag{3.61}$$

Explicitly, this is

$$w(x,t) = \frac{1}{Z_{x,t}(\sigma^2)} \int_{-\infty}^{\infty} \frac{x-y}{t}\, \exp(-\frac{1}{\sigma^2}[\frac{(x-y)^2}{2t} + H(y)])\, dy, \tag{3.62}$$

where

$$Z_{x,t}(\sigma^2) = \int_{-\infty}^{\infty} \exp(-\frac{1}{\sigma^2}[\frac{(x-y)^2}{2t} + H(y)])\, dy. \tag{3.63}$$

The remarkable thing about this solution is that it has a solution in the limit $\sigma^2 \to 0$ of zero viscosity.

Theorem 3.4 *The equation for the velocity of a gas moving with no viscous forces is*

$$\frac{\partial w}{\partial t} + w\frac{\partial w}{\partial x} = 0. \tag{3.64}$$

Consider the initial value problem with $w = h(x)$ when $t = 0$. Let $H'(x) = h(x)$ and let

$$E_{x,t}(y) = \frac{(y-x)^2}{2t} + H(y). \tag{3.65}$$

Then the solution obtained by taking the zero viscosity limit is $w = h(y)$, where y is the point at which the absolute minimum of $H(y)$ is assumed.

Proof: At every point y where the derivative of $E_{x,t}(y)$ is equal to zero we have the characteristic equation

$$x = y + h(y)t. \tag{3.66}$$

The theorem gives the solution only at the points x, t for which there is a unique y where the function $E_{x,t}(y)$ assumes its absolute minimum. For most x and t there will be a single such y. In this case, for small σ^2 the function

$$\delta_{\sigma^2}(y) = \frac{1}{Z_{x,t}(\sigma^2)} \exp(-\frac{1}{\sigma^2} E_{x,t}(y)) \tag{3.67}$$

is an approximate delta function concentrated at the point y where the absolute minimum is assumed. The other critical points will give a negligible contribution. So the value of the solution in the limit $\sigma^2 \to 0$ is the value of the integrand at this point, namely

$$w = \frac{x-y}{t}. \tag{3.68}$$

Since y satisfies the characteristic equation we have $w = h(y)$.

In the case when $h'(y) > 0$, the equation $x = y + h(y)t$ has a unique solution for all x and $t > 0$. This is when the slow particles are behind the fast particles. This is reflected in the present picture by the fact that $E_{x,t}(y)$ is concave up and so has a unique local minimum. However in the case when $h'(y) < 0$ at some point the equation $x = y + h(y)t$ can have several solutions, and the function $E_{x,t}(y)$ can have several local minima. This is when the fast particles are behind the slow particles. They catch up and form a shock. For most x and t there will be a unique global minimum, and this determines the solution. However as x varies for fixed t, the critical point that gives the global minimum can jump, and the solution has a shock discontinuity.

Here is a very simple example. Consider fast particles travelling at velocity v_0 that have just caught up with stationary particles. Take the initial condition to be $h(y) = v_0$ for $y < 0$ and $h(y) = 0$ for $y > 0$. The characteristics are $x = y + v_0 t$ for $y < 0$ and $x = y$ for $y > 0$. There is a shock ambiguity immediately in the region where $0 < x < v_0 t$. However this is resolved by taking the zero viscosity limit. The function $H(y)$ satisfies $H(y) = v_0 y$ for $y < 0$ and $H(y) = 0$ for $y > 0$. The function $E_{x,t}(y) = (x - y)^2/(2t) + H(y)$. For $y < 0$ the minimum value is $v_0(v_0 t/2 + y)$. For $y > 0$ the minimum value is 0. Thus the $y < 0$ characteristic is preferred when $y < -v_0 t/2$, that is, when $x < v_0 t/2$. The shock front thus moves at velocity $v_0/2$, with fast particles moving at velocity v_0 piling up in back and with unsuspecting stationary particles sitting in front.

3.7 Diffusion with drift

We can look more generally at linear diffusion equations with variable coefficients. Consider, for instance, the *backward equation*

$$\frac{\partial u}{\partial t} = Lu = \frac{1}{2}\sigma(x)^2\frac{\partial^2 u}{\partial x^2} + a(x)\frac{\partial u}{\partial x}. \tag{3.69}$$

There is a corresponding *forward equation*

$$\frac{\partial \rho}{\partial t} = L^\dagger \rho = \frac{1}{2}\frac{\partial^2 \sigma(y)^2 \rho}{\partial y^2} - \frac{\partial a(y)\rho}{\partial y}. \tag{3.70}$$

In physics the forward equation is also known as the *Fokker-Planck equation.*

Both these equations describe the probability density $p(x, y, t)$ for a particle to diffuse from x to near y in time t. The backward equation is the equation satisfied as a function of the initial position. Its solution is of the form

$$u(x, t) = \int_{-\infty}^{\infty} p(x, y, t) f(y)\, dy \tag{3.71}$$

Here f is a function of the final position, and the solution represents the expected value of f as a function of the initial position.

The forward equation is an equation for a density. It is in the form of a conservation law. We shall see that the solution of the forward equation is

$$\rho(y, t) = \int_{-\infty}^{\infty} p(x, y, t)\rho_0(x)\, dx \tag{3.72}$$

Here ρ_0 is the initial density, and the solution represents the density as a function of the final position. Note that the solutions are given by the same transition probabilities, but with the roles of the initial and final position reversed.

Here is how to establish this connection between the backward equation and the forward equation. We can solve the backward equation starting with the solution $u(z, t - s)$ at time $t - s$. This gives

$$u(x, t) = \int_{-\infty}^{\infty} p(x, y, s)u(y, t - s)\, dz. \tag{3.73}$$

Thus

$$\frac{\partial u(x, t)}{\partial t} = \int_{-\infty}^{\infty} p(x, y, s)Lu(y, t - s)\, dy. \tag{3.74}$$

Let s approach t. This gives

$$\frac{\partial u(x, t)}{\partial t} = \int_{-\infty}^{\infty} p(x, y, t)Lf(y)\, dy. \tag{3.75}$$

This implies that

$$\int_{-\infty}^{\infty} \frac{\partial \rho(y, t)}{\partial t} f(y)\, dy = \int_{-\infty}^{\infty} \rho(y, t)Lf(y)\, dy = \int_{-\infty}^{\infty} L^\dagger \rho(y, t)f(y)\, dy. \tag{3.76}$$

The last equation comes from integrating by parts. We thus see that $\rho(y,t)$ as defined by the integral is indeed a solution of the forward equation.

In general such diffusion equations are difficult to solve. However it is not so difficult to find a *stationary* or *equilibrium* solution of the forward equation. If the current

$$J = a(y)\rho - \frac{1}{2}\frac{\partial \sigma(y)^2 \rho}{\partial y} = 0, \tag{3.77}$$

then ρ is a steady state solution. This situation is called *detailed balance*, since it says that the drift current is exactly balanced by the diffusion current at each point. This equation can be solved with just one integration.

There is a special case when it is possible to find an explicit solution of the time-dependent equation. This is for $a(y) = -\lambda y$, where $\lambda > 0$ is a constant *relaxation rate*. This represents a diffusion that likes to stay near the origin in space. If it strays too far from the origin, then the drift $-\lambda y$ brings it back. This can be seen by solving the characteristic equation for case of zero diffusion. The equation is $dy/dt = -\lambda y$ with $y = x$ when $t = 0$. It has solution $y = xe^{-\lambda t}$. With diffusion constant σ_1^2 the backward equation is

$$\frac{\partial u}{\partial t} = \frac{\sigma_1^2}{2}\frac{\partial^2 u}{\partial x^2} - \lambda x \frac{\partial u}{\partial x} \tag{3.78}$$

and the corresponding forward equation is

$$\frac{\partial \rho}{\partial t} = \frac{\sigma_1^2}{2}\frac{\partial^2 \rho}{\partial y^2} + \frac{\partial \lambda y \rho}{\partial y} \tag{3.79}$$

The way to solve this is to establish a relation with the usual diffusion equation. To examine this, consider the function $u(x,t) = w(h(t)x, g(t))$. If w satisfies the diffusion equation $\partial w/\partial \tau = (\sigma_1^2/2)\partial^2 w/\partial z^2$, then u satisfies the equation

$$\frac{\partial u}{\partial t} = \frac{g'(t)}{h(t)^2}\frac{\sigma_1^2}{2}\frac{\partial^2 u}{\partial x^2} + \frac{h'(t)}{h(t)} x \frac{\partial u}{\partial x}. \tag{3.80}$$

It would be nice to get rid of the time dependence. Take $h'(t)/h(t) = -\lambda$. Then $h(t) = e^{-\lambda t}$. Take $g'(t) = h(t)^2 = e^{-2\lambda t}$. Then $g(t) = (1 - e^{-2\lambda t})/(2\lambda)$. The constants of integration have been chosen so that when t is small $h(t)$ is close to one and $g(t)$ is close to t. Thus this is a solution of the backward equation that is close to the solution of the heat equation when t is small. The explicit formula $u(x,t)$ for the solution of the backward equation is determined by the transition probabilities

$$p(x,y,t) = \frac{1}{\sqrt{2\pi\sigma_1^2 g(t)}} \exp(-\frac{(y - h(t)x)^2}{2\sigma_1^2 g(t)}). \tag{3.81}$$

The explicit formula for the solution $\rho(y,t)$ of the forward equation is determined by the same transition probabilities, reversing the roles of the variables.

It is now easy to determine the long time behavior of the solution of the forward equation. The particle is started off with initial distribution $\rho_0(x)$. It

diffuses, but it also drifts toward the origin with an average velocity $-\lambda y$. Since $h(t) = e^{-\lambda t}$ approaches zero, the solution loses memory of its initial condition. The time to lose memory is a multiple of $1/\lambda$. Eventually the random diffusion is balanced on the average by the drift. Since $g(t) = (1-e^{-2\lambda t})/(2\lambda)$ approaches $1/(2\lambda)$, the solution approaches an equilibrium given explicitly by

$$\rho(y) = \frac{1}{\sqrt{\pi\sigma_1^2/\lambda}} \exp(-\frac{\lambda y^2}{\sigma_1^2}). \tag{3.82}$$

This is a Gaussian with variance $\sigma_1^2/(2\lambda)$. As one might expect, as the restoring drift proportional to λ becomes larger, the variance becomes smaller.

One interpretation of this forward equation is as a velocity distribution of a particle. This model is called the *Ornstein-Uhlenbeck* process. The motion of the particle is influenced by a friction force proportional to the velocity and by thermal diffusion. The motion of the particle in time is given by

$$m\frac{dv}{dt} = -\gamma v + \text{ thermal noise.} \tag{3.83}$$

The relation between the relaxation rate λ and the friction coefficient γ is $\lambda = \gamma/m$. Therefore the relaxation time is $\Delta t = 2/\lambda = 2m/\gamma$, a very small but non-zero quantity. In equilibrium the velocity of the particle is random with the above Gaussian distribution at each fixed time. The variance $(\Delta v)^2 = \sigma_1^2/(2\lambda) = m\sigma_1^2/(2\gamma)$ of the Gaussian velocity distribution is determined by requiring that the average kinetic energy is determined by the temperature. This says that $(1/2)m(\Delta v)^2 = (1/2)kT$, where kT is the energy corresponding to absolute temperature T. So the original velocity diffusion parameter in the Ornstein-Uhlenbeck process must have been $\sigma_1^2 = 2\lambda kT/m = 2\gamma kT/m^2$.

If we take the distance travelled in a relaxation time to be given by $(\Delta x)^2 = (\Delta v\,\Delta t)^2 = (kT/m)(2m/\gamma)\Delta t = (2kT/\gamma)\Delta t$, then we get the Einstein formula $\sigma^2 = 2kT/\gamma$. The relation between the diffusion coefficients for position and for velocity is thus $\sigma^2 = \sigma_1^2(\Delta t/2)^2$.

3.8 Reaction-diffusion equations

Nonlinear diffusion equations produce new phenomena, such as solutions with a determined propagation speed. A typical example of a reaction diffusion equation is

$$\frac{\partial u}{\partial t} = \mu\frac{\partial^2 u}{\partial x^2} + f(u). \tag{3.84}$$

The first term on the right is the diffusion term, and the second term on the right is the reaction term. The physical interpretation is that u is the concentration of some chemical. The chemical diffuses with diffusion constant $\mu > 0$, but it also is produced by a reaction that itself depends on the amount of the chemical that is present. This is a non-linear equation.

A classic example is Fisher's equation, when $f(u) = k(u-u^2)$. The state $u = 0$ represents no concentration of the chemical, while the state $u = 1$ represents

a state when the reaction is completed. The constant $k > 0$ is the reaction rate. When u is between 0 and 1 the reaction is taking place, and the concentration in increasing. Fisher's equation also has similar interpretations in ecology, where it models the spatial spreading of some trait.

Let us look for a solution that represents a burning front that moves from left to right. Thus the solution should be near 1 for large negative x and near 0 for large positive x. The interface should be moving to the right as the reaction takes place with some velocity $c > 0$. We can try a solution of the form

$$u(x,t) = g(x - ct). \tag{3.85}$$

This represents a wave travelling at velocity c. The equation for $y = g(z)$ is seen to be

$$\mu \frac{d^2y}{dz^2} = -c\frac{dy}{dz} - f(y). \tag{3.86}$$

The question is whether there is a velocity c for which the solution y stays between 0 and 1 and tends to 1 at $-\infty$ and to 0 at ∞.

This can be thought of as a problem of the motion of a particle under the influence of a force. In this interpretation z is the time parameter. The dependent variable y is the position of the particle. Its velocity is $v = dy/dz$. The frictional force is $-cv$. The position dependent force is $-f(y) = -ky(1-y)$. Near $y = 1$ the position dependent force looks like a $k(y-1)$, while near $y = 0$ it looks like $-ky$. We start with a solution with $y < 1$ and $v < 0$ such that y approaches 1 and v approaches zero as z approaches minus infinity. We need to make the friction c strong enough so that we can be sure that the solution remains with $y > 0$ and does not overshoot. We shall see that the condition for this to happen is that $c \geq 2\sqrt{\mu k}$.

The argument uses the equations $dy/dz = v$ and $\mu dv/dz = -cv - f(y)$. From the second equation we see that $\mu dv/dz > -cv - ky$. This is a linear expression that is easier to analyze. We want to argue that there is an $a < 0$ such that the velocity v always satisfies $0 > v > ay$. In this case the velocity v will approach zero as y approaches zero, and the solution will not overshoot.

It will turn out that it is sufficient to take a to be a solution of $\mu a^2 + ca + k = 0$. Such an $a < 0$ always exists if c satisfies the condition.

We need to show that it impossible that the solution ever reaches the boundary $v = ay$. If it were so, then it would exit through this boundary. Consider the exit point. From $dy/dz = ay$ and $\mu dv/dz > -cay - ky$ we would have $dv/dz > (1/\mu)(-cay - ky) = a^2 y = a\,dy/dz$. This would imply that the solution instead would enter through this boundary, which is a contradiction.

The conclusion for the original reaction diffusion equations is that they have traveling wave solutions, but only with velocities $c \geq 2\sqrt{\mu k}$. If the non-linear front is to exist at all, it has to move rather rapidly. However it has been shown that for an initial function with values between 0 and 1 on some bounded interval, equal to 1 on the left of the interval and to 0 on the right of the interval, the front moves at the minimum possible velocity $c = 2\sqrt{\mu k}$.

The lesson is that a combination of reaction and diffusion can produce a wave that travels at a constant speed. The speed depends both on the diffusion

constant μ and on the reaction rate k, so this shows that progress of the wave is due to the two effects acting together.

When c is very large, one can find an explicit formula for the traveling wave. Let $z = cw$ and write the equation as

$$\frac{\mu}{c^2}\frac{d^2y}{dw^2} = -\frac{dy}{dw} - ky(1-y). \tag{3.87}$$

Take the limit as c goes to infinity. The resulting equation is a first order differential equation that may be solved explicitly. There is a solution that satisfies the boundary conditions for large positive and negative w. This solution is defined up to a shift in w. This solution may be used to construct the traveling wave in a rather explicit form.

3.9 Problems

1. Check that the Gaussian $1/\sqrt{2\pi\sigma^2 t}\exp(-x^2/(2\sigma^2 t))$ is a solution of the diffusion equation for $t > 0$. Fix t. What is the integral of this solution from $-\infty$ to ∞ with respect to x?

2. Show the equivalence of the two alternate forms for the law of conservation of energy.

3. We expect that for fixed density, an increase in temperature is accompanied by an increase in internal energy. What would go wrong with the heat equation if $\partial u/\partial T$ were negative?

4. Show that $1/(\pi t)\mathrm{sech}(x/t)$ is an approximate delta function.

5. Let ϕ be an initial condition for the heat equation. Say that it is a positive function that vanishes outside a bounded interval. Show that the solution $u(x,t)$ for fixed x and large t behaves asymptotically like a function of t that approaches zero as t gets large. Find this function explicitly.

6. Use the detailed balance formula to find the stationary solution of the general forward diffusion equation. Show that it can be taken positive. Say that the diffusion coefficient satisfies $0 < c_1 < \sigma(y)^2 < c_2$ and that the drift $a(y)$ satisfies $a(y) \le -\epsilon < 0$ for large positive y and $a(y) \ge \epsilon > 0$ for large negative y. Show that the stationary solution has finite integral.

7. Use the detailed balance formula to find the equilibrium in the special case of the Ornstein-Uhlenbeck forward equation. Check that this coincides with the result obtained in the text.

8. Find the explicit form of the traveling wave solution $u(x,t) = g(x-ct)$ of Fisher's equation in the limit of large c. Take the solution with $g(0) = 1/2$. The solution will depend on the parameters k and c.

Chapter 4

The Laplace equation

4.1 Classification

The traditional classification of partial differential equations is into three types: hyperbolic, parabolic, and elliptic. In two dimensions the linear second order real constant coefficient partial differential equations fall into one of these three types.

The standard example of a *hyperbolic* equation is the wave equation

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}. \tag{4.1}$$

The typical property of a hyperbolic equation is an upper bound on the speed of propagation. In the case of the wave equation this bound is the speed c. The typical problem for a hyperbolic equation is an initial value problem or an initial value-boundary value problem. Note that solutions need not be smooth. If an initial condition is not smooth, then as it moves along it will typically continue not to be smooth.

The standard example of a *parabolic* equation is the heat equation

$$\frac{\partial u}{\partial t} = \frac{\sigma^2}{2} \frac{\partial^2 u}{\partial x^2}. \tag{4.2}$$

The typical problem for a parabolic equation is the initial value problem or an initial value-boundary value problem. However this problem will have nice properties only in one direction of time. In general the solutions of a parabolic equation will be smooth, since the solutions represent a sort of dissipation in the course of time. Note that the propagation speed will not be bounded above, though on the average the solution will spread out rather slowly (as the square root of time).

The standard example of an *elliptic* equation is the Laplace equation

$$\frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0. \tag{4.3}$$

The typical problem for an elliptic equation is a boundary value problem. In general the solutions of an elliptic equation will be smooth, even analytic. This chapter is a brief introduction to the Laplace equation.

It is important to note that not all important partial differential equations fit into this classification. For example, the Schrödinger equation of quantum mechanics is not real. The equation is

$$\frac{\partial u}{\partial t} = i\frac{\sigma^2}{2}\frac{\partial^2 u}{\partial x^2}, \tag{4.4}$$

which is like the heat equation, but with imaginary time. In this case the diffusion coefficient is $\sigma^2 = \hbar/m$, where $\hbar$ is Planck's constant and m is a mass. The properties of the Schrödinger equation are very different from those of the heat equation. There is no preferred direction of time in which the solution gets smoothed. The solutions behave more like waves. However there is no maximum propagation speed; instead there is an entire infinite range of possible propagation velocities. This kind of equation is called *dispersive*.

4.2 The mean value property

Perhaps the most famous partial differential equation is the *Laplace equation*. Often it is written

$$\nabla^2_{\mathbf{x}} u = 0, \tag{4.5}$$

where $\mathbf{x} = (x, y)$. In polar coordinates the *Laplace operator* takes the form

$$\nabla^2_{\mathbf{x}} = \frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{1}{r^2}\frac{\partial^2}{\partial \theta^2}. \tag{4.6}$$

There are many interpretations of the Laplace equation, usually as determining some sort of equilibrium. A common interpretation is as the equation for a steady state distribution of temperature. Another interpretation is as an equation for electric potential.

It is easy to find solutions of the Laplace equation, which are also called *harmonic* functions. Some standard examples are $e^x \cos y$, $\ln(x^2 + y^2)$, and $\tan^{-1}(y/x)$. However only the first is defined at every point in the plane.

Let $\mathbf{x} = (x, y)$ be a point in the plane, and let $M_{\mathbf{x},r}(f)$ be the mean value of f on the circle of radius r centered at $\mathbf{x}$. Then $M_{\mathbf{x},r}(u)$ satisfies the equation

$$\nabla^2_{\mathbf{x}} M_{\mathbf{x},r}(r) = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} M_{\mathbf{x},r}. \tag{4.7}$$

The proof of this identity is left as an exercise.

It follows from this identity that if we take u to be a solution of the Laplace equation, then

$$\frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} M_{\mathbf{x},r}(u) = 0. \tag{4.8}$$

It is easy to solve this ordinary differential equation Thus $r\partial M_{\mathbf{x},r}(u)/\partial r = C(\mathbf{x})$ and $M_{\mathbf{x},r}(u) = A(\mathbf{x}) + C(\mathbf{x}) \ln r$. If we assume that u is continuous at $\mathbf{x}$ with value $u(\mathbf{x})$, then also $M_{\mathbf{x},r}(u)$ is continuous at $\mathbf{x}$ with the same value. So this means that $M_{\mathbf{x},r}(u) = A(\mathbf{x}) = u(\mathbf{x})$. This proves the following *mean value property.*

Theorem 4.1 *Let u be a solution of the Laplace equation in the plane. Let $r > 0$ and $M_{\mathbf{x},r}(u)$ be the average of u over the circle of radius r centered at $\mathbf{x}$. Then*

$$u(\mathbf{x}) = M_{\mathbf{x},r}(u) \tag{4.9}$$

Corollary 4.1 *Let u be a solution of the Laplace equation in some region. Then u cannot assume a maximum value (or a minimum value) at a single interior point.*

The theorem and corollary make sense in the physical interpretation of the solution as a distribution of temperature. It seems reasonable that there could not be a hot spot at an interior point, since then heat would flow away and there would not be an equilibrium.

4.3 The Poisson formula

Here we look at the solution of the equation in a disk of radius one. We shall see that the appropriate formulation is as a *boundary value problem.* One interpretation of the Laplace equation is the steady state distribution of temperature in a region when the boundary of the region is held at specified temperature.

Another differential operator, the *Euler operator*, will be useful. This is

$$E = x\frac{\partial}{\partial x} + y\frac{\partial}{\partial y} = r\frac{\partial}{\partial r}. \tag{4.10}$$

A nice exercise is to show that the Euler operator and Laplace operator acting on an arbitrary function f are related by

$$\nabla^2_{\mathbf{x}} E f = E\nabla^2_{\mathbf{x}} f + 2\nabla^2_{\mathbf{x}} f. \tag{4.11}$$

The reader should be comfortable doing this exercise in either Cartesian or polar coordinates. This leads to a nice lemma.

Lemma 4.1 *Let u be a solution of the Laplace equation. Then the result Eu of applying the Euler operator is also a solution of the Laplace equation.*

In order to solve the boundary value problem for the unit disk, we look for a solution that is singular at a point on the unit circle, for instance, at this point $(x, y) = (a, b)$, where $a^2 + b^2 = 1$. An appropriate solution is obtained from the solution $\log(x^2 + y^2) = \log r^2 = 2 \log r$ by translation. This solution

is $\log((x-a)^2+(y-b)^2)$. Now we apply the Euler operator and obtain the solution

$$\frac{2x(x-a)+2y(y-b)}{(x-a)^2+(y-b)^2} = \frac{x^2+y^2+(x-a)^2+(y-a)^2-1}{(x-a)^2+(y-b)^2}. \tag{4.12}$$

If we subtract 1, change the sign, and divide by 2π, we obtain the *Poisson kernel*

$$p(x,y,a,b) = \frac{1}{2\pi}\frac{1-(x^2+y^2)}{(x-a)^2+(y-b)^2}. \tag{4.13}$$

This has the property that it is a solution of the Laplace equation that is singular at (a,b) but is equal to zero at all other points of the circle $x^2+y^2=1$.

Let $a=\cos(\phi)$ and $b=\sin(\phi)$. The Poisson kernel may be expressed in polar coordinates $x=r\cos(\theta)$ and $y=r\sin(\theta)$. This is accomplished as follows. The square of the length of the vector $(a,b)-(x,y)$ is $(x-a)^2+(y-b)^2$. On the other hand, it is also the scalar product of the vector with itself, which by the distributive law is

$$(a,b)\cdot(a,b)-2(a,b)\cdot(x,y)+(x,y)\cdot(x,y) = 1-2r\cos(\theta-\phi)+r^2. \tag{4.14}$$

This shows that the Poisson kernel is

$$p(r,\theta-\phi) = \frac{1}{2\pi}\frac{1-r^2}{1-2r\cos(\theta-\phi)+r^2}. \tag{4.15}$$

For each $r<1$ the Poisson kernel

$$p(r,\theta) = \frac{1}{2\pi}\frac{1-r^2}{1-2r\cos(\theta)+r^2}. \tag{4.16}$$

is is a nice function of θ. We want to show that it is an approximate δ function as r tends to one.

First note that the Poisson kernel is always positive. Furthermore, when $\cos\theta$ is not equal to one, the kernel satisfies the bound

$$p(r,\theta) \le \frac{1}{2\pi}\frac{1-r^2}{1-\cos^2\theta}. \tag{4.17}$$

Thus it approaches zero as r tends to one except at the place where $\cos\theta=1$. Of course at this place it approaches infinity as r tends to one.

The final observation is that the integral of the Poisson kernel around the circle from zero to 2π is one. This follows from a calculation using the standard device for finding the integral of a rational function of $\cos\theta$. It follows that the Poisson kernel acts as an approximate delta function as $r\to 1$.

Theorem 4.2 *The solution of the Laplace equation in the unit disk with boundary value f on the unit circle is given in Cartesian coordinates by*

$$u(x,y) = \int_0^{2\pi} p(x,y,\cos\phi,\sin\phi)f(\cos\phi,\sin\phi)\,d\phi. \tag{4.18}$$

It is given in polar coordinates by

$$u(r,\theta) = \int_0^{2\pi} p(r,\theta-\phi) f(\phi)\, d\phi. \tag{4.19}$$

4.4 Problems

1. Let

$$M_{(x,y),r}(f) = \frac{1}{2\pi}\int_0^{2\pi} f(x + r\cos\theta, y + r\sin\theta)\, d\theta. \tag{4.20}$$

Prove the identity

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2}\right) M_{(x,y),r}(f) = \frac{1}{r}\frac{\partial}{\partial r} r \frac{\partial}{\partial r} M_{(x,y),r}(f). \tag{4.21}$$

used to show that the solution of the Laplace equation in two dimensions satisfies the mean value property.

2. Prove that a solution u of the Laplace equation in three dimensions satisfies the mean value property: for each point and each radius r, the value at the point is the average of the values on the sphere of radius r centered at the point. That is, prove that

$$u(x,y,z) = M_{(x,y,z),r}(u) \tag{4.22}$$

Hint: Use the identity

$$\left(\frac{\partial^2}{\partial x^2} + \frac{\partial^2}{\partial y^2} + \frac{\partial^2}{\partial z^2}\right) M_{(x,y,z),r}(u) = \frac{1}{r^2}\frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} M_{(x,y,z),r}(u). \tag{4.23}$$

3. Show that for each $r < 1$ the integral of the Poisson kernel $p(r,\theta)$ around the unit circle is equal to one. Hint: The standard trick for integrating a rational function of $\cos(\theta)$ is to make the substitution $z = \tan(\theta/2)$.

4. Let

$$p(x,y) = \frac{1}{\pi}\frac{y}{y^2 + x^2} \tag{4.24}$$

be defined for $y > 0$. Let f be a bounded continuous function. Show that the bounded solution of the Laplace equation in the half-space $y > 0$ with boundary value f at $y = 0$ is given by

$$u(x,y) = \int_{-\infty}^{\infty} p(x-z,y) f(z)\, dz. \tag{4.25}$$

Hint: There are two tasks. The first is to show that $p(x,y)$ is harmonic. Then $p(x-z,y)$ will be harmonic for each z, and so will $u(x,y)$. The second is to show that $p(x,y)$ is an approximate delta function of x as y tends to zero.

Chapter 5

The Schrödinger equation

5.1 Complex numbers

This chapter is not a full treatment of the Schrödinger equation. The main purpose is only to compare the Schrödinger equation with the heat equation. The strange thing about the Schrödinger equation is that it involves complex numbers.

A complex number is a number of the form $x + iy$, where i with $i^2 = -1$ is a square root of minus one. One may regard complex numbers as vectors in the plane. Addition of complex numbers is ordinary vector addition. The absolute value of a complex number is the usual length of the vector. Multiplication is given by the formula $(x + iy)(x' + iy') = (xx' - yy') + i(yx' + xy')$. If we use polar coordinates in the plane to write $x = r\cos(\theta)$ and $y = r\sin(\theta)$, then this becomes

$$(x + iy)(x' + iy') = r[(\cos(\theta)x' - \sin(\theta)y') + i(\sin(\theta)x' + \cos(\theta)y')]. \quad (5.1)$$

Multiplication by a complex number thus represents a planar rotation by angle θ followed by a scale change resulting from multiplication by r.

Every complex number $z = x + iy$ has a conjugate $\overline{z} = x - iy$. The conjugation operation has nice properties: the conjugate of a sum is the sum of the conjugates, and the conjugate of a product is the product of the conjugates. Furthermore, the conjugate is related to the absolute value by the relation $\overline{z}z = |z|^2$. In the polar representation the conjugate of $z = x+iy = r[\cos(\theta)+i\sin(\theta)]$ is obtained by taking the negative of the angle, so $\overline{z} = x-iy = r[\cos(-\theta)+i\sin(-\theta)]$.

The notion of complex exponential is a central concept. This is introduced by the following theorem.

Theorem 5.1 *There is a unique definition of $e^{i\theta}$ that has the property that*

$$\frac{de^{i\theta}}{d\theta} = ie^{i\theta} \quad (5.2)$$

with $e^{i0} = 1$. This definition is

$$e^{i\theta} = \cos(\theta) + i\sin(\theta). \tag{5.3}$$

The definition indicated in the theorem gives the definition of the exponential of a pure imaginary complex number. It is then natural to define the exponent of an arbitrary complex number $z = x + iy$ by

$$e^z = e^{x+iy} = e^x e^{iy}. \tag{5.4}$$

5.2 The Schrödinger equation for free motion

The Schrödinger equation for free motion is

$$\frac{\partial u}{\partial t} = i\frac{\sigma^2}{2}\frac{\partial^2 u}{\partial x^2}. \tag{5.5}$$

It is just the heat equation with the diffusion coefficient multiplied by i. In quantum mechanics the diffusion coefficient is $\sigma^2 = \hbar/m$, where m is a mass and $\hbar$ is Planck's constant. Planck's constant is a small number that is the characteristic feature of equations from quantum mechanics. If m is the mass of the electron, then the corresponding diffusion coefficient σ^2 is about one cm^2 per second.

How does one interpret an equation involving complex numbers? What is the interpretation of the "wave function" that solves the Schrödinger equation? The answer is not immediately obvious. However the absolute value squared of the wave function is real and in fact positive. The accepted interpretation of this is as a probability density. This is

$$\rho = |u|^2. \tag{5.6}$$

It satisfies the conservation law

$$\frac{\partial \rho}{\partial t} + \frac{\partial J}{\partial x} = 0, \tag{5.7}$$

where

$$J = \sigma^2 \frac{1}{2i}\left(\overline{u}\frac{\partial u}{\partial x} - \frac{\partial \overline{u}}{\partial x}u\right). \tag{5.8}$$

So one can think of ρ as describing a density with associated current J. The current may also be expressed as $J = v\rho$, where v is a velocity vector field given by σ^2 times the imaginary part of the logarithmic derivative $(1/u)\partial u/\partial x$.

The initial value problem for the Schrödinger equation for free motion has an explicit solution. This can be taken over directly from the solution for the heat equation. It is thus

$$u(x,t) = \frac{1}{\sqrt{2\pi i\sigma^2 t}}\int_{-\infty}^{\infty} \exp(\frac{i(x-y)^2}{2\sigma^2 t}) f(y)\, dy. \tag{5.9}$$

Because of the factor of i in the exponent this is no longer a Gaussian, but rather some complicated expression involving sines and cosines.

This solution takes a simpler form for large t. We can write it as

$$u(x,t) = \frac{1}{\sqrt{2\pi i\sigma^2 t}} \exp(\frac{ix^2}{2\sigma^2 t}) \int_{-\infty}^{\infty} \exp(\frac{-ixy}{\sigma^2 t}) \exp(\frac{iy^2}{2\sigma^2 t}) f(y)\, dy. \tag{5.10}$$

Consider the situation when $f(y)$ vanishes outside of a bounded region. Then the factor $\exp(iy^2/(2\sigma^2 t)$ goes to one uniformly as t approaches infinity for the y in this region. Define the *Fourier transform* of f to be

$$\hat{f}(k) = \int_{-\infty}^{\infty} e^{-iky} f(y)\, dy. \tag{5.11}$$

Then for large t the solution is approximately

$$u(x,t) = \frac{1}{\sqrt{2\pi i\sigma^2 t}} \exp(\frac{ix^2}{2\sigma^2 t}) \hat{f}(\frac{x}{\sigma^2 t}). \tag{5.12}$$

Thus in the same approximation

$$\rho(x,t) = \frac{1}{2\pi\sigma^2 t} |\hat{f}(\frac{x}{\sigma^2 t})|^2. \tag{5.13}$$

This approximate solution for large t represents the result of an explosion in a relatively small bounded region at time zero. The density satisfies the equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial (v\rho)}{\partial x} = 0, \tag{5.14}$$

where $v = x/t$ is the velocity of the exploding particles. These particles are moving freely, as may be seen by the equation

$$\frac{\partial v}{\partial t} + v\frac{\partial v}{\partial x} = 0 \tag{5.15}$$

satisfied by the velocity.

The conclusion of this discussion is that the solution of the Schrödinger equation for free motion in the limit of long time is equivalent to the free motion of a gas of particles. The proportion of particles with a given velocity is given by the magnitude of the Fourier transform of the initial condition.

The Schrödinger equation for motion in a potential energy field is

$$\frac{\partial u}{\partial t} = i\frac{\sigma^2}{2}\frac{\partial^2 u}{\partial x^2} - i\phi(x)u, \tag{5.16}$$

where $\phi(x)$ is the potential energy divided by $\hbar$. If ϕ vanishes outside of a bounded region, then there are two qualitatively different kinds of solutions possible. A *bound state* solution has the property that for each bounded region the time average of the probability associated with that region converges to a constant. The wave is trapped by the attractive potential energy field. A *scattering state* solution, on the other hand, eventually leaves the bounded region and escapes the influence of the potential energy. Thus the scattering state solution eventually resembles the solution of the Schrödinger equation for free motion.

5.3 Problems

1. Consider the Schrödinger equation for motion in a potential energy field. Prove the conservation law for $\rho = |u|^2$ for this case. Hint: Write $\rho = \overline{u}u$.

2. Show that every function of the form $\rho(x,t) = h(x/t)/t$ is a solution of the equation

$$\frac{\partial \rho}{\partial t} + \frac{\partial((x/t)\rho)}{\partial x} = 0. \tag{5.17}$$

Chapter 6

Diffusion and equilibrium

6.1 Forward and backward equations

This chapter treats the diffusion equation in one space dimension, with special regard for the time independent problem. This reduces to an ordinary differential equation, so it is possible to give a rather complete analysis.

The context is diffusion where the diffusion $\sigma(x)^2$ and the drift $a(x)$ can depend on position x in space. We recall the basic facts. The *backward equation* is

$$\frac{\partial u}{\partial t} = Lu = \frac{1}{2}\sigma(x)^2\frac{\partial^2 u}{\partial x^2} + a(x)\frac{\partial u}{\partial x}. \tag{6.1}$$

There is a corresponding *forward equation*

$$\frac{\partial \rho}{\partial t} = L^\dagger \rho = \frac{1}{2}\frac{\partial^2 \sigma(y)^2 \rho}{\partial y^2} - \frac{\partial a(y)\rho}{\partial y}. \tag{6.2}$$

In physics the forward equation is also known as the *Fokker-Planck equation.*

Both these equations describe the probability density $p(x, y, t)$ for a particle to diffuse from x to near y in time t. The backward equation is the equation satisfied as a function of the initial position. Its solution is of the form

$$u(x,t) = \int_{-\infty}^{\infty} p(x,y,t) f(y)\, dy \tag{6.3}$$

Here f is a function of the final position, and the solution represents the expected value of f as a function of the initial position.

The forward equation is an equation for a density. It is in the form of a conservation law. The solution of the forward equation is

$$\rho(y,t) = \int_{-\infty}^{\infty} p(x,y,t)\rho_0(x)\, dx \tag{6.4}$$

Here ρ_0 is the initial density, and the solution represents the density as a function of the final position. Note that the solutions are given by the same transition probabilities, but with the roles of the initial and final position reversed.

In general such diffusion equations are difficult to solve. However it is not so difficult to find a *stationary* or *equilibrium* solution of the forward equation. If the current

$$J = a(y)\rho - \frac{1}{2}\frac{\partial \sigma(y)^2 \rho}{\partial y} = 0, \tag{6.5}$$

then ρ is a steady state solution. This situation is called *detailed balance*, since it says that the drift current is exactly balanced by the diffusion current at each point. This equation can be solved with just one integration. Fix a point y_0 and let

$$I(y) = \int_{y_0}^{y} \frac{2}{\sigma(z)^2} a(z)\, dz. \tag{6.6}$$

Then the solution is

$$\rho(y) = C \frac{2}{\sigma(y)^2} \exp(I(y)). \tag{6.7}$$

6.2 Positive recurrence

The diffusion process is called *positive recurrent* if there is a probability density that is invariant under the time development. For the problem that we are considering, the condition for positive recurrence is that we can take $C > 0$ with

$$\int_{-\infty}^{\infty} \rho(y)\, dy = C \int_{-\infty}^{\infty} \frac{2}{\sigma(y)^2} \exp(I(y))\, dy < \infty. \tag{6.8}$$

Then we can take C so that $\rho(y)$ is a probability density. This condition is satisfied if $I(y)$ approaches $-\infty$ sufficiently rapidly as y approaches $\pm\infty$. This happens when $a(y)$ is sufficiently negative for large positive y and is sufficiently positive for large negative y. This says that there is a drift toward the center that confines the particles and keeps them from wandering off too far too often. The standard example is the Ornstein-Uhlenbeck process.

It is interesting to constrast the solution of the homogeneous forward equation with that for the homogeneous backward equation. The forward equation always has the solution $L\rho = 0$, but only in the positive recurrent case can the ρ be interpreted as a probability density with total integral one. The backward equation always has constant solutions, for instance the constant 1. Thus $L1 = 0$ is always true, but this gives no particularly useful information.

We can also look at diffusion in a bounded region $a < x < b$. Then we have to describe what happens to a diffusing particle when it reaches the boundary. With *Dirichlet* or *absorbing* boundary conditions, the particle is absorbed by the boundary and it never returns to the region. This boundary condition is described by setting $p(x, y, t) = 0$ when x is on the boundary and y is in the interior. In terms of the differential equation this says that the solution $u(x, t)$ of the backward equation satisfies $u(x, t) = 0$ for x on the boundary. It turns out that it is also true that the solution $\rho(y, t)$ of the forward satisfies $\rho(y, t) = 0$ zero for y on the boundary.

For Dirichlet boundary conditions the equilibrium density $\rho(y)$ vanishes for y on the boundary. Therefore it vanishes in the entire region. There is no invariant probability density in the interior of the region. This is physically intuitive, because the particles will eventually wander out of the region and never return.

With *Neumann* or *reflecting* or *insulating* boundary conditions the situation is different. A particle that reaches the boundary just bounces off and returns to the region. This boundary condition is described by setting the current $a(y)\rho(y,t) - \partial(\sigma(y)^2/2\rho(y,t))/\partial y$ equal to 0 for y on the boundary. This says that there is no flow into or out from the region. (It may be shown that the corresponding condition on the forward equation is just $\partial u(x,t)/\partial x = 0$.)

For Neumann boundary conditions the equilibrium solution $\rho(y)$ given above automatically has zero current. Furthermore, the integral defining the normalization constant will converge, since the integral is only over a bounded interval. Therefore the equilibrium density may be adjusted to define a probability density. This is physically reasonable, since the diffusing particles are trapped in the region, and it is plausible their probability distribution approaches equilibrium in the limit of large time. This is the case of positive recurrence, when the particles keep coming back to near the same place with a stable frequency. The simplest example is Brownian motion (constant diffusion, zero drift) on a bounded interval with reflecting boundary conditions. The invariant probability density is then constant. The next simplest example is Brownian motion with non-zero drift. Then the solution is an exponential.

6.3 Transience

The other extreme of behavior of a diffusion is when it is *transient*. This is when the diffusing particles eventually leave each bounded region in the interior of the interval and never return. Thus on the average, they spend only a finite amount of time in each such region before escaping permanently.

The analysis of the transient case uses bounded solutions of the stationary backward equation. For generality we look at the case when the region is an interval $a < x < b$, considering that a or b may be infinite.

The equation is

$$Lu(x) = \frac{\sigma(x)^2}{2}\frac{d^2}{dx^2}u(x) + a(x)u(x) = 0. \tag{6.9}$$

Let

$$s(x) = \int_{x_0}^{x} \exp(-I(y))\, dy. \tag{6.10}$$

This is a solution of the homogeneous equation $Lu = 0$. Let

$$h(x) = \frac{s(x) - s(a)}{s(b) - s(a)}. \tag{6.11}$$

This has the interpretation as the probability that the diffusing particle hits b before it hits a. This quantity is well-defined provided that $-s(a) < \infty$ (the particle escapes to a) or $s(b) < \infty$ (the particle escapes to b) or both (the particle escapes to a or b). If on the other hand both $-s(a) = \infty$ and $s(b) = \infty$, then this is no longer the transient case, and this probability is not defined.

Note that $-s(a) < \infty$ and $s(b) = \infty$, then $h(x) = 0$. This is the case when the particle is sure to escape to a. Similarly, if $s(b) < \infty$ and $-s(a) = \infty$, then $h(x) = 1$. This is the case when the particle is sure to escape to b. In the case when both $-s(a) < \infty$ and $s(b) < \infty$ the function $h(x)$ is a non-constant bounded solution of the homogeneous equation that is equal to zero when $x = a$ and is equal to one when $x = b$. There is a non-zero chance for permanent escape in either direction, and so $h(x)$ increases from 0 to 1 as x runs from a to b.

In the transient case we define the *Green's function*

$$G(x, y) = \int_0^\infty p(x, y, t)\, dt \tag{6.12}$$

It is a measure of the total amount of time that the particle starting at x spends near y, on the average. Let $f(y)$ be a function of position, and let

$$u(x) = \int_{-\infty}^\infty G(x, y) f(y)\, dy = \int_0^\infty u(x, t)\, dt. \tag{6.13}$$

Here $u(x, t)$ is the solution of the backward equation with $u(x, 0) = f(x)$. It follows that

$$Lu(x) = \int_0^\infty Lu(x, t)\, dt = \int_0^\infty \frac{\partial u(x, t)}{\partial t}\, dt = -f(x). \tag{6.14}$$

This shows that such a Green's function may be used to give a solution u of the equation $Lu = -f$. The function $f(y)$ has the interpretation as the rate of reward when the diffusing particle is at y, and $u(x)$ has the interpretation as the total reward in the future history when the particle starts at x.

Note that there is a mathematical ambiguity in solving the backward equations $Lu = -f$, since the backward equation $Lu = 0$ has non-zero solutions. Therefore we want to insist that the solution vanish at in at least one direction, so as to have a chance of uniquely specifying the solution.

We want to calculate the Green's function. The ordinary differential equation is

$$\frac{\sigma(x)^2}{2} \frac{d^2}{dx^2} u(x) + a(x) u(x) = -f(x). \tag{6.15}$$

The general solution is

$$u(x) = \int_a^x (s(y) - s(x)) \rho(y) f(y)\, dy + A(s(x) - s(a)) + B. \tag{6.16}$$

In this equation $\rho(y) = 2/\sigma(y)^2 \exp(I(y))$ is the density without the normalization constant. If we want the solution to vanish at the boundary points, then

we must have $B = 0$ and A satisfying

$$0 = \int_a^b (s(y) - s(b))\rho(y)f(y)\,dy + A(s(b) - s(a)). \tag{6.17}$$

Thus

$$u(x) = \int_a^x (s(y) - s(x))\rho(y)f(y)\,dy + \frac{s(x) - s(a)}{s(b) - s(a)} \int_a^b (s(b) - s(y))\rho(y)f(y)\,dy. \tag{6.18}$$

This can be written in a more symmetric form as

$$u(x) = \frac{s(b) - s(x)}{s(b) - s(a)} \int_a^x (s(y) - s(a))\rho(y)f(y)\,dy + \frac{s(x) - s(a)}{s(b) - s(a)} \int_x^b (s(b) - s(y))\rho(y)f(y)\,dy. \tag{6.19}$$

This can also be written

$$u(x) = (1 - h(x)) \int_a^x (s(y) - s(a))\rho(y)f(y)\,dy + h(x) \int_x^b (s(b) - s(y))\rho(y)f(y)\,dy. \tag{6.20}$$

This gives the correct Green's function even when the escape to infinity is only in one direction. The requirement is that $-s(a) < \infty$ or $s(b) < \infty$ or both. If, for instance, $-s(a) < \infty$ but $s(b) = \infty$, then the limit in the original formula for the Green's function gives

$$u(x) = \int_a^x (s(y) - s(a))\rho(y)f(y)\,dy + (s(x) - s(a)) \int_x^b \rho(y)f(y)\,dy. \tag{6.21}$$

This is the case of escape to a. Similarly, if $s(b) < \infty$ but $-s(a) = \infty$, then

$$u(x) = (s(b) - s(x)) \int_a^x \rho(y)f(y)\,dy + \int_x^b (s(b) - s(y))\rho(y)f(y)\,dy. \tag{6.22}$$

This is the case of escape to b. If $s(b) - s(a) < \infty$, then escape is possible in either direction, and we can use the formula in the original form.

Thus for the case of diffusion on the line, the condition for transience is that either we have escape to plus infinity when

$$\int_0^\infty \exp(-I(y))\,dy < \infty, \tag{6.23}$$

or escape to minus infinity when

$$\int_{-\infty}^0 \exp(-I(y))\,dy < \infty, \tag{6.24}$$

or both. This condition is satisfied if $I(y)$ approach ∞ sufficiently rapidly either as y approaches ∞ or as y approaches $-\infty$. This happens when $a(y)$ is sufficiently positive for large positive y or is sufficiently negative for large negative

y. This says that there is a drift away from the center that helps eventually get rid of the particles. The standard example is Brownian motion on the line (constant diffusion) with non-zero constant drift a.

We can also look at the Green's function from the point of view of the forward equation. Let $q(x)$ be a rate of production of diffusing particles. Then the integral

$$r(x) = \int_0^\infty q(x)G(x,y)\,dx \tag{6.25}$$

is the density of particles in the steady state. This is a steady state solution of the equation $\partial\rho/\partial t = L^\dagger\rho + q$, so it is a solution of the equation $L^\dagger r = -q$. From this we see that there are two kinds of equilibrium, corresponding to positive recurrence and transience. In the positive recurrent case the solution of $L^\dagger\rho = 0$ represents the equilibrium of a closed system. In the transient case the solution of $L^\dagger r = -q$ represents the equilibrium of an open system, where the particles pumped in by the source described by q leave by going off to infinity or to an absorbing boundary.

We can also look at diffusion in a bounded region $a < x < b$. Then we have to describe what happens to a diffusing particle when it reaches the boundary. With Dirichlet or absorbing boundary conditions, the particle is absorbed by the boundary and it never returns to the region. For Dirichlet boundary conditions the typical behavior is transience. This is because if the particle ever reaches the boundary, then it never returns. This is reflected in the mathematics by the fact that the Green's function is well-defined. The standard example is Brownian motion (constant diffusion and drift) on an interval with Dirichlet boundary conditions on both ends. It is particularly easy to evaluate the Green's function in this case.

With Neumann or reflecting or insulating boundary conditions the situation is different. A particle that reaches the boundary just bounces off and returns to the region. The particle spends an infinite amount of time in the region. Thus for Neumann boundary conditions the Green's function is not normally expected to exist.

6.4 Null recurrence

Positive recurrence is when the particles stay around permanently, and transience is when the particles eventually leave permanently. The mathematical characterization of positive recurrence is that there is a solution ρ of $L^\dagger\rho = 0$ that is a probability density. The mathematical characterization of transience is that the operator L has an inverse given by a positive Green's function that approaches zero at the boundary. (The relevant equation in the first case is homogeneous; in the second case it is inhomogeneous.) Both physically and mathematically these are rather different kinds of behavior.

There is yet another kind of behavior that is intermediate. This is when the diffusion is *null recurrent*. The particles keep coming back, but less and less frequently, so that there is no stationary probability distribution. This

seems like a rather special situation, and indeed it is. However the most famous diffusion, Brownian motion in one dimension (constant diffusion, zero drift), is null recurrent. The invariant density is constant, so that it cannot be made into a probability measure. On the other hand, there is no Green's function that is positive and approaches zero at infinity. We shall see later that there is a Green's function, but its properties are not quite so pleasant.

6.5 Problems

1. Consider diffusion on the line with constant diffusion and drift of the form $-\lambda x^3 + m^2 x$ with $\lambda > 0$ and $m^2 > 0$. Find the invariant probability density. The normalization constant may be defined as a definite integral. Where is the density maximal?

2. Consider diffusion on the bounded interval from a to b with constant diffusion, constant drift, and reflecting boundary conditions. Find the invariant probability density. In this case one can calculate the normalization constant.

3. Find the solution of the Dirichlet problem for the stationary diffusion equation on the interval from a to b in the transient case. That is, find the solution of $Lu = 0$ with given boundary values $u(a)$ and $u(b)$. (Hint: Express the solution in terms of the hitting probabilities $h(x)$.)

4. Find the Green's function $G(x, y)$ for diffusion on the line with constant diffusion and non-zero drift $a > 0$. Sketch the solution as a function of y and discuss the interpretation of the solution in terms of the time spent near the point y.

5. In the case of escape only at the right hand point b the Green's function is given by

$$u(x) = \int_a^b G(x,y) f(y)\, dy = (s(b) - s(x)) \int_a^x \rho(y) f(y)\, dy + \int_x^b (s(b) - s(y)) \rho(y) f(y)\, dy. \tag{6.26}$$

   The limit of this as x approaches the other end point a is

$$u(a) = \int_a^b (s(b) - s(y) \rho(y) f(y)\, dy \tag{6.27}$$

   which typically a non-zero constant. Explain the physical meaning of this limit. Why is it non-zero in this case and zero in the case when escape to either end point is possible? What is this constant limit in the case of the diffusion in the preceding problem?

6. Consider diffusion with constant diffusion and zero drift on the bounded interval from a to b with absorbing boundary conditions. Find the Green's function. Take x close to one boundary point. Sketch $G(x, y)$ as a function of y and interpret this physically.

7. Consider diffusion with constant diffusion and non-zero drift on the bounded interval from a to b with absorbing boundary conditions. Find the Green's function.

8. Consider a diffusion whose diffusion constant is bounded above, so that $\sigma(y)^2 \leq M$. If the diffusion is positive recurrent, then

$$\int_{-\infty}^{\infty} \exp(I(y))\, dy \leq M \int_{-\infty}^{\infty} \frac{1}{\sigma(y)^2} \exp(I(y))\, dy < \infty. \tag{6.28}$$

If the diffusion is transient, then either

$$\int_{0}^{\infty} \exp(-I(y))\, dy < \infty \tag{6.29}$$

or

$$\int_{-\infty}^{0} \exp(-I(y))\, dy < \infty. \tag{6.30}$$

Show that such a diffusion cannot be both positive recurrent and transient.

Chapter 7

Fourier series

7.1 Periodic functions

Consider a function (real or complex valued) that is periodic with period L and that may be written as a series of the form

$$f(x) = c_0 + \sum_{n=1}^{\infty} 2a_n \cos(2\pi nx/L) + \sum_{n=1}^{\infty} 2b_n \sin(2\pi nx/L). \tag{7.1}$$

The factor of 2 in this definition is not standard, but it will have the advantage of making the various formulas for Fourier coefficients internally consistent. Then this function is said to have a Fourier series representation.

The meaning of the Fourier series is that the function can be analyzed in terms of its components with various *angular frequencies* or *wave numbers*. The first terminology is often used when x represents time, and the second is sometimes preferred when x represents space. The wave number associated with the nth coefficient is $k = 2\pi n/L$. Thus the cosine term can be written $\cos(kx)$. The spatial frequency is $k/(2\pi) = n/L$, and the spatial period is $(2\pi)/k = L/n$. As x changes by a period the corresponding trigonometric function goes through a complete rotation.

In applications when the variable represents time one often writes $\cos(\omega t)$, where ω is the angular frequency. The angular frequency is $\omega = 2\pi n/T$, where T is the fundamental period in time. The frequency of the nth mode is $\omega/(2\pi) = n/T$, and the corresponding period is $(2\pi)/\omega = T/n$.

The first task is to find a formula for the coefficients of a function having a Fourier series representation. The calculation of these coefficients involves the use of trigonometric identities. Recall that the trigonometric functions satisfy well-known *angle sum identities*:

$$\cos(A \pm B) = \cos(A)\cos(B) \mp \sin(A)\sin(B) \tag{7.2}$$

and

$$\sin(A \pm B) = \sin(A)\cos(B) \pm \cos(A)\sin(B). \tag{7.3}$$

From these identities it is easy to add or subtract and obtain the *product identities*:

$$2\cos(A)\cos(B) = \cos(A+B) + \cos(A-B) \tag{7.4}$$

and

$$2\sin(A)\cos(B) = \sin(A+B) + \sin(A-B) \tag{7.5}$$

and

$$2\sin(A)\sin(B) = \cos(A-B) - \cos(A+B). \tag{7.6}$$

These identities make it easy to calculate integrals of products of trigonometric functions. In particular, they lead to the *orthogonality relations*

$$\int_0^L \cos(2\pi nx/L)\cos(2\pi mx/L)\,dx = (L/2)\delta_{mn} \tag{7.7}$$

and

$$\int_0^L \sin(2\pi nx/L)\cos(2\pi mx/L)\,dx = 0 \tag{7.8}$$

and

$$\int_0^L \sin(2\pi nx/L)\sin(2\pi mx/L)\,dx = (L/2)\delta_{mn} \tag{7.9}$$

when $m \geq 1$ and $n \geq 1$. Here δ_{mn} is the *Kronecker delta* that is equal to 1 when $m = n$ and 0 otherwise.

The orthogonality relations allow the calculation of the various coefficients. The coefficient c_0 associated with zero frequency is obtained by averaging f over the interval. Since each trigonometric function associated with non-zero frequency has average zero, this gives

$$c_0 = \frac{1}{L}\int_0^L f(y)\,dy, \tag{7.10}$$

The coefficients a_n is obtained by multiplying by $\cos(2\pi nx/L)$ and averaging. Similarly, b_n is obtained by multiplying by $\sin(2\pi nx/L)$ and averaging. From the orthogonality relations it follows that

$$a_n = \frac{1}{L}\int_0^L \cos(2\pi ny/L) f(y)\,dy, \tag{7.11}$$

and

$$b_n = \frac{1}{L}\int_0^L \sin(2\pi ny/L) f(y)\,dy, \tag{7.12}$$

There are various other ways of writing the Fourier series representation. For instance, suppose that all the numbers are real, and write $a_n = r_n\cos(\phi_n)$ and $b_n = r_n\sin(\phi_n)$. Then

$$f(x) = c_0 + \sum_{n=1}^{\infty} 2r_n\cos(2\pi nx/L - \phi_n). \tag{7.13}$$

This shows that the series representation may be regarded as involving phase shifted cosines. The phase shift ϕ_n depends on the frequency.

The representation may also be written in the form

$$f(x) = \frac{1}{L}\int_0^L f(y)\,dy + \frac{1}{L}\sum_{n=1}^{\infty}\int_0^L 2\cos(2\pi n(x-y)/L)f(y)\,dy \tag{7.14}$$

This shows directly how the terms in the series depend on the function f that is being expanded.

Sometimes it is convenient to make the change of variable $\theta = 2\pi x/L$. This reduces the Fourier series to the case when the period is 2π. Then if we write out the coefficients, the Fourier series representation says that

$$f(\theta) = \frac{1}{2\pi}\int_0^{2\pi} f(\phi)\,d\phi + \frac{1}{\pi}\sum_{n=1}^{\infty}\int_0^{2\pi}(\cos(n\theta)\cos(n\phi)+\sin(n\theta)\sin(n\phi))f(\phi)\,d\phi. \tag{7.15}$$

Sometimes this is written in terms of the delta function as

$$\delta(\theta-\phi) = \frac{1}{2\pi}[1 + 2\sum_{n=1}^{\infty}(\cos(n\theta)\cos(n\phi)+\sin(n\theta)\sin(n\phi))]. \tag{7.16}$$

However this is just an abbreviation for the version obtained by multiplying by $f(\phi)$ and integrating.

It is generally true that there is a sense in which the Fourier series of a function converges to the function, but making this precise involves some technicalities. The functions need not be continuous, but a precise formulation of the class of functions that is allowed requires considerable theoretical preparation. The following theorem and its proof gives at least some idea of the situation.

Theorem 7.1 *Every continuous periodic function is uniquely determined by its Fourier coefficients. If the infinite series of coefficients is absolutely convergent, then the Fourier series converges absolutely to the function.*

Proof: We consider the case when the period is 2π. The idea is to prove a rigorous version of the delta function identity. For this introduce a parameter r with $0 \le r < 1$. Consider

$$p(r,\theta-\phi) = \frac{1}{2\pi}[1 + 2\sum_{n=1}^{\infty} r^n(\cos(n\theta)\cos(n\phi)+\sin(n\theta)\sin(n\phi))]. \tag{7.17}$$

If we abbreviate $\theta' = \theta - \phi$, then we can also write this as

$$p(r,\theta') = \frac{1}{2\pi}[1 + 2\sum_{n=1}^{\infty} r^n\cos(n(\theta')]. \tag{7.18}$$

We can sum this series. The way to do this is to multiply both sides by $\cos(\theta')$ and use the identity for a product of cosines to obtain an equation for

the unknown quantity $q = 2\pi p(r, \theta')$. The equation that results is

$$\cos(\theta')q = \frac{1}{r}\frac{q-1}{2} + r\frac{q+1}{2}. \tag{7.19}$$

This equation may be solved for q. The final result is

$$p(r, \theta') = \frac{1}{2\pi}\frac{1-r^2}{1-2r\cos(\theta')+r^2}. \tag{7.20}$$

This is an approximate delta function as r approaches 1. The integral property is obvious from the original series representation. The positivity and concentration property follow easily from an examination of the formula.

If f is a continuous periodic function, this shows that

$$f(\theta) = \lim_{r\to 1}\int p(r, \theta-\phi)f(\phi)\,d\phi. \tag{7.21}$$

In other words, the series converges in the sense that

$$f(\theta) = \frac{1}{2\pi}\int_0^{2\pi} f(\phi)\,d\phi + \lim_{r\to 1}\sum_{n=1}^{\infty}\frac{1}{2\pi}\int_0^{2\pi} r^n(\cos(n\theta)\cos(n\phi)+\sin(n\theta)\sin(n\phi))f(\phi)\,d\phi. \tag{7.22}$$

Thus

$$f(\theta) = c_0 + \lim_{r\to 1}\sum_{n=1}^{\infty}(2a_n r^n\cos(n\theta) + 2b_n r^n\sin(n\theta)). \tag{7.23}$$

The coefficients determine the function.

If the series of coefficients is absolutely convergent, then since the sine and cosine functions are bounded by one, it is possible to take the limit as r approaches one. This gives the absolutely convergent series

$$f(\theta) = c_0 + \sum_{n=1}^{\infty}(2a_n\cos(n\theta) + 2b_n\sin(n\theta)). \tag{7.24}$$

7.2 The Laplace equation in a disk

A by product of the proof is the solution of the boundary value problem for the Laplace equation in the unit disk. We expand the boundary value function in a Fourier series

$$f(\theta) = c_0 + \sum_{n=1}^{\infty}(2a_n\cos(n\theta) + 2b_n\sin(n\theta)). \tag{7.25}$$

The Laplace equation in polar coordinates is

$$\frac{1}{r}\frac{\partial}{\partial r}r\frac{\partial u}{\partial r} + \frac{1}{r^2}\frac{\partial^2 u}{\partial\theta^2} = 0. \tag{7.26}$$

From this we see that $r^n \cos(n\theta)$ and $r^n \sin(n\theta)$ are solutions. We reject the solutions when $n < 0$ since they are singular at the origin. The solution with the given boundary value is

$$u(r,\theta) = c_0 + \sum_{n=1}^{\infty} (2a_n r^n \cos(n\theta) + 2b_n r^n \sin(n\theta)). \tag{7.27}$$

This is also

$$u(r,\theta) = \int_0^{2\pi} p(r,\theta-\phi) f(\phi)\, d\phi. \tag{7.28}$$

7.3 Complex form of a Fourier series

It is often more convenient to write the Fourier expansion in a complex form. The expansion takes the form

$$f(x) = \sum_{n=-\infty}^{\infty} c_n \exp(2\pi i n x/L), \tag{7.29}$$

where

$$c_n = \frac{1}{L}\int_0^L \exp(-2\pi i n y/L) f(y)\, dy. \tag{7.30}$$

The relation with the previous notation is that $c_n = a_n - ib_n$ and $c_{-n} = a_n + ib_n$ for $n \ge 1$.

In the complex form of the Fourier series the orthogonality relations take the form

$$\int_0^L \exp(-2\pi i m x/L) \exp(2\pi i n x/L) = \delta_{mn}. \tag{7.31}$$

Thus one can derive the form of the coefficients by multiplying $f(x)$ by $\exp(-2\pi i m x/L)$ and integrating.

It is also sometimes convenient to think of the sum as being a sum over frequencies that are multiples of an angular frequency difference.

$$\Delta k = \frac{2\pi}{L}. \tag{7.32}$$

Thus each angular frequency $k = n\Delta k$ for some integer n. Also, since for large period L the angular frequency difference Δk is very small, it is convenient to deal with $\hat{f}(k)$ defined by $c_k = \hat{f}(k)\Delta k/2\pi$. This quantity, the *Fourier transform*, has a chance of remaining non-zero in the limit of large period and small frequency difference. The formula then takes the elegant form

$$f(x) = \sum_k \hat{f}(k) \exp(ikx) \frac{\Delta k}{2\pi} \tag{7.33}$$

where

$$\hat{f}(k) = \int_{-L/2}^{L/2} \exp(-iky) f(y)\, dy. \tag{7.34}$$

Notice that the weight of each term in the series is the *frequency difference*

$$\frac{\Delta k}{2\pi} = \frac{1}{L}. \tag{7.35}$$

As $L \to \infty$ and $\Delta k \to 0$ the formulas that emerge are those of the Fourier transform. The sum over discrete frequencies weighted by frequency difference is replaced by an integral over all frequencies.

7.4 Boundary conditions

Fourier series are useful for representing periodic functions. In many problems in which the independent variable represents space, one does not have periodic functions, but instead functions that satisfy a *boundary condition* on some interval, say from 0 to L'.

One boundary condition is when the values at the end points of an interval are specified. In the case of a heat condition problem, this corresponds to fixing the temperature at the end points of a rod. If we subtract a linear function, then we may reduce this to the case when the values at the end points of the interval are zero. This is called the *Dirichlet boundary condition*.

Another boundary condition is when the derivatives at the end points are required to be zero. In the case of a heat condition problem, this corresponds to insulating the rod, so that the heat flow is zero. This is called the *Neumann boundary condition*.

The trick for using Fourier series in these cases is to set $L = 2L'$ and extend the function to be periodic with period L. The two special cases correspond to when the periodic function is taken to be are odd or even.

In the odd case, one obtains

$$f(x) = \sum_{n=1}^{\infty} 2b_n \sin(\pi n x/L'), \tag{7.36}$$

where

$$b_n = \frac{1}{L'} \int_0^{L'} \sin(\pi n y/L') f(y)\, dy. \tag{7.37}$$

This is the useful representation when the function is required to vanish at the end points.

In the even case, one obtains the representation

$$f(x) = c_0 + \sum_{n=1}^{\infty} 2a_n \cos(\pi n x/L'). \tag{7.38}$$

The coefficient c_0 is obtained by averaging over the interval. Thus

$$c_0 = \frac{1}{L'} \int_0^{L'} f(y)\, dy, \tag{7.39}$$

The coefficients a_n is given by

$$a_n = \frac{1}{L'} \int_0^{L'} \cos(\pi n y / L') f(y)\, dy. \tag{7.40}$$

This is the useful representation when the derivative of the function is required to vanish at the end points.

In summary: when we consider only the interval from 0 to L' the functions are no longer periodic. However in the case of the sine expansion all the functions $\sin(n\pi x/L')$ vanish at 0 and at L'. Correspondingly, in the cosine expansion all the functions $\cos(n\pi x/L')$ have derivatives that vanish at 0 and at L'. Thus we have the correct functions for the Dirichlet boundary condition in the first case and for the Neumann boundary condition in the second case.

7.5 The wave equation

Consider the boundary value problem for the wave equation on the interval from 0 to L' where the boundary condition is that the value is held fixed at zero at both ends. This is the vibrating string problem. The equation is

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2} \tag{7.41}$$

for $0 \le x \le L'$. The boundary conditions are $u(0,t) = 0$ and $u(L',t) = 0$, and the initial conditions are $u(x,0) = f(x)$ and $\partial u/\partial t(x,0) = g(x)$.

Let $k_n = \pi n/L'$ be the wave number of the nth mode in the Fourier series expansion. Expand

$$f(x) = \sum_{n=1}^{\infty} 2b_n \sin(k_n x) \tag{7.42}$$

and

$$g(x) = \sum_{n=1}^{\infty} 2\dot{b}_n \sin(k_n x). \tag{7.43}$$

Then the solution is in the form

$$u(x,t) = \sum_{n=1}^{\infty} 2b_n(t) \sin(k_n x). \tag{7.44}$$

The choice of the sine expansion is appropriate to the boundary conditions at the end points. For later use, we note that the integral of $g(x)$ is given by a cosine expansion

$$G(x) = -\sum_{n=1}^{\infty} 2\dot{b}_n \frac{1}{k_n} \cos(k_n x). \tag{7.45}$$

The partial differential equation says that

$$\frac{d^2 b_n(t)}{dt^2} = -c^2 k_n^2 b_n(t). \tag{7.46}$$

Let $\omega_n = ck_n$. The solution is

$$b_n(t) = \cos(\omega_n t) b_n + \frac{1}{\omega_n} \sin(\omega_n t) \dot{b}_n. \tag{7.47}$$

Thus the solution is

$$u(x,t) = \sum_{n=1}^{\infty} [2b_n \cos(\omega_n t) + 2\dot{b}_n \frac{1}{\omega_n} \sin(\omega_n t)] \sin(k_n x). \tag{7.48}$$

In the Fourier analysis of the wave equation we see that the high wave number in space corresponds to high frequency in time. The term in the solution that has wave number $k = \pi n/L'$ has angular frequency

$$\omega = ck. \tag{7.49}$$

Rapid spatial variation translates into rapid time variation.

We can use the product identities to write the solution in a form with a more geometrical interpretation. We obtain

$$u(x,t) = \sum_{n=1}^{\infty} b_n(\sin(k_n(x+ct))+\sin(k_n(x-ct)))+\sum_{n=1}^{\infty} \dot{b}_n \frac{1}{ck_n}(\cos(k_n(x-ct))-\cos(k_n(x+ct)). \tag{7.50}$$

Extend f and g to be odd functions that are periodic of period $2L'$. Then this may be summed to obtain

$$u(x,t) = \frac{1}{2}(f(x+ct) + f(x-ct)) + \frac{1}{2c}(G(x+ct) - G(x-ct)). \tag{7.51}$$

Here $G'(x) = g(x)$. This is just the d'Alembert solution with the initial condition taken to be these periodic extensions.

The solution consists of waves that travel back and forth in the interval from 0 to L', reflecting off the boundary points with a sign change. This way of representing the solution shows that these reflections are equivalent to appropriate waves travelling freely in the infinite space interval that arrive from outside the interval in just such a way as to simulate these reflections.

7.6 The heat equation

Consider the boundary value problem for the heat equation on the interval from 0 to L' where the temperature is held fixed at the two end points. The equation is

$$\frac{\partial u}{\partial t} = \frac{\sigma^2}{2} \frac{\partial^2 u}{\partial x^2} \tag{7.52}$$

for $0 \le x \le L'$. The boundary conditions are $u(0,t) = a$ and $u(L',t) = b$, and the initial condition is $u(x,0) = f(x)$.

If we can solve the equation for the case when $a = b = 0$, then we can solve it in general, just by adding the function $a(1 - x/L') + bx/L'$. So we may as well restrict ourself to this case. This is the Dirichlet boundary equation.

Again the natural course is expand the initial condition in a Fourier sine series. The reason for the choice of the sine function is that it is an eigenfunction of the second differentiation operator with the given boundary conditions. Thus

$$\frac{\partial^2}{\partial x^2} \sin(k_n x) = -k_n^2 \sin(k_n x). \tag{7.53}$$

The choice $k_n = n\pi/L'$ satisfies the boundary conditions. The eigenvalue corresponding to the eigenfunction of wave number k_n is equal to $-k_n^2$.

Thus we use

$$f(x) = \sum_{n=1}^{\infty} 2b_n \sin(k_n x). \tag{7.54}$$

The reason this is useful is that the solution may be represented in the form

$$u(x,t) = \sum_{n=1}^{\infty} 2b_n(t) \sin(k_n x). \tag{7.55}$$

This is because the partial differential equation says that

$$\frac{db_n(t)}{dt} = -\frac{\sigma^2}{2} k_n^2 b_n(t) = -\lambda_n b_n(t), \tag{7.56}$$

where $\lambda_n = (\sigma^2/2)k_n^2$. This has solution

$$b_n(t) = \exp(-\lambda_n t) b_n. \tag{7.57}$$

Thus the solution is

$$u(x,t) = \sum_{n=1}^{\infty} 2 \exp(-\lambda_n t) b_n \sin(k_n x). \tag{7.58}$$

This solution is important because it displays a number of essential features of the problem. The most important thing to notice is that all the coefficients approach zero rapidly with t. This says that heat is flowing so as to bring the system in equilibrium with its environment. Furthermore, the higher the frequency, the smaller the coefficient. This says that the high frequencies get damped out, and the solution becomes more and more smooth. There is no problem with the convergence of this series when $t > 0$. The explicit formula for the damping rate as a function of wave number $k = \pi n/L'$ is

$$\lambda = \frac{\sigma^2}{2} k^2 \tag{7.59}$$

Thus the mode with wave number k decays according to an exponential law $\exp(-\lambda t)$.

This formula is particularly useful for t large, since in that case relatively few terms of the Fourier series are needed to give accurate results. There is another way of writing this formula that gives accurate results for small t. In order to obtain this formula, we need the calculation of an integral, the integral that gives the Fourier transform $\hat{g}(k,t)$ of the Gaussian

$$g(x,t) = \frac{1}{\sqrt{2\pi\sigma^2 t}} \exp(-\frac{x^2}{\sigma^2 t}). \tag{7.60}$$

This is

$$\hat{g}(k,t) = \int_{-\infty}^{\infty} g(z,t)\cos(kz)\,dz = \exp(-\frac{\sigma^2 t}{2}k^2). \tag{7.61}$$

This integral can be calculated by solving the ordinary differential equation for $\hat{g}(k,t)$ as a function of k. This ordinary differential equation may be derived by differentiating the integral expression for $\hat{g}(k,t)$ with respect to k and then using integration by parts to express the result again in terms of $\hat{g}(k,t)$.

For the present application we take $k = \pi n/L'$. We insert the formula in the solution and get

$$u(x,t) = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} g(z,t)\cos(k_n z)2b_n \sin(k_n x)\,dz. \tag{7.62}$$

Next we use the product formulas and the fact that $g(z)$ is even to write this as

$$u(x,t) = \sum_{n=1}^{\infty} \int_{-\infty}^{\infty} g(z,t)2b_n \sin(k_n(x-z))\,dz. \tag{7.63}$$

This can be resummed to get

$$u(x,t) = \int_{-\infty}^{\infty} g(z,t)f(x-z)\,dz = \int_{-\infty}^{\infty} g(x-w,t)f(w)\,dw. \tag{7.64}$$

Here f is extended to be odd and periodic with period $2L'$.

It is also revealing to write this answer in terms of the original f on the interval from 0 to L'. This expression is

$$u(x,t) = \int_0^{L'} \sum_m [g(x-w+2mL') - g(x+w+2mL')]f(w)\,dw. \tag{7.65}$$

This solutions shows that the temperature evolution in the interval from 0 to L' satisfying the boundary condition is equivalent to a temperature evolution in the entire infinite interval with appropriate initial conditions that maintain the boundary conditions.

7.7 Problems

1. Consider a periodic function with period 2π. Expand it using complex Fourier coefficients. The theorem that a continuous periodic function is determined by its Fourier coefficients may be proved in this context. It says that

$$f(\theta) = \lim_{r \to 1} \sum_{n=-\infty}^{\infty} c_n r^{|n|} e^{in\theta}. \tag{7.66}$$

Here $r < 1$ so that the series converges. If $\sum_n |c_n| < \infty$, then we can take the limit and get

$$f(\theta) = \sum_{n=-\infty}^{\infty} c_n e^{in\theta}. \tag{7.67}$$

The proof is much simpler, since the series that needs to be summed to get the Poisson kernel is a geometric series. Carry out this proof in detail.

Hint: Start with the expression

$$\sum_{n=-\infty}^{\infty} c_n r^{|n|} e^{in\theta} = \sum_{n=-\infty}^{\infty} \frac{1}{2\pi} \int_0^{2\pi} r^{|n|} e^{in(\theta-\phi)} f(\phi)\, d\phi, \tag{7.68}$$

interchange sum and integral, and sum the appropriate geometric series.

2. Consider the boundary value problem for the heat equation, but with the insulating boundary conditions $\partial u/\partial x(0,t) = 0$ and $\partial u/\partial x(L',t) = 0$. These boundary conditions are the Neumann boundary conditions. Find the solution using the Fourier cosine series. Find the limit of the solution as t approaches infinity. In this case, unlike in the case of Dirichlet boundary conditions, the final distribution of temperature depends on the initial condition. Describe this dependence explicitly.

Chapter 8

Fourier transforms

8.1 The Fourier transform

The Fourier transform representation is

$$f(x) = 2\int_0^\infty [a(k)\cos(kx) + b(k)\sin(kx)]\,\frac{dk}{2\pi}. \tag{8.1}$$

The coefficients in the Fourier transform are defined for $k \geq 0$ by

$$a(k) = \int_{-\infty}^{\infty} \cos(ky) f(y)\,dy \tag{8.2}$$

and

$$b(k) = \int_{-\infty}^{\infty} \sin(ky) f(y)\,dy \tag{8.3}$$

The difference from Fourier series is that the functions are not periodic but extend over all x. The frequencies then are continuous, so the representation involves an integral over frequencies rather than a sum.

If f is an even function, then we have as a special case

$$f(x) = \int_0^\infty \cos(kx) a(k)\,\frac{dk}{\pi}. \tag{8.4}$$

where the cosine transform is

$$a(k) = 2\int_0^\infty \cos(ky) f(y)\,dy. \tag{8.5}$$

If f is an odd function, then we have as a special case

$$f(x) = \int_0^\infty \sin(kx) b(k)\,\frac{dk}{\pi}. \tag{8.6}$$

where the sine transform is

$$b(k) = 2 \int_0^\infty \sin(ky) f(y)\, dy. \tag{8.7}$$

We can take these to be the definitions of the cosine and sine transforms for functions defined on the half-line. These definitions of cosine and sine transforms differ from the most common definition. They amount to defining the transform to be related to the ordinary Fourier transform of the even or odd extension. However they have the advantage that the tables for transforms are the same in all cases.

There is also a complex form of the Fourier transform. The Fourier transform representation is

$$f(x) = \int_{-\infty}^\infty e^{ikx} \hat{f}(k)\, \frac{dk}{2\pi}. \tag{8.8}$$

The Fourier transform is defined by

$$\hat{f}(k) = \int_{-\infty}^\infty e^{-iky} f(y)\, dy. \tag{8.9}$$

For $k \geq 0$ we can write $\hat{f}(k) = a(k) - ib(k)$ and $\hat{f}(-k) = a(k) + ib(k)$. Then this gives the relation between the complex form and the real form. The complex form is more convenient to use. However one must keep in mind that complex exponentials are just a way of talking about sines and cosines.

The following theorem is the fundamental result about Fourier transforms.

Theorem 8.1 *Consider an integrable function f and its Fourier transform $\hat{f}$ defined by*

$$\hat{f}(k) = \int_{-\infty}^\infty e^{-iky} f(y)\, dy. \tag{8.10}$$

Then the function may be recovered from the Fourier transform. In fact,

$$f(x) = \lim_{\epsilon \to 0} \int_{-\infty}^\infty e^{ikx} \hat{f}(k) e^{-\epsilon|k|}\, \frac{dk}{2\pi}. \tag{8.11}$$

If $\hat{f}$ is also integrable, then

$$f(x) = \int_{-\infty}^\infty e^{ikx} \hat{f}(k)\, \frac{dk}{2\pi}. \tag{8.12}$$

Proof: It is straightforward to compute that for each $\epsilon > 0$ we have

$$\int_{-\infty}^\infty e^{ikx} \hat{f}(k) e^{-\epsilon|k|}\, \frac{dk}{2\pi} = \int_{-\infty}^\infty \delta_\epsilon(y - x) f(y)\, dy, \tag{8.13}$$

where

$$\delta_\epsilon(y) = \frac{1}{\pi} \frac{\epsilon}{y^2 + \epsilon^2}. \tag{8.14}$$

However this is easily seen directly to be an approximate delta function. So the limit as $\epsilon \to 0$ is $f(x)$.

Here are some famous Fourier transforms. Let $H(x)$ be the function that is 1 for $x > 0$ and 0 for $x < 0$. Then the Fourier transform of $H(x)e^{-\epsilon x}$ is

$$\int_0^\infty e^{-ikx} e^{-\epsilon x}\, dx = -i\frac{1}{k - i\epsilon}. \tag{8.15}$$

The function $H(-x)e^{\epsilon x}$ is obtained by reflecting about the origin on the x axis. Therefore its Fourier transform is obtained by reflecting about the origin of the k axis. Therefore it is

$$\int_{-\infty}^0 e^{-ikx} e^{\epsilon x}\, dx = i\frac{1}{k + i\epsilon}. \tag{8.16}$$

It easily follows that the Fourier transform of the sum and difference are

$$\int_{-\infty}^\infty e^{-ikx} e^{-\epsilon|x|}\, dx = \frac{2\epsilon}{k^2 + \epsilon^2} \tag{8.17}$$

and

$$\int_{-\infty}^\infty e^{-ikx} \mathrm{sign}(x) e^{-\epsilon|x|}\, dx = -2i\frac{k}{k^2 + \epsilon^2}. \tag{8.18}$$

If a function $f(x)$ has Fourier transform $g(k)$, then the function $g(x)$ has Fourier transform $2\pi f(-k)$. From this we see that

$$\int_{-\infty}^\infty e^{-ikx} \frac{1}{x - i\epsilon}\, dx = 2\pi i H(-k) e^{\epsilon k} \tag{8.19}$$

and

$$\int_{-\infty}^\infty e^{-ikx} \frac{1}{x + i\epsilon}\, dx = -2\pi i H(k) e^{-\epsilon k} \tag{8.20}$$

Similarly,

$$\int_{-\infty}^\infty e^{-ikx} \frac{1}{\pi} \frac{\epsilon}{x^2 + \epsilon^2}\, dx = e^{-\epsilon|k|} \tag{8.21}$$

and

$$\int_{-\infty}^\infty e^{-ikx} \frac{x}{x^2 + \epsilon^2}\, dx = -\pi i \mathrm{sign}(k) e^{-\epsilon|k|} \tag{8.22}$$

These last two have interesting limits. If we let ϵ tend to zero, we see that the Fourier transform of $\delta(x)$ is 1. The Fourier transform of the principal value $1/x$ is $-\pi i \mathrm{sign}(k)$.

Another famous Fourier transform is the Fourier transform of the Gaussian kernel

$$g(x,t) = \frac{1}{\sqrt{2\pi\sigma^2 t}} \exp(-\frac{x^2}{2\sigma^2 t}). \tag{8.23}$$

This was computed in the previous chapter. The result is that

$$\hat{g}(k,t) = \exp(-\frac{\sigma^2 t k^2}{2}). \tag{8.24}$$

A particularly simple Fourier transform is that of the approximate delta function that is $\delta_\epsilon(x) = 1/(2\epsilon)$ for $|x| \le \epsilon$ and zero otherwise. The result is that $\hat{\delta}_\epsilon(k) = \sin(\epsilon k)/(\epsilon k)$.

Of course, for each of these Fourier transforms there is a corresponding inverse Fourier transform relation. Furthermore, the smoother the function, the less high frequencies in the representation. Take for example the various approximate delta functions.

For the Gaussian we have

$$g(x,t) = \int_{-\infty}^{\infty} e^{ikx} e^{-\frac{\sigma^2 t k^2}{2}} \frac{dk}{2\pi}. \tag{8.25}$$

The Gaussian is very smooth, and its Fourier transform goes to zero very rapidly at high frequency.

For the Cauchy distribution we have

$$\frac{1}{\pi}\frac{\epsilon}{x^2+\epsilon^2} = \int_{-\infty}^{\infty} e^{ikx} e^{-\epsilon|k|} \frac{dk}{2\pi}. \tag{8.26}$$

Again this is smooth, and high frequencies make a small contribution.

For the two-sided exponential we have

$$\frac{1}{2\epsilon} e^{-\frac{|x|}{\epsilon}} = \int_{-\infty}^{\infty} e^{ikx} \frac{1}{1+\epsilon^2 k^2} \frac{dk}{2\pi}. \tag{8.27}$$

This function has a slope discontinuity at the origin. In order to synthesize it from cosines, it is necessary to employ relatively high frequencies. Thus the Fourier transform only has quadratic decay at infinity.

For the step function $\delta_\epsilon(x)$, equal to $1/(2\epsilon)$ for $|x| \le \epsilon$ and zero otherwise, the Fourier representation is

$$\delta_\epsilon(x) = \int_{-\infty}^{\infty} e^{ikx} \frac{\sin(\epsilon k)}{\epsilon k} \frac{dk}{2\pi}. \tag{8.28}$$

Since this function is discontinuous, it needs lots of high frequencies. The Fourier transform only decays like the first power of k.

In each case the limit is the delta function with Fourier transform 1. The delta function is so discontinuous that its Fourier transform requires all frequencies weighted equally.

The principal utility of the Fourier transform is due to the fact that it transforms shifts into multiples. Thus the Fourier transform of $f(x-a)$ is $e^{-iak}\hat{f}(k)$. Thus

$$f(x-a) = \int_{-\infty}^{\infty} e^{ikx} e^{-ika} \hat{f}(k) \frac{dk}{2\pi}. \tag{8.29}$$

This contains the formula for the Fourier transform of a derivative as a limiting case. If we consider $(f(x+a)-f(x))/a$ and take the limit, then we get that the Fourier transform of $df(x)/dx$ is $ik\hat{f}(k)$. Thus

$$\frac{d}{dx}f(x) = \int_{-\infty}^{\infty} e^{ikx} ik\hat{f}(k)\,\frac{dk}{2\pi}. \tag{8.30}$$

Of course this formula can also be seen directly. It should be noted that the role of multiplication by i can be seen by writing the exponential in terms of trigonometric functions by $\exp(ikx) = \cos(kx) + i\sin(kx)$. Then $ik\exp(ikx) = -k\sin(kx) + ik\cos(kx)$. This is of course just a summary of the usual results of differentiating sines and cosines.

The second derivative is given by doing this twice, so the effect on the frequency is multiplication by $-k^2$. Thus

$$\frac{d^2}{dx^2}f(x) = \int_{-\infty}^{\infty} e^{ikx}(-k^2)\hat{f}(k)\,\frac{dk}{2\pi}. \tag{8.31}$$

Another consequence of the shift relation is seen by taking a weighted integral of the amount of shift. A consequence is that the Fourier transform of the convolution $f * g$ is multiplication of the Fourier transforms. Recall that the convolution of two functions is

$$(f*g)(x) = \int_{-\infty}^{\infty} f(x-a)g(a)\,da. \tag{8.32}$$

Thus we can always represent a convolution as

$$(f*g)(x) = \int_{-\infty}^{\infty} e^{ikx}\hat{f}(k)\hat{g}(k)\,\frac{dk}{2\pi}. \tag{8.33}$$

8.2 The Poisson summation formula

The Poisson summation formula gives a way of using the Fourier transform to sum a Fourier series. It produces a periodic function with period L whose Fourier coefficients are the values of the Fourier transform at the discrete frequencies $2\pi n/L$.

Theorem 8.2 *Let f be a function with Fourier transform $\hat{f}$. Then*

$$\sum_m f(x+mL) = \frac{1}{L}\sum_k \hat{f}(k)e^{ikx}, \tag{8.34}$$

where the sum on the left is over integer m, and the sum on the right is over $k = 2\pi n/L$ with integer n.

The proof of the theorem is just to compute the Fourier coefficient of the periodic function on the left. This is

$$c_n = \frac{1}{L}\int_0^L \sum_m f(x+mL)e^{-ikx}\,dx = \frac{1}{L}\int_{-\infty}^{\infty} f(y)e^{-iky}\,dy. \tag{8.35}$$

The theorem can be used to sum a Fourier series $\sum_n c_n e^{2\pi i n x/L}$. All that one has to do is to find a known Fourier transform $\hat{f}$ such that $c_n = \hat{f}(2\pi n/L)$. Then the Poisson summation formula gives an explicit construction of a periodic function with the given series as its sum.

An example is given by the Fourier series $\sum_n \exp(-\lambda_n t)e^{ik_n t}$ that comes up in the solution of the heat equation on a periodic interval of length L. Here $k_n = 2\pi n/L$ and $\lambda_n = (\sigma^2/2)k_n^2$. We recognize the Fourier coefficients as the values of $\hat{g}(k,t)$ at the values k_n where $g(x,t)$ is the Gaussian. Hence the sum of the series is $\sum_m g(x+mL,t)L$. Let c_n be the Fourier coefficients of the initial function f, so that $c_n = \int_0^{2\pi} e^{-iky} f(y)\,dy$. Then the solution of the initial value problem is

$$\sum_n c_n \exp(-\lambda_n t)e^{ik_n t} = \int_0^{2\pi} \sum_m g(x-y+mL,t)f(y)\,dy. \tag{8.36}$$

8.3 The heat equation

Consider the heat equation

$$\frac{\partial u}{\partial t} = \frac{\sigma^2}{2}\frac{\partial^2 u}{\partial x^2} \tag{8.37}$$

for all real x. The initial condition is $u(x,0) = f(x)$.

Take the Fourier transform. This gives

$$\frac{d\hat{u}(k,t)}{dt} = \frac{\sigma^2}{2}(-k^2)\hat{u}(k,t) \tag{8.38}$$

with initial condition $\hat{u}(k,0) = \hat{f}(k)$. The solution is

$$\hat{u}(k,t) = \exp(-\frac{\sigma^2}{2}k^2 t)\hat{f}(k). \tag{8.39}$$

This is the product of two functions of k. The time dependent factor deemphasizes the high frequencies, so the solution is expected to be very smooth. Indeed, the inverse transform is a convolution.

$$u(x,t) = \int_{-\infty}^{\infty} g(x-a,t)f(a)\,da, \tag{8.40}$$

where $g(x,t)$ is the Gaussian kernel.

8.4 The wave equation

Consider the wave equation on the infinite interval.

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}. \tag{8.41}$$

The initial conditions are $u(x,0) = f(x)$ and $\partial u/\partial t(x,0) = g(x)$.

Expand

$$f(x) = \int_{-\infty}^{\infty} e^{ikx} \hat{f}(k) \, \frac{dk}{2\pi} \tag{8.42}$$

and

$$g(x) = \int_{-\infty}^{\infty} e^{ikx} \hat{g}(k) \, \frac{dk}{2\pi}. \tag{8.43}$$

Then the solution is in the form

$$u(x,t) = \int_{-\infty}^{\infty} e^{ikx} \hat{u}(k,t) \, \frac{dk}{2\pi}. \tag{8.44}$$

The partial differential equation says that

$$\frac{d^2 \hat{u}(k,t)}{dt^2} = -c^2 k^2 \hat{u}(k,t). \tag{8.45}$$

This has solution

$$\hat{u}(k,t) = \cos(ckt)\hat{f}(k) + \frac{1}{ck} \sin(ckt)\hat{g}(k). \tag{8.46}$$

Thus the solution is

$$u(x,t) = \int_{-\infty}^{\infty} e^{ikx} \cos(ckt)\hat{f}(k) \, \frac{dk}{2\pi} + \int_{-\infty}^{\infty} e^{ikx} \frac{\sin(ckt)}{ck} \hat{g}(k) \, \frac{dk}{2\pi}. \tag{8.47}$$

These inverse transforms are easy to calculate. The first integral is immediate. Since $\cos(ckt) = (e^{ickt} + e^{-ickt})/2$, we need only calculate the effect of multiplying a Fourier transform by a complex exponential. However this we know to be a shift on the original function f. The second integral is also not difficult. We recall that the Fourier transform of the approximate delta function $\delta_\epsilon(x)$ is

$$\frac{1}{2\epsilon} \int_{-\epsilon}^{\epsilon} \exp(-ikx) \, dx = \frac{\sin(\epsilon k)}{\epsilon k}. \tag{8.48}$$

Thus the Fourier transform of $t\delta_{ct}(x)$ is $\sin(ctk)/(ck)$. The second term is the convolution of $t\delta_{ct}$ with g. The final answer is

$$u(x,t) = \frac{1}{2}(f(x+ct) + f(x-ct)) + \frac{1}{2c} \int_{|x-y| \le ct} g(y) \, dy. \tag{8.49}$$

This is the d'Alembert solution again.

8.5 The Laplace transform

The Laplace transform of $f(t)$ is a function of a complex variable $s = c + i\omega$ where $c > 0$ is taken sufficiently large. It is the same as the Fourier transform of the function $H(t)\exp(-ct)f(t)$ evaluated at ω.

Thus we have the definition

$$f^L(s) = \int_0^\infty e^{-st} f(t)\, dt \tag{8.50}$$

and the inversion formula

$$f(t) = \frac{1}{2\pi}\int_{-\infty}^\infty e^{(c+i\omega)t} f^L(c + i\omega)\, d\omega. \tag{8.51}$$

We can write also write this in real form. Thus we can define

$$a(\omega) = \int_0^\infty e^{-ct}\cos(\omega t) f(t)\, dt \tag{8.52}$$

and

$$b(\omega) = \int_0^\infty e^{-ct}\sin(\omega t) f(t)\, dt. \tag{8.53}$$

Then

$$f(t) = \frac{1}{\pi}\int_0^\infty e^{ct}[a(\omega)\cos(\omega t) + b(\omega)\sin(\omega t)]\, d\omega. \tag{8.54}$$

From this we see that the Laplace transform is also a representation in terms of oscillatory functions; however they only are used to represent the function for $t \geq 0$. This allows the introduction of the exponential damping factor e^{-ct} for large $c > 0$.

The Laplace transform is most often used for problems involving time. In such problems the initial value problem is more common than the boundary value problem, and the Laplace transform is the proper tool for this situation. The operators in question tend to be somewhat different. The reason is that the functions are defined only for $t \geq 0$. Since this is a boundary point, something needs to be done to define shifts when the boundary is involved.

It is easy to use integration by parts to see that

$$f'^L(s) = sf^L(s) - f(0). \tag{8.55}$$

However it is revealing to look at this result as a consequence of relations involving shifts.

The forward shifted function $H(t-a)f(t-a)$ for $a \geq 0$ has Laplace transform $e^{-sa}f^L(s)$. This is a nice simple result. However if we use this forward shift to compute the derivative, then we have

$$\frac{H(t-a)f(t-a) - f(t)}{-a} = \frac{f(t-a) - f(t)}{-a} + \frac{1 - H(t-a)}{a} f(t-a). \tag{8.56}$$

The second term on the right involves an approximate delta function. Thus when we take Laplace transforms and then take the limit as $a \to 0$, we see that s times the Laplace transform of f is the Laplace transform of f' plus $f(0)$.

The backward shifted and truncated function $f(t+a)$ for $a \geq 0$ has Laplace transform $e^{sa}[f^L(s) - \int_0^a f(t)\,dt]$. The extra term is significant. If we take the limit as $a \to 0$ of the Laplace transform of $(f(t+a) - f(t))/a$, then we get $sf^L(s) - f(0)$ which is the Laplace transform of f'.

We get the same result using the forward shift or the backward shift, though for somewhat different reasons. It is the forward shift that has the simple Laplace transform, while it is the backward shift that gives the derivative without any correction.

The result extends to the second derivative in a routine way. If we take the Laplace transform of $f''(t)$ we get $s[sf^L(s) - f(0)] - f'(0)]$. This may also be written as $s^2 f^L(s) - sf(0) - f'(0)$.

If we weight the forward shift appropriately, then we get a forward or causal convolution. This is

$$(f * g)(t) = \int_0^\infty H(t-a)f(t-a)g(a)\,da = \int_0^t f(t-a)g(a)\,da. \tag{8.57}$$

For this case, the Laplace transform of the convolution is the product of the Laplace transforms of the individual functions.

Here is a comparison of the Laplace and Fourier transform methods on a simple example. Consider the equation

$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \tag{8.58}$$

with initial condition $u(x,0) = f(x)$.

The Fourier transform of this equation is

$$\frac{d\hat{u}(k,t)}{dt} + iak\hat{u}(k,t) = 0. \tag{8.59}$$

The solution is

$$\hat{u}(k,t) = e^{-iakt}\hat{f}(k). \tag{8.60}$$

Thus the solution is given by a shift $u(x,t) = f(x-at)$.

The Laplace transform of the same equation is

$$su^L(x,s) - f(x) + a\frac{du^L(x,s)}{dx} = 0. \tag{8.61}$$

This is an inhomogeneous equation that may be solved by introducing the integrating factor $\exp(sx/a)$. The general solution is

$$u^L(x,s) = \frac{1}{a}\int_{-\infty}^x \exp(-s(x-y)/a)f(y)\,dy + C(s)\exp(-sx/a). \tag{8.62}$$

The first term is the convolution of $H(x)\exp(-sx/a)$ with $f(x)$. If we take these both to be integrable functions, then the convolution is also integrable.

The second term grows exponentially, so it is tempting to take the constant of integration to be zero. If we do this, we see that

$$u^L(x,s) = \int_0^\infty e^{-st} f(x-at)\,dt. \tag{8.63}$$

We recover the same solution.

8.6 Problems

1. Write out the details of the calculation in the proof of the inversion theorem for the Fourier transform. That is, show that if the frequency integral is weighted by $e^{-\epsilon|k|}$, then the original function is convolved with an approximate delta function.

2. Consider the equation
$$\frac{\partial u}{\partial t} + a\frac{\partial u}{\partial x} = 0 \tag{8.64}$$
with initial condition $u(x,0) = f(x)$. Write the equation for the function $\hat{u}^L(k,s)$ obtained by taking both the Fourier and the Laplace transform. Solve this equation. Then find $u(x,t)$ by inverting the Laplace transform and then the Fourier transform.

Chapter 9

Gradient and divergence

9.1 Multi-dimensional geometry

The natural operations for multi-variable calculus are the gradient and divergence. We consider a *orthogonal coordinate system* $u_1, \ldots, u_n$, where the curves of constant coordinate values are orthogonal at each point. At each point, let $\mathbf{e}_1, \ldots, \mathbf{e}_n$ be the unit vectors in the coordinate directions. Let $h_1\,du_1, \ldots, h_n\,du_n$ be the differentials in the coordinate directions for computing lengths. Then the gradient of a function f in the ith direction is $(1/h_i)\partial f/\partial u_i$.

The general definition of the gradient of a function is

$$\nabla f = \mathbf{e}_1 \frac{1}{h_1}\frac{\partial f}{\partial u_1} + \cdots \mathbf{e}_n \frac{1}{h_n}\frac{\partial f}{\partial u_n}. \tag{9.1}$$

This is a vector field.

Example: In two-dimensional Cartesian coordinates the gradient is

$$\nabla f = \mathbf{e}_x \frac{\partial}{\partial x} f + \mathbf{e}_y \frac{\partial}{\partial y} f. \tag{9.2}$$

Example: In polar coordinates r, θ the differentials giving length are dr and $r\,d\theta$. So the gradient is

$$\nabla f = \mathbf{e}_r \frac{\partial}{\partial r} f + \mathbf{e}_\theta \frac{1}{r}\frac{\partial}{\partial \theta} f. \tag{9.3}$$

Example: In three-dimensional Cartesian coordinates the gradient is

$$\nabla f = \mathbf{e}_x \frac{\partial}{\partial x} f + \mathbf{e}_y \frac{\partial}{\partial y} f + \mathbf{e}_z \frac{\partial}{\partial z} f. \tag{9.4}$$

Example: One of the most useful cases is that of spherical polar coordinates in three dimensions. In this case we follow the convention that the co-latitude is θ and the longitude is ϕ. The reader should be warned that the opposite convention is also used in many places. In any case, the conversion from Cartesian

coordinates is $z = r\cos\theta$, $x = r\cos\phi\sin\theta$, $y = r\sin\phi\sin\theta$. The three length elements are dr, $r\,d\theta$, and $r\sin\theta\,d\phi$. The $\sin\theta$ in the last expression is due to the fact that near a pole even a large change in longitude does not translate into a great distance. The factors in the gradient thus 1, $1/r$, and $1/(r\sin\theta)$. The gradient is

$$\nabla f = \mathbf{e}_r \frac{\partial}{\partial r} f + \mathbf{e}_\theta \frac{1}{r} \frac{\partial}{\partial \theta} f + \mathbf{e}_\phi \frac{1}{r\sin\theta} \frac{\partial}{\partial \phi} f. \tag{9.5}$$

Let $w = h_1 \cdots h_n$, so that

$$dV = h_1\,du_1 \cdots h_n\,du_n = w\,du_1\,\cdots\,du_n \tag{9.6}$$

is the area or volume element. Thus in two dimensions the area element is $dV = dx\,dy = r\,dr\,d\theta$. In three dimesions the volume element is $dV = dx\,dy\,dz = r^2\sin(\theta)\,dr\,d\theta\,d\phi$.

We want to define the divergence $\nabla \cdot \mathbf{v}$ of a vector field

$$\mathbf{v} = v_1\mathbf{e}_1 + \cdots v_n\mathbf{e}_n \tag{9.7}$$

in such a way that the integration by parts formula

$$\int_R f \nabla\cdot\mathbf{v}\,dV = -\int_R \nabla f\cdot\mathbf{v}\,dV \tag{9.8}$$

is true whenever f vanishes at the boundary of the region. The resulting definition of the divergence of a vector field is

$$\nabla\cdot\mathbf{v} = \frac{1}{w}\frac{\partial}{\partial u_1}(\frac{1}{h_1} w\,v_1) + \cdots + \frac{1}{w}\frac{\partial}{\partial u_n}(\frac{1}{h_n} w\,v_n). \tag{9.9}$$

This is a scalar.

Example: In Cartesian coordinates the divergence is given by

$$\nabla\cdot\mathbf{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y}. \tag{9.10}$$

Example: In polar coordinates $w = r$. So the divergence is given by

$$\nabla\cdot\mathbf{v} = \frac{1}{r}\frac{\partial r v_r}{\partial r} + \frac{1}{r}\frac{\partial v_\theta}{\partial \theta}. \tag{9.11}$$

Example: In three dimensional Cartesian coordinates the divergence is given by

$$\nabla\cdot\mathbf{v} = \frac{\partial v_x}{\partial x} + \frac{\partial v_y}{\partial y} + \frac{\partial v_z}{\partial z}. \tag{9.12}$$

Example: In spherical polar coordinates the factor in the volume element is $w = r^2\sin\theta$. The divergence of a vector field is

$$\nabla\cdot\mathbf{v} = \frac{1}{r^2}\frac{\partial}{\partial r}(r^2 v_r) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\theta}(\sin\theta v_\theta) + \frac{1}{r\sin\theta}\frac{\partial}{\partial\phi} v_\phi. \tag{9.13}$$

The following two theorems are the key properties of the divergence. The first is the product rule for differentiating.

Theorem 9.1 *The divergence of a product is given by*

$$\nabla \cdot (f\mathbf{v}) = \nabla f \cdot \mathbf{v} + f \nabla \cdot \mathbf{v}. \tag{9.14}$$

The other result is the divergence theorem.

Theorem 9.2

$$\int_R \nabla \cdot \mathbf{v} \, dV = \int_{\partial R} \mathbf{v} \cdot d\mathbf{A}. \tag{9.15}$$

Here R is a region and ∂R is its boundary. Also, we write the normal surface area element as

$$d\mathbf{A} = \sum_i \mathbf{e}_i \, (-1)^{(n-1)(i-1)} \frac{1}{h_i} w \, du_{i+1} \cdots du_n \, du_1 \cdots du_{i-1}. \tag{9.16}$$

The most important cases of the theorem are $n = 2$ and $n = 3$. For $n = 2$ the normal boundary length element is

$$d\mathbf{A} = \mathbf{e}_1 h_2 \, du_2 - \mathbf{e}_2 h_1 \, du_1. \tag{9.17}$$

For $n = 3$ the normal surface area element is

$$d\mathbf{A} = \mathbf{e}_1 h_2 \, du_2 \, h_3 \, du_3 + \mathbf{e}_2 h_3 \, du_3 \, h_1 \, du_1 + \mathbf{e}_3 h_1 \, du_1 \, h_2 \, du_2. \tag{9.18}$$

Consequently, for $n = 2$ the divergence theorem is

$$\int_R \nabla \cdot \mathbf{v} \, w \, du_1 \, du_2 = \int_{\partial R} v_1 \, h_2 \, du_2 - v_2 \, h_1 \, du_1, \tag{9.19}$$

where $w = h_1 h_2$. For $n = 3$ the divergence theorem is

$$\int_R \nabla \cdot \mathbf{v} \, w \, du_1 \, du_2 \, du_3 = \int_{\partial R} v_1 \, h_2 \, du_2 \, h_3 \, du_3 + v_2 \, h_3 \, du_3 \, h_1 \, du_1 + v_3 \, h_1 \, du_1 \, h_2 \, du_2, \tag{9.20}$$

where $w = h_1 h_2 h_3$.

Example: The divergence theorem in two dimensions in Cartesian coordinates says that

$$\int_R \nabla \cdot \mathbf{v} \, dx \, dy = \int_{\partial R} v_x \, dy - v_y \, dx. \tag{9.21}$$

Example: The divergence theorem in two dimensions in polar coordinates is

$$\int_R \nabla \cdot \mathbf{v} \, r \, dr \, d\theta = \int_{\partial R} v_r \, r \, d\theta - v_\theta \, dr. \tag{9.22}$$

Example: The divergence theorem in three dimensions using Cartesian coordinates is

$$\int_R \nabla \cdot \mathbf{v} \, dx \, dy \, dz = \int_{\partial R} v_x \, dy \, dz + v_y \, dz \, dx + v_z \, dx \, dy. \tag{9.23}$$

Example: The divergence theorem in three dimensions using spherical polar coordinates is

$$\int_R \nabla \cdot \mathbf{v}\, r^2 \sin(\theta)\, dr\, d\theta\, d\phi = \int_{\partial R} v_r\, r^2 \sin(\theta)\, d\theta\, d\phi + v_\theta\, r \sin(\theta)\, d\phi\, dr + v_\phi\, r\, dr\, d\theta. \tag{9.24}$$

The divergence theorem as stated here uses heavily the notions of length and area and volume. However it may be proved by using a result that is completely independent of these notions. Let $\alpha_i = (1/h_i) w v_i$. Then the divergence theorem takes the form

$$\int_R \sum_i \frac{\partial \alpha_i}{\partial u_i}\, du_1 \cdots du_n = \int_{\partial R} \sum_i \alpha_i\, (-1)^{(n-1)(i-1)}\, du_{i+1} \cdots du_n\, du_1 \cdots du_{i-1}. \tag{9.25}$$

This is a generalization of the fundamental theorem of calculus.

The preceding two theorems give an important *integration by parts* formula.

Theorem 9.3

$$\int_R f \nabla \cdot \mathbf{v}\, dV + \int_R \nabla f \cdot \mathbf{v}\, dV = \int_{\partial R} f \mathbf{v} \cdot d\mathbf{A}. \tag{9.26}$$

This theorem is the key to many results about partial differential equations.

The *Laplace operator* is defined by taking the divergence of the gradient. This is explicitly given by

$$\nabla^2 f = \sum_i \frac{1}{w} \frac{\partial}{\partial u_i} \frac{w}{h_i^2} \frac{\partial}{\partial u_i} f. \tag{9.27}$$

Example: In two dimensions the Laplace operator is

$$\nabla^2 f = \frac{\partial^2}{\partial x^2} f + \frac{\partial^2}{\partial y^2} f. \tag{9.28}$$

Example: In two dimensions the Laplace operator is also given by

$$\nabla^2 f = \frac{1}{r} \frac{\partial}{\partial r} r \frac{\partial}{\partial r} f + \frac{1}{r^2} \frac{\partial^2}{\partial \theta^2} f. \tag{9.29}$$

Example: The three-dimensional result is

$$\nabla^2 f = \frac{\partial^2}{\partial x^2} f + \frac{\partial^2}{\partial y^2} f + \frac{\partial^2}{\partial z^2} f. \tag{9.30}$$

Example: It is a pleasant exercise to work out the Laplace operaor in spherical polar coordinates. The result is

$$\nabla^2 f = \frac{1}{r^2} \frac{\partial}{\partial r} r^2 \frac{\partial}{\partial r} f + \frac{1}{r^2} [\frac{1}{\sin\theta} \frac{\partial}{\partial \theta} \sin\theta \frac{\partial}{\partial \theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial \phi^2}] f. \tag{9.31}$$

9.2 Gas dynamics

In this section we look at the physics of conservation laws. The most important ones, of course, are conservation of mass, of momentum, and of energy.

A *conservation law* is an equation of the form

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{J} = 0. \tag{9.32}$$

The interpretation of this equation is most easily seen in its integrated form. This is

$$\frac{d}{dt}\int_R u\, dV + \int_{\partial R} \mathbf{J} \cdot d\mathbf{A} = 0. \tag{9.33}$$

This says that the change in the quantity is given by the amount of current flowing in through the boundary.

The simplest example is the equation of *conservation of mass*. In this case the dependent variable ρ is the *density*. The current is $\mathbf{J} = \mathbf{v}\rho$, where $\mathbf{v}$ is the *velocity*. The equation is

$$\frac{\partial \rho}{\partial t} + \nabla \cdot (\mathbf{v}\rho) = 0. \tag{9.34}$$

In integrated form this says that

$$\frac{d}{dt}\int_R \rho\, dV = -\int_{\partial R} \rho \mathbf{v} \cdot d\mathbf{A}. \tag{9.35}$$

An increase in mass within the region can only take place if there is material flowing in through the boundary.

A much more complicated example is the equation of *conservation of momentum*. Here the quantity of interest is the momentum density $\mathbf{v}\rho$. The convective current is then $\mathbf{v}\rho\mathbf{v}$. This is a matrix with components $v_i \rho v_j$. Thus the j component of momentum ρv_j is carried along at velocity v_i. There is also a current due to the pressure equal to p times the identity matrix I. This current is in the same direction as the velocity and is proportional to the pressure p. (We assume for simplicity that there are no viscous forces.) The equation is

$$\frac{\partial \rho \mathbf{v}}{\partial t} + \nabla \cdot (\mathbf{v}\rho\mathbf{v} + pI) = 0. \tag{9.36}$$

This can also be written explicitly in the form

$$\frac{\partial \rho v_j}{\partial t} + \sum_i \nabla_i (v_i \rho v_j + p\delta_{ij}) = \frac{\partial \rho v_j}{\partial t} + \sum_i \nabla_i (v_i \rho v_j) + \nabla_j p = 0. \tag{9.37}$$

We see that a pressure gradient changes the momentum in the opposite direction to the gradient. This can also be written in integrated form. It says that

$$\frac{d}{d}\int_R \rho \mathbf{v}\, dV = -\int_{\partial R} \mathbf{v}\rho\, \mathbf{v} \cdot d\mathbf{A} - \int_{\partial R} p\, d\mathbf{A}. \tag{9.38}$$

The momentum in a certain region increases if moving fluid is being transported in or if there is a pressure difference between opposite sides of the boundary.

We can use the equation of conservation of mass to write the equation in a somewhat different form:

$$\rho[\frac{\partial \mathbf{v}}{\partial t} + (\mathbf{v} \cdot \nabla)\mathbf{v}] + \nabla p = 0. \tag{9.39}$$

For a particle with

$$\frac{d\mathbf{x}}{dt} = \mathbf{v} \tag{9.40}$$

the acceleration is

$$\frac{d^2\mathbf{x}}{dt^2} = \frac{d\mathbf{v}}{dt} = \frac{\partial \mathbf{v}}{\partial t} + (\frac{d\mathbf{x}}{dt} \cdot \nabla)\mathbf{v}. \tag{9.41}$$

Therefore this is the equation mass (per volume) times acceleration equals force (per volume), where the force (per volume) is the negative of the gradient of the pressure. The equations of conservation of mass and momentum involve the dependent variables ρ and $\mathbf{v}$. If the pressure p is given as a function of ρ, then they form a closed system.

Let $c^2 = \partial p/\partial \rho$. Consider the linear approximation to these equations. Suppose that ρ is close to a constant ρ_0, and let $u = (\rho - \rho_0)/\rho_0$. The equations become

$$\frac{\partial u}{\partial t} + \nabla \cdot \mathbf{v} = 0 \tag{9.42}$$

and

$$\frac{\partial \mathbf{v}}{\partial t} + c^2 \nabla u = 0. \tag{9.43}$$

As a consequence we see that u satisfies the *wave equation*

$$\frac{\partial^2 u}{\partial t^2} = c^2 \nabla^2 u. \tag{9.44}$$

The remaining conservation law in a fluid is the law of *conservation of energy*. The energy density of a fluid is a sum of a kinetic energy part and an internal energy part. It is $\rho e = (1/2)\rho \mathbf{v}^2 + \rho u$. Here e is the energy per mass. The u is the internal energy per mass, a function of the density and temperature. The current $\mathbf{J}$ has three parts. The first is just $\rho e \mathbf{v}$, which describes how the energy density is transported at velocity $\mathbf{v}$. The second is $p\mathbf{v}$, which describes the work on the system. Finally the third is the heat flow J_q. This is given by

$$J_q = -\lambda \nabla T, \tag{9.45}$$

a quantity proportional to the temperature gradient. Again we neglect effects of viscosity. The conservation law takes the form

$$\frac{\partial \rho e}{\partial t} + \nabla \cdot (\mathbf{v}\rho e + J_q + p\mathbf{v}) = 0. \tag{9.46}$$

By using the laws of conservation of mass and momentum, this can be written in the alternate form

$$\rho[\frac{\partial u}{\partial t} + \mathbf{v} \cdot \nabla u] + \nabla \cdot J_q + p\nabla \cdot \mathbf{v} = 0. \tag{9.47}$$

This is a complicated system of equations. The dependent variables are ρ, $\mathbf{v}$, and T. In order to get a closed system, we need to know how p may be expressed as a function of ρ and T. Furthermore, we need to know how u may be expressed as a function of ρ and T.

Consider the special case when ρ is constant and $\mathbf{v}$ is zero. Then we can consider the energy equation by itself. Furthermore, we can think of the internal energy u as a function of T. The equation takes the simple form

$$\rho\frac{\partial u}{\partial t} + \nabla \cdot J_q = 0. \tag{9.48}$$

Let $c = \partial u/\partial T$. Then this equation becomes the *heat equation*

$$\rho c\frac{\partial T}{\partial t} = \lambda\nabla^2 T. \tag{9.49}$$

It says that the change in internal energy is given entirely by the heat flow. Consequently, the change in temperature is related to the gradient of the temperature.

9.3 Sound speed

The purpose of this section is to show that the sound speed in a gas is comparable to the velocities of the individual molecules. Thus it is much faster than the fluid velocity, which is an average velocity for many molecules in a small region near a given point.

The sound speed c is given by

$$c^2 = \frac{\partial p}{\partial \rho}. \tag{9.50}$$

In many situations in fluid dynamics the pressure p is related to the density ρ by

$$p = A\rho^\gamma, \tag{9.51}$$

where A is a constant and γ is an exponent a bit larger than one. This says that a pressure increase is related to a density increase. In fact, the proportional increases are related by

$$\frac{\partial p}{\partial \rho} = \gamma\frac{p}{\rho}. \tag{9.52}$$

Thus we get

$$c^2 = \gamma\frac{p}{\rho}. \tag{9.53}$$

If ρ is the mass of the particles per unit volume, and if m is the mass of a single particle, then ρ/m is the number of particles per unit volume. According to the gas law, the pressure is

$$p = \frac{\rho}{m} kT. \tag{9.54}$$

Here T is the absolute temperature, and kT is the corresponding energy. The constant k is Boltzmann's constant. From this we see that the sound speed c is given by

$$c^2 = \gamma \frac{kT}{m}. \tag{9.55}$$

The energy of a particle is $(1/2)m\mathbf{v}^2$. It has an average squared velocity $\langle \mathbf{v}^2 \rangle$ given by

$$\frac{1}{2} m \langle \mathbf{v}^2 \rangle = \frac{3}{2} kT. \tag{9.56}$$

From this we see that the sound velocity c is given by

$$c^2 = \frac{1}{3} \gamma \langle \mathbf{v}^2 \rangle. \tag{9.57}$$

Thus the sound velocity is of the same general order of magnitude as the velocity of motion of the individual molecules. The overall fluid velocity is an average motion, and it is usually much less.

Chapter 10

Spherical harmonics

10.1 Circular harmonics

In this section we review the facts about two-dimensional space and its rotational symmetry. A *harmonic* u of degree n is a polynomial solution of the Laplace equation that is homogeneous of degree n. Thus it is a solution of

$$\nabla^2 u = 0 \tag{10.1}$$

and

$$r\frac{\partial}{\partial r}u = nu. \tag{10.2}$$

The harmonics are multiples of 1 for $n = 0$ and are linear combinations of $r^n \cos(n\theta)$ and $r^n \sin(n\theta)$ for $n = 1, 2, 3, \ldots$.

A *circular harmonic* Y of degree ℓ is the restriction of a harmonic to the unit circle. The relation between the solid spherical harmonic and the surface spherical harmonic is

$$u = r^n Y. \tag{10.3}$$

The circular harmonics are multiples of 1 for $n = 0$ and are linear combinations of $\cos(n\theta)$ and $\sin(n\theta)$ for $n = 1, 2, 3, \ldots$.

The most imporant fact about the space of circular harmonics of degree n is that it is invariant under all rotations of the plane that keep the origin fixed. This is because the two equations that define this space are themselves invariant under rotations. We now review familiar properties of the circular harmonics from a somewhat different point of view. The advantage of this is that the results will generalize to three dimensions.

Theorem 10.1 *For each n each circular harmonic Y satisfies*

$$\frac{\partial^2}{\partial\theta^2}Y = -n^2 Y. \tag{10.4}$$

Thus it is an eigenfunction of the angular part of the Laplacian with eigenvalue $-n^2$.

Proof: The function $u = r^n Y$ satisfies $\nabla^2 u = 0$ and $r\partial/\partial r\, u = nu$. The Laplace operator may be written

$$\nabla^2 = \frac{1}{r^2}[r\frac{\partial}{\partial r} r \frac{\partial}{\partial r} + \frac{\partial^2}{\partial \theta^2}]. \tag{10.5}$$

The result follows by applying this operator to u.

Theorem 10.2 *If Y and Y' are circular harmonics of degree $n \neq n'$, then they are orthogonal in the sense that*

$$\int_0^{2\pi} Y(\theta) Y'(\theta)\, d\theta = 0. \tag{10.6}$$

Proof: Let L be the angular part of the Laplace operator. Then

$$LY = -n^2 Y \tag{10.7}$$

and similarly for Y'. Furthermore, if we integrate by parts we get the identity

$$\int LY\, Y'\, d\theta = \int Y\, LY'\, d\theta. \tag{10.8}$$

It follows that

$$-n^2 \int Y\, Y'\, d\theta = -n'^2 \int Y\, Y'\, d\theta. \tag{10.9}$$

The only way this can happen when $n \neq n'$ is for the integral to be zero.

10.2 Expansions in circular harmonics

This section continues the study of two-dimensional rotational symmetry. The fundamental theorem about circular harmonics is that every function defined on the unit circle may be expanded in terms of circular harmonics. Thus we have the representation

$$f(\theta) = c_0 + \sum_{n=1}^{\infty} 2a_n \cos(n\theta) + 2b_n \sin(n\theta). \tag{10.10}$$

Thus every function may be written as a sum of eigenfunctions of the angular part of the Laplacian.

For $r < 1$ define the Poisson kernel

$$p_r(\theta) = \frac{1}{2\pi} \frac{1 - r^2}{1 - 2r\cos(\theta) + r^2}. \tag{10.11}$$

Then the Poisson kernel may be written as a sum of powers of r times cosines by

$$p_r(\theta) = \frac{1}{2\pi}[1 + \sum_{n=0}^{\infty} r^n 2\cos(n\theta)]. \tag{10.12}$$

The key result that leads to the convergence of Fourier series is the following.

Theorem 10.3 *Let f be a continuous function on the unit circle. Then*

$$f(\theta) = \lim_{r \to 1} \frac{1}{2\pi} [\int_0^{2\pi} f(\theta')\, d\theta' + \sum_{n=1}^{\infty} r^n \int_0^{2\pi} 2\cos(n(\theta - \theta')) f(\theta')\, d\theta']. \quad (10.13)$$

It is based on the fact that the Poisson kernel is an approximate delta function. We shall see that there is a three dimensional analog of this result as well.

10.3 Spherical harmonics

In this section we consider three dimensional space and its rotational symmetry. A *solid spherical harmonic* u of degree ℓ is a polynomial solution of the Laplace equation that is homogeneous of degree ℓ. Thus it is a solution of

$$\nabla^2 u = 0 \quad (10.14)$$

and

$$r \frac{\partial}{\partial r} u = \ell y. \quad (10.15)$$

A *surface spherical harmonic* Y of degree ℓ is the restriction of a solid spherical harmonic to the unit sphere. The relation between the solid spherical harmonic and the surface spherical harmonic is

$$u = r^\ell Y. \quad (10.16)$$

The most important fact about the space of spherical harmonics of degree ℓ is that it is invariant under all rotations of space that keep the origin fixed. This is because the two equations that define this space are themselves invariant under rotations. In practice we often write the spherical harmonics in spherical polar coordinates with $x = r\sin(\theta)\cos(\phi)$, $y = r\sin(\theta)\sin(\phi)$ and $z = r\cos(\theta)$. However since this choice of coordinates does not display the rotational symmetry explicitly, the expressions get rather complicated.

Theorem 10.4 *For each ℓ each surface spherical harmonic Y satisfies*

$$[\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin(\theta) \frac{\partial}{\partial\theta} + \frac{1}{\sin^2(\theta)} \frac{\partial^2}{\partial\phi^2}] Y = -\ell(\ell+1) Y. \quad (10.17)$$

Thus it is an eigenfunction of the angular part of the Laplacian with eigenvalue $-\ell(\ell+1)$.

Proof: The function $u = r^\ell Y$ satisfies $\nabla^2 u = 0$ and $r\partial/\partial r\, u = \ell u$. The Laplace operator may be written

$$\nabla^2 = \frac{1}{r^2} [r \frac{\partial}{\partial r} r \frac{\partial}{\partial r} + r \frac{\partial}{\partial r}] + \frac{1}{r^2} [\frac{1}{\sin\theta} \frac{\partial}{\partial\theta} \sin\theta \frac{\partial}{\partial\theta} + \frac{1}{\sin^2\theta} \frac{\partial^2}{\partial\phi^2}]. \quad (10.18)$$

The result follows by applying this operator to u.

Theorem 10.5 *If Y and Y' are surface spherical harmonics of degree $\ell \neq \ell'$, then they are orthogonal in the sense that*

$$\int_0^{2\pi} \int_0^{\pi} Y(\theta, \phi) Y'(\theta, \phi) \, \sin(\theta) \, d\theta \, d\phi = 0. \tag{10.19}$$

Proof: Let L be the angular part of the Laplace operator. Then

$$LY = -\ell(\ell + 1)Y \tag{10.20}$$

and similarly for Y'. Furthermore, if we integrate by parts we get the identity

$$\int LY \, Y' \sin(\theta) \, d\theta \, d\phi = \int Y \, LY' \sin(\theta) \, d\theta \, d\phi. \tag{10.21}$$

It follows that

$$-\ell(\ell + 1) \int Y \, Y' \sin(\theta) \, d\theta \, d\phi = -\ell'(\ell' + 1) \int Y \, Y' \sin(\theta) \, d\theta \, d\phi. \tag{10.22}$$

The only way this can happen when $\ell \neq \ell'$ is for the integral to be zero.

It may be shown that the dimension of the space of spherical harmonics of degree ℓ is $2\ell + 1$. Here are the first few cases.

For $\ell = 0$ the space of spherical harmonics consists of the constant functions.

For $\ell = 1$ the space of solid spherical harmonics is the collection of all linear functions $ax + by + cz$. The corresponding surface spherical harmonics are the functions

$$Y = ax + by + cz = a \sin(\theta) \cos(\phi) + b \sin(\theta) \sin(\phi) + c \cos(\theta) \tag{10.23}$$

on the unit sphere $x^2 + y^2 + z^2 = 1$. This looks like a fairly complicated expression. However, there is a change of coordinates so that the vector is in the z direction. In this new coordinate system we would have the rather simple result

$$Y = cz = c \cos(\theta). \tag{10.24}$$

If we look at the magnitude of Y as a function of θ, we see that as we go around the sphere in latitude, the magnitude of Y goes from 1 at the poles to 0 at the equator. Thus the angular distribution of an $\ell = 1$ spherical harmonic has two lobes. This harmonic is often called a dipole.

For $\ell = 2$ the space of solid spherical harmonics consists of all quadratic functions $ax^2 + by^2 + cz^2 + 2dxy + 2eyz + 2fxz$ with $a + b + c = 0$. The diagonal terms are

$$a \sin^2(\theta) \cos^2(\phi) + b \sin^2(\theta) \sin^2(\phi) + c \cos^2(\theta) \tag{10.25}$$

with $a + b + c = 1$. They can also be written as the sum of two terms

$$(a - b)/2[\sin^2(\theta) \cos(2\phi)] + c/2[2 \cos^2(\theta) - \sin^2(\theta)]. \tag{10.26}$$

The off diagonal terms are

$$d \sin^2(\theta) \sin(2\phi) + 2e \cos(\theta) \sin(\theta) \sin(\phi) + 2f \cos(\theta) \sin(\theta) \cos(\phi). \tag{10.27}$$

We can always choose a new coordinate system in which the quadratic form is diagonal, equal to $ax^2 + by^2 + cz^2$ with $a + b + c = 1$. If $a = b$ then the solution is a multiple of $2z^2 - x^2 - y^2 = 2\cos^2(\theta) - \sin^2(\theta)$. If we plot the magnitude of this as a function of the latitude, then we get a clover leaf pattern. In the case when $a \neq b$ there is also a dependence on longitude, but this is also in the form of a clover leaf. This harmonic is called a quadrupole.

For $\ell = 3$ the space of solid spherical harmonics consists of all linear combinations of the 10 monomials $x^3, y^2x, z^2x, y^3, x^2y, z^2y, z^3, x^2z, y^2z, xyz$ that satisfy three equations.

The geometric interpretations of the first three cases $\ell = 0$, $\ell = 1$, and $\ell = 2$ are particularly simple. Of course $\ell = 0$ stands for spherically symmetric. An $\ell = 1$ spherical harmonic is just the restriction of a linear function to the sphere, so it is $\cos(\gamma)$, where the angle γ is measured from the direction in which the linear function is increasing. An $\ell = 2$ spherical harmonic is the restriction of a quadratic form to the unit sphere, with the added restriction that its average over the sphere is zero.

These spaces of spherical harmonics come up in many areas of science, and they have various names. The first few spaces $\ell = 0$, $\ell = 1$, $\ell = 2$ are often associated with the names monopole, dipole, quadrupole. In chemistry the spaces $\ell = 0$, $\ell = 1$, $\ell = 2$, $\ell = 3$ go by the names S, P, D, F. (One might think that S stands for spherically symmetric and P for polar, but this is not so. The names come from spectroscopy, where they were abbreviations: sharp, principle, diffuse, fine.)

For each ℓ there is a one-dimensional subspace that consists of spherical harmonics that are also invariant under rotations about the z axis. These are called the zonal harmonics. These are polynomials that are homogeneous of degree ℓ, harmonic, and that depend only on z and $x^2 + y^2$. In spherical polar coordinates the corresponding surface spherical harmonics depend only on latitude θ and not on longitude ϕ.

Obviously for $\ell = 0$ the zonal harmonics are again the constant functions.

For $\ell = 1$ the zonal harmonics consist of the multiples of $z = \cos(\theta)$.

For $\ell = 2$ the zonal harmonics consist of the multiples of $2z^2 - (x^2 + y^2) = 2\cos^2(\theta) - \sin^2(\theta)$.

For $\ell = 3$ the zonal harmonics consist of the multiples of $2z^3 - 3z(x^2 + y^2) = 2\cos^3(\theta) - 3\cos(\theta)\sin^2(\theta)$.

10.4 Expansions in spherical harmonics

This section continues the study of three-dimensional rotational symmetry. The fundamental theorem about spherical harmonics is that every function defined on the unit sphere may be expanded in terms of spherical harmonics. Thus we have the representation

$$f(\theta, \phi) = \sum_{\ell=0}^{\infty} \sum_{m} a_{\ell m} Y_{\ell,m}(\theta, \phi). \tag{10.28}$$

Thus every function may be written as a sum of eigenfunctions of the angular part of the Laplacian. This section is devoted to understanding how this comes about.

The function

$$\frac{1}{|\mathbf{x}|} = \frac{1}{\sqrt{x^2 + y^2 + z^2}} \tag{10.29}$$

is harmonic except at the origin. This is easily seen by noting that this is $1/r$ in spherical polar coordinates.

Consider the point $\mathbf{e}$ at the north pole of the unit sphere in three dimensions. The function

$$\frac{1}{|\mathbf{x} - \mathbf{e}|} = \frac{1}{\sqrt{x^2 + y^2 + (z-1)^2}} \tag{10.30}$$

is a harmonic function except at the north pole. In fact, it is a translate of the first example.

We can write this also in spherical polar coordinates. We note that $|\mathbf{x} - \mathbf{e}|$ is the square root of the dot product of $\mathbf{e} - \mathbf{x}$ with itself. We obtain

$$\frac{1}{|\mathbf{x} - \mathbf{e}|} = \frac{1}{\sqrt{1 - 2r\cos(\theta) + r^2}}. \tag{10.31}$$

Take $r < 1$ and expand this in a Taylor series in powers of r. We obtain

$$\frac{1}{\sqrt{1 - 2r\cos(\theta) + r^2}} = \sum_{\ell=0}^{\infty} r^\ell P_\ell(\cos(\theta)), \tag{10.32}$$

where the P_ℓ are the *Legendre polynomials*. Each $P_\ell(\cos(\theta))$ is a polynomial of degree ℓ in $\cos(\theta)$. Thus $P_0(\cos(\theta)) = 1$, $P_1(\cos(\theta)) = \cos(\theta)$, $P_2(\cos(\theta)) = (3\cos^2(\theta) - 1)/2$, $P_3(\cos(\theta)) = (5\cos^3(\theta) - 3\cos(\theta))/2$.

We can also write these polynomials in a slightly differerent form, with every term homogeneous of degree ℓ in powers of $\cos(\theta)$ and $\sin^2(\theta)$. Thus $P_0(\cos(\theta)) = 1$, $P_1(\cos(\theta)) = \cos(\theta)$, $P_2(\cos(\theta) = (2\cos^2(\theta) - \sin^2(\theta))/2$, $P_3(\cos(\theta) = (2\cos^3(\theta) - 3\cos(\theta)\sin^2(\theta))/2$, and so on. Thus they are just certain special multiples of the zonal harmonics.

Theorem 10.6 *Each term $r^\ell P_\ell(\cos(\theta))$ is a harmonic function that is homogeneous of degree ℓ.*

Proof: For each t the function

$$\frac{1}{|t\mathbf{x} - \mathbf{e}|} = \frac{1}{\sqrt{1 - 2tr\cos(\theta) + t^2 r^2}}. \tag{10.33}$$

is harmonic. Therefore for each t

$$\frac{1}{\sqrt{1 - 2tr\cos(\theta) + t^2 r^2}} = \sum_{\ell=0}^{\infty} t^\ell r^\ell P_\ell(\cos(\theta)) \tag{10.34}$$

is harmonic. It follows that each coefficient is harmonic.

Theorem 10.7 *For $r < 1$ define the Poisson kernel*

$$p_r(\theta) = \frac{1}{4\pi} \frac{1 - r^2}{(1 - 2r\cos(\theta) + r^2)^{\frac{3}{2}}}. \tag{10.35}$$

Then the Poisson kernel may be written as a sum of powers of r times zonal spherical harmonics by

$$p_r(\theta) = \sum_{\ell=0}^{\infty} r^\ell \frac{2\ell + 1}{4\pi} P_\ell(\cos(\theta)). \tag{10.36}$$

Proof: Apply the operator $r\partial/\partial r$ to

$$\frac{1}{\sqrt{1 - 2r\cos(\theta) + r^2}} = \sum_{\ell=0}^{\infty} r^\ell P_\ell(\cos(\theta)), \tag{10.37}$$

multiply by two, and add the original expression. Finally divide by 4π.

Theorem 10.8 *Let f be a continuous function on the unit sphere in three dimensional space. Then the value of f at the north pole $\mathbf{e}$ is*

$$f(\mathbf{e}) = \lim_{r \to 1} \int_0^{2\pi} \int_0^{\pi} p_r(\theta) f(\theta, \phi) \sin(\theta) \, d\theta \, d\phi. \tag{10.38}$$

Proof: All that one needs to do is to check that the Poisson kernel is an approximate delta function. This is left as an exercise.

Theorem 10.9 *Let f be a continuous function on the unit sphere in three dimensional space. Then*

$$f(\theta, \phi) = \lim_{r \to 1} \sum_{\ell=0}^{\infty} r^\ell \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} (2\ell + 1) P_\ell(\cos(\gamma)) f(\theta', \phi') \sin(\theta') \, d\theta' \, d\phi', \tag{10.39}$$

where γ is the angle between the points θ, ϕ and θ', ϕ' on the sphere, so

$$\cos(\gamma) = \sin(\theta)\sin(\theta')\cos(\phi - \phi') + \cos(\theta)\cos(\theta'). \tag{10.40}$$

.

Proof: By rotating coordinates it is sufficient to prove this when the angle $\theta = 0$. Then the value of the function is taken at the north pole.

Let us assume that the series converges. Then we can take the limit as $r \to 1$ and get

$$f(\theta, \phi) = \sum_{\ell=0}^{\infty} \frac{1}{4\pi} \int_0^{2\pi} \int_0^{\pi} (2\ell + 1) P_\ell(\cos(\gamma)) f(\theta', \phi') \sin(\theta') \, d\theta' \, d\phi'. \tag{10.41}$$

This is the expansion in spherical harmonics. We can also write this as

$$f(\mathbf{x}) = \sum_{\ell=0}^{\infty} \frac{1}{4\pi} \int (2\ell + 1) P_\ell(\mathbf{x} \cdot \mathbf{x}') f(\mathbf{x}') \, dS(\mathbf{x}') \tag{10.42}$$

where the points are all on the unit sphere, and the integral is with respect to area on the unit sphere.

10.5 The multipole expansion

One of the most famous equations in physics is the Poisson equation

$$\nabla_{\mathbf{x}}^2 u = -s(\mathbf{x}). \tag{10.43}$$

It describes, among other things, the electric potential u due to a charge distribution $s(\mathbf{x})$. We shall see in the next chapter that the solution of this equation is

$$u(\mathbf{x}) = \int \frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|} s(\mathbf{x}')\, dV(\mathbf{x}'). \tag{10.44}$$

We shall use the fact that when $|\mathbf{x}'| < |\mathbf{x}|$ we have the expansion

$$\frac{1}{|\mathbf{x}-\mathbf{x}'|} = \sum_{\ell=0}^{\infty} \frac{|\mathbf{x}'|^\ell}{|\mathbf{x}|^{\ell+1}} P_\ell(\frac{\mathbf{x}\cdot\mathbf{x}'}{|\mathbf{x}||\mathbf{x}'|}). \tag{10.45}$$

When $|\mathbf{x}| = 1$ is the north pole vector this is true by the definition of Legendre polynomials given above. However it is easy to derive the general case from this by multiplying this vector by a scalar and rotating.

Insert this in the solution of the Poisson equation. We obtain the *multipole expansion*

$$\int \frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|} s(\mathbf{x}')\, dV(\mathbf{x}') = \frac{1}{4\pi} \sum_{\ell=0}^{\infty} m_\ell(\frac{\mathbf{x}}{|\mathbf{x}|}) \frac{1}{|\mathbf{x}|^{\ell+1}}. \tag{10.46}$$

where

$$m_\ell(\frac{\mathbf{x}}{|\mathbf{x}|}) = \int |\mathbf{x}'|^\ell P_\ell(\frac{\mathbf{x}}{|\mathbf{x}|}\cdot\frac{\mathbf{x}'}{|\mathbf{x}'|}) s(\mathbf{x}')\, dV(\mathbf{x}') \tag{10.47}$$

The ℓ order coefficient in this expansion is a surface spherical harmonic of degree ℓ times $1/|\mathbf{x}|^{\ell+1}$.

The $\ell = 0$ term is the monopole term. The coefficient is the total charge

$$m_0 = \int s(\mathbf{x}')\, dV(\mathbf{x}'). \tag{10.48}$$

This term drops off for large distance like $1/|\mathbf{x}|$.

If the total charge is zero, then the dominant term is the dipole term with $\ell = 1$. The coefficient of this term is

$$m_1(\frac{\mathbf{x}}{|\mathbf{x}|}) = \int \frac{\mathbf{x}}{|\mathbf{x}|}\cdot\mathbf{x}' s(\mathbf{x}')\, dV(\mathbf{x}'). \tag{10.49}$$

It drops off for large distances like $1/|\mathbf{x}|^2$.

It can happen that the dipole term is also zero. This would be true, for instance, if the source were even under reflection. Then the leading term is the quadrupole term with $\ell = 2$. The coefficient of this term is

$$m_2(\frac{\mathbf{x}}{|\mathbf{x}|}) = \frac{1}{2}\int \left(3(\frac{\mathbf{x}}{|\mathbf{x}|}\cdot\mathbf{x}')^2 - |\mathbf{x}'|^2\right) s(\mathbf{x}')\, dV(\mathbf{x}'). \tag{10.50}$$

It drops off for large distances like $1/|\mathbf{x}|^3$.

Chapter 11

Sources

11.1 Equilibrium Green's functions: one dimension

This chapter deals with linear equations with a inhomogeneous source term. The solution is required to satisfy homogeneous boundary condition. In certain circumstances the solution of the equation is uniquely specified and is given by an inverse operator. This operator is an integral operator given by what is known as a Green's function. This is the continuous analog of a matrix.

The general scheme is the following. A differential operator L is defined for certain functions u satisfying homogeneous boundary conditions. Often if the boundary conditions are specified correctly, then the equations $Lu = s$ has a unique solution. This solution is $u = L^{-1}s$. In many cases it is given by a function

$$u(x) = L^{-1}s(x) = \int G(x, x')s(x')dx'. \tag{11.1}$$

This function $G(x, x')$ is the Green's function that specifies the inverse. Thus it gives a solution for an arbitrary source.

In this and the following sections we consider the Laplace operator in Euclidean space. The goal is to find for each function s a solution of

$$\nabla^2_{\mathbf{x}} u + s(\mathbf{x}) = 0. \tag{11.2}$$

If we can somehow give boundary conditions that specify a unique such solution, then it should be given by a Green's function $G(\mathbf{x}, \mathbf{x}')$ with

$$-\nabla^2_{\mathbf{x}} \int G(\mathbf{x}, \mathbf{x}')s(\mathbf{x}')dV(\mathbf{x}') = s(\mathbf{x}). \tag{11.3}$$

Let us begin with the one dimensional case. Then the problem is

$$-\frac{d^2u}{dx^2} = s(x). \tag{11.4}$$

It is easy to solve this equation. An obvious integration gives

$$u(x) = \int_{-\infty}^{x} \int_{-\infty}^{y} s(z)\, dz\, dy + Cx + D. \tag{11.5}$$

Then integration by parts gives

$$u(x) = \int_{-\infty}^{x} (y - x)s(y)\, dy + Cx + D. \tag{11.6}$$

The integral in the first term has the following interpretation. Say that the positive source is at point y. Then the temperature to the left of y is zero. However the temperature at point x to the right of y is negative and proportional to $y - x$. Thus all heat is flowing to the right. We can add another term that gives heat flowing to the left. This is the role of the $Cx + D$. The boundary conditions determine the values of C and D.

One possible Green's function is given by taking $C = D = 0$. This is

$$G^R(x, y) = -H(x - y)(x - y), \tag{11.7}$$

where H denotes the Heaviside function that is 1 on the positive axis and 0 on the negative axis. The heat from the source flows only to the right.

Another possible Green's function is given by taking the heat to flow to the left. This is

$$G^L(x, y) = H(y - x)(x - y). \tag{11.8}$$

We can also take a Green's function where the heat flows equally in both directions. This is

$$G(x, y) = -\frac{1}{2}|x - y|. \tag{11.9}$$

All of these Green's functions are somewhat peculiar, since they go to $-\infty$ as $|x|$ goes to infinity.

Another way of thinking about the Green's function is the following. If we can solve the equation

$$-\frac{d^2}{dx^2} G(x, y) = \delta(x - y) \tag{11.10}$$

with appropriate boundary conditions, then we have found the Green's function. This is because we can then multiply both sides with $s(y)$ and integrate with respect to y. So we need to know how to get a function whose second derivative is a delta function. One way to approach this is with approximate delta functions.

Recall how to get an approximate delta function $\delta_\epsilon(x)$. Take a positive function $\delta_1(x)$ with integral one and define $\delta_\epsilon(x) = \delta_1(x/\epsilon)/\epsilon$.

Here is how to get the integral $H_\epsilon(x)$ of an approximate delta function. Take an increasing function $H_1(x)$ that increases a total of one. Define $H_\epsilon(x) = H(x/\epsilon)$.

There is a similar way to get the two-fold integral $A_\epsilon(x)$ of an approximate delta function. Take a concave up function $A_1(x)$ whose slope increases by one. Define $A_\epsilon(x) = \epsilon A_1(x/\epsilon)$.

As an example, take the symmetric function $A_\epsilon(x) = (1/2)\sqrt{x^2+\epsilon^2}$. The second derivative of this is an approximate delta function. Therefore

$$\frac{d^2}{dx^2} A_\epsilon(x-y) = \delta_\epsilon(x-y). \tag{11.11}$$

Now we can multiply by $s(y)$ and integrate with respect to y. This gives

$$\frac{d^2}{dx^2} \int_{-\infty}^{\infty} A_\epsilon(x-y)s(y)\,dy = \int_{-\infty}^{\infty} \delta_\epsilon(x-y)s(y)\,dy. \tag{11.12}$$

Take the limit as $\epsilon \to 0$. This gives

$$\frac{d^2}{dx^2} \int_{-\infty}^{\infty} \frac{1}{2}|x-y|s(y)\,dy = s(x). \tag{11.13}$$

We see that the Green's function is

$$G(x,y) = D - \frac{1}{2}|x-y|, \tag{11.14}$$

where D is an arbitrary additive constant. This is essentially the same answer that we got before in the case when the heat flows from the source in equal amounts in both directions.

We see that in one dimension there is no particularly natural boundary condition for the Green's function. One can always add the $Cx + D$ term that adds a total heat flow and changes the zero of temperature. However there is always the odd feature that the temperature goes to negative infinity at large distances.

11.2 Equilibrium Green's functions: two dimensions

Let us now go to two dimensions. The spherically symmetric solutions of the Laplace equation are given by

$$\frac{1}{r}\frac{d}{dr} r \frac{d}{dr} u = 0. \tag{11.15}$$

The solution of this equation is

$$u(r) = C\ln(r) + D = C\ln(\frac{r}{r_0}), \tag{11.16}$$

where $D = -C\ln(r_0)$. The additive constant D corresponds to an arbitrary choice of scale r_0 with respect to which length is measured.

We want to find which value of the constant C gives the Green's function. We can do this by using an approximate delta function. This will be obtained

by using an approximation to the logarithm function. We use the function $\ln(\sqrt{r^2+\epsilon^2})$. First we obtain the increasing function

$$r\frac{d}{dr}\ln(\sqrt{r^2+\epsilon^2}) = \frac{r^2}{(r^2+\epsilon^2)}. \tag{11.17}$$

This function rises from 0 to 1 as r ranges from 0 to ∞. The quantity of interest is

$$\frac{1}{r}\frac{d}{dr}r\frac{d}{dr}\ln(\sqrt{r^2+\epsilon^2}) = \frac{2\epsilon^2}{(r^2+\epsilon^2)^2}. \tag{11.18}$$

Take the integral of this over two dimensional space with respect to the volume element $r\,dr\,d\theta$. This can be done by inspection using the fact that increasing function obtained before rises from 0 to 1. The result is 2π. Therefore the quantity of interest is 2π times the delta function in two dimensions.

The conclusion is that

$$-\nabla_{\mathbf{x}}^2 \int -\frac{1}{2\pi}\ln(\sqrt{|\mathbf{x}-\mathbf{x}'|^2+\epsilon^2})s(\mathbf{x}')\,dV(\mathbf{x}') = \int \delta_\epsilon(\mathbf{x}-\mathbf{x}')s(\mathbf{x}')dV(\mathbf{x}'). \tag{11.19}$$

Let $\epsilon \to 0$. We obtain

$$-\nabla_{\mathbf{x}}^2 \int -\frac{1}{2\pi}\ln(|\mathbf{x}-\mathbf{x}'|)s(\mathbf{x}')\,dV(\mathbf{x}') = s(\mathbf{x}). \tag{11.20}$$

Since we can always put in an additive constant, the Green's function in two dimensions can be taken to be

$$G(\mathbf{x},\mathbf{x}') = -\frac{1}{2\pi}\ln(\frac{|\mathbf{x}-\mathbf{x}'|}{r_0}) = \frac{1}{2\pi}\ln(\frac{r_0}{|\mathbf{x}-\mathbf{x}'|}). \tag{11.21}$$

This function is positive within the disk of radius r_0 about the source point $\mathbf{x}'$. However it goes to minus infinity at large distances, albeit slowly.

11.3 Equilibrium Green's functions: three dimensions

Let us now go to three dimensions. The spherically symmetric solutions of the Laplace equation are given by

$$\frac{1}{r^2}\frac{d}{dr}r^2\frac{d}{dr}u = 0. \tag{11.22}$$

The solution of this equation is

$$u(r) = C\frac{1}{r} + D. \tag{11.23}$$

Now there is a natural choice for the additive constant D. We take it to be zero. The remaining part can be interpreted as the contribution from the source. In three dimensions we are thus able to separate the source from the environment.

We want to find which value of the constant C gives the Green's function. We can do this by using an approximate delta function. This will be obtained by using an approximation $1/\sqrt{r^2 + \epsilon^2}$. First we obtain the increasing function

$$-r^2 \frac{d}{dr} \frac{1}{\sqrt{r^2 + \epsilon^2}} = \frac{r^3}{(r^2 + \epsilon^2)^{\frac{3}{2}}}. \tag{11.24}$$

This rises from 0 to 1 as we go from $r = 0$ to infinity. We can continue the computation and get

$$-\frac{1}{r^2} \frac{d}{dr} r^2 \frac{d}{dr} \frac{1}{\sqrt{r^2 + \epsilon^2}} = \frac{3\epsilon^2}{(r^2 + \epsilon^2)^{\frac{5}{2}}}. \tag{11.25}$$

If we take the integral of this over three dimensional space with respect to the volume element $r^2\, dr\, \sin(\theta)\, d\theta\, d\phi$, we can use the fact that the increasing function rises by one to obtain the value 4π. Therefore this represents 4π times the delta function in three dimensions.

The conclusion is that

$$-\nabla_{\mathbf{x}}^2 \int \frac{1}{4\pi} \frac{1}{\sqrt{|\mathbf{x} - \mathbf{x}'|^2 + \epsilon^2}} s(\mathbf{x}')\, dV(\mathbf{x}') = \int \delta_\epsilon(\mathbf{x} - \mathbf{x}') s(\mathbf{x}') dV(\mathbf{x}'). \tag{11.26}$$

Let $\epsilon \to 0$. We obtain

$$-\nabla_{\mathbf{x}}^2 \int \frac{1}{4\pi} \frac{1}{|\mathbf{x} - \mathbf{x}'|} s(\mathbf{x}')\, dV(\mathbf{x}') = s(\mathbf{x}). \tag{11.27}$$

The conclusion is that the Green's function for the three-dimensional Laplace operator is

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi} \frac{1}{|\mathbf{x} - \mathbf{x}'|}. \tag{11.28}$$

This function is positive and approaches zero as $\mathbf{x}$ tends to infinity. This nice behavior is due to the fact that there is a lot of room in three dimensional space. A hot spot or a impurity concentration can steadily diffuse in space without requiring some special sink at infinity. The solution of the original problem

$$\nabla_{\mathbf{x}}^2 u + s(\mathbf{x}) = 0 \tag{11.29}$$

in the three-dimensional case is

$$u(\mathbf{x}) = \int \frac{1}{4\pi} \frac{1}{|\mathbf{x} - \mathbf{x}'|} s(\mathbf{x}') dV(\mathbf{x}'). \tag{11.30}$$

11.4 Causal Green's functions: diffusion

One class of Green's functions consists of causal Green's functions, where the task is to solve a problem forward in time. For example, the problem may have the form

$$\frac{\partial u}{\partial t} - Au = s(t) \tag{11.31}$$

with $u = 0$ when $t = 0$. Then it is easy to see that the solution is

$$u(t) = \int_0^t v(t;t')\,dt', \tag{11.32}$$

where $v(t;t')$ is the solution of the equation

$$\frac{\partial v}{\partial t} - Av = 0 \tag{11.33}$$

with initial condition $v(t';t') = s(t')$. Thus the Green's function is

$$G(t,t') = H(t-t')v(t;t') \tag{11.34}$$

This result is known as Duhamel's principle. The fact that this Green's functions satisfies $G(t,t') = 0$ for $t' > t$ is the reason for the term "causal". This says that the future cannot affect the past. From a mathematical point of view a causal Green's function is the analog of a triangular matrix.

Example: Consider the n-dimensional heat equation for $t > 0$ and arbitrary $\mathbf{x}$. The boundary condition is that the solution vanish at $t = 0$. The equation is

$$\left(\frac{\partial u}{\partial t} - \frac{1}{2}\sigma^2\nabla_{\mathbf{x}}^2\right) u = \frac{1}{2}\sigma^2 s(x,t). \tag{11.35}$$

By Duhamel's principle, the solution is

$$u(\mathbf{x},t) = \frac{1}{2}\sigma^2 \int_0^t \int g(\mathbf{x}-\mathbf{x}', t-t')s(\mathbf{x}',t')\,dV(\mathbf{x}')\,dt', \tag{11.36}$$

where

$$g(\mathbf{x},t) = \frac{1}{(\sqrt{2\pi\sigma^2 t})^n}\exp(-\frac{\mathbf{x}^2}{2\sigma^2 t}) \tag{11.37}$$

is the Gaussian kernel in n dimensions. This is just the product of the one-dimensional Gaussian kernels. Thus the Green's function for the time-dependent problem is

$$G(\mathbf{x},t;\mathbf{x}',t') = g(\mathbf{x}-\mathbf{x}', t-t')H(t-t'). \tag{11.38}$$

This solution can also be written in terms of the lag $\tau = t - t'$ as

$$u(\mathbf{x},t) = \frac{1}{2}\sigma^2 \int_0^t \int g(\mathbf{x}-\mathbf{x}', \tau)\ s(\mathbf{x}', t-\tau)\,dV(\mathbf{x}')\,d\tau, \tag{11.39}$$

Consider the case when the source $s(\mathbf{x})$ is independent of time. Then the solution is the convolution of

$$\frac{1}{2}\sigma^2 \int_0^t g(\mathbf{x},\tau)\,d\tau \tag{11.40}$$

with the source. It is interesting to attempt to take the limit as $t \to \infty$. But there is a problem with convergence at $t = \infty$. The integral in question is

$$\frac{\sigma^2}{2}\int_0^\infty g(\mathbf{x},\tau)\,d\tau = \frac{\sigma^2}{2}\int_0^\infty \frac{1}{(2\pi\sigma^2\tau)^{\frac{n}{2}}}\exp(-\frac{|\mathbf{x}|^2}{2\sigma^2\tau})\,d\tau. \tag{11.41}$$

This converges at $t = \infty$ only if the dimension n is three or more. In this case we can evaluate it explicitly. Make the substitution $\tau = |x|^2/(2\sigma^2)u$. This gives the result

$$\frac{\sigma^2}{2}\int_0^\infty g(\mathbf{x},\tau)\,d\tau = \frac{1}{4\pi^{\frac{n}{2}}|\mathbf{x}|^{n-2}}\int_0^\infty \frac{1}{u^{\frac{n}{2}}}e^{-\frac{1}{u}}\,du. \tag{11.42}$$

We can also write this as

$$\frac{\sigma^2}{2}\int_0^\infty g(\mathbf{x},\tau)\,d\tau = \frac{1}{4\pi^{\frac{n}{2}}|\mathbf{x}|^{n-2}}2\int_0^\infty a^{n-3}e^{-a^2}\,da. \tag{11.43}$$

This is infinite for $n = 1$ and $n = 2$. However it is finite for $n = 3$, and for this case we get

$$\frac{\sigma^2}{2}\int_0^\infty g(\mathbf{x},\tau)\,d\tau = \frac{1}{4\pi|\mathbf{x}|}. \tag{11.44}$$

This gives the usual Green's function for three dimensional static problems.

Let us look at what happens in the one and two dimensional problems for large t. First consider the case of one dimension. We have

$$\frac{\sigma^2}{2}\int_0^t g(x,\tau)\,d\tau = \frac{\sigma^2}{2}\int_0^t \frac{1}{(2\pi\sigma^2\tau)^{\frac{1}{2}}}\exp(-\frac{x^2}{2\sigma^2\tau})\,d\tau. \tag{11.45}$$

For each t this is positive. With a change of variable this becomes

$$\frac{\sigma^2}{2}\int_0^t g(x,\tau)\,d\tau = \frac{1}{4\pi^{\frac{1}{2}}}|x|\int_0^{\frac{2\sigma^2 t}{x^2}} \frac{1}{u^{\frac{1}{2}}}e^{-\frac{1}{u}}\,du. \tag{11.46}$$

Integrate by parts. This gives

$$\frac{\sigma^2}{2}\int_0^t g(x,\tau)\,d\tau = -\frac{1}{2\pi^{\frac{1}{2}}}|x|\int_0^{\frac{2\sigma^2 t}{x^2}} \frac{1}{u^{\frac{3}{2}}}e^{-\frac{1}{u}}\,du + \frac{1}{(2\pi)^{\frac{1}{2}}}\sqrt{\sigma^2 t}\exp(-\frac{x^2}{2\sigma^2 t}). \tag{11.47}$$

As $t \to \infty$ the first term converges to $-\frac{1}{2}|x|$. This is the negative static Green's function that we saw before. However as $t \to \infty$ the second term is growing like the square root of the time, and its limit is $+\infty$. So in some very rough sense the static Green's function needs to have an infinite constant added to it in order to resemble the result of solving the time dependent equation for large time.

The case of two dimensions is similar. We have

$$\frac{\sigma^2}{2}\int_0^t g(x,\tau)\,d\tau = \frac{\sigma^2}{2}\int_0^t \frac{1}{2\pi\sigma^2\tau}\exp(-\frac{x^2}{2\sigma^2\tau})\,d\tau. \tag{11.48}$$

By a change of variable we see that

$$\frac{\sigma^2}{2}\int_0^t g(x,\tau)\,d\tau = \frac{1}{4\pi}\int_0^{2\sigma^2 t/|\mathbf{x}|^2} \frac{1}{u}e^{-\frac{1}{u}}\,du. \tag{11.49}$$

Integrate by parts. This gives

$$\frac{\sigma^2}{2}\int_0^t g(x,\tau)\,d\tau = \frac{1}{4\pi}\int_0^{2\sigma^2 t/|\mathbf{x}|^2} \ln(u)\frac{1}{u^2}e^{-\frac{1}{u}}\,du + \frac{1}{4\pi}\ln(\frac{2\sigma^2 t}{|\mathbf{x}|^2})\exp(-\frac{|\mathbf{x}|^2}{2\sigma^2 t}). \tag{11.50}$$

As $t \to \infty$ the first term converges to a constant. This constant is $1/(4\pi)$ times the integral

$$\int_0^\infty \ln(u)\frac{1}{u^2}e^{-\frac{1}{u}}\,du = -\int_0^\infty \ln(t)e^{-t}\,dt, \tag{11.51}$$

which is Euler's constant. The second term is

$$\frac{1}{2\pi}\ln(\frac{\sqrt{2\sigma^2 t}}{|\mathbf{x}|})\exp(-\frac{|\mathbf{x}|^2}{2\sigma^2 t}). \tag{11.52}$$

For large t this is the static Green's function plus a term that is growing like the logarithm of t. So again there is increase, but it is very slow.

This result has a physical interpretation in the diffusion picture. In one dimensional and two dimensional diffusion the particles being continually emitted at the source do not ever succeed in permanently escaping. There is no way of reaching equilibrium when particles are continually being injected, short of having some sort of vacuum at infinity. The particles persist in coming back; this is what is called the null recurrent case in diffusion theory.

However in three dimensions there is so much room that the particles will eventually escape permanently and never return to near the source. So there is an equilibrium between the source emitting particles and the vast expanses of three-dimensional space ready to receive them. This is what is called the transient case in diffusion theory.

The interpretation is the heat picture is similar. A steady source of heat in a localized part of an infinite rod will make the rod hotter and hotter. A steady source of heat in a localized part of an infinite plate will make the plate hotter and hotter, though very slowly. However a steady source of heat in a localized part of an infinite solid object will dissipate it throughout space, and the solid will achieve an equilibrium temperature.

11.5 Causal Green's functions: wave motion

There is also a Duhamel's principle for equations that are second order in time. Say that the problem has the form

$$\frac{\partial^2 u}{\partial t^2} - Au = s(t) \tag{11.53}$$

with $u = 0$ and $\partial u/\partial t = 0$ when $t = 0$. Then it is easy to see that the solution is

$$u(t) = \int_0^t v(t;t')\,dt', \tag{11.54}$$

where $v(t;t')$ is the solution of the equation

$$\frac{\partial^2 v}{\partial t^2} - Av = 0 \tag{11.55}$$

with initial conditions $v(t';t') = 0$ and $\partial v/\partial t(t';t') = s(t')$. This says that the source is continuously emitting waves.

Example: Consider the one-dimensional wave equation for $t > 0$ and arbitrary x. The boundary condition is that the solution and its time derivative vanish at $t = 0$. The equation is

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right) u = s(x,t). \tag{11.56}$$

By Duhamel's principle, the solution is

$$u(x,t) = \int_0^t \frac{c}{2} \int_{x-c(t-t')}^{x+c(t-t')} s(x',t')\, dx' dt'. \tag{11.57}$$

This is an integral over a triangle in space-time with one vertex at x, t and the other two vertices at $x \pm ct, 0$. Consider the case when the source is independent of time. We can perform the t' integral. When $|x - x'| \le c(t - t')$ the integrand is one. This happens for $t' \le t - |x - x'|/c$. So the result is

$$u(x,t) = \frac{1}{2} \int_{x-ct}^{x+ct} (ct - |x - x'|) s(x')\, dx'. \tag{11.58}$$

Let us look at the limit when ct approaches infinity. We see that there is a problem: there is a ct term in the solution. Only if we discard this term do we get the solution of the one-dimensional static problem, but then the Green's function is negative.

Duhamel's principle also works for the three-dimensional wave equation. This is the equation for electrical potential u when the electric charge is s.

$$\left(\frac{1}{c^2}\frac{\partial u^2}{\partial t^2} - \nabla_{\mathbf{x}}^2\right) u = s(\mathbf{x},t). \tag{11.59}$$

According to Duhamel's principle, the solution of the source problem is

$$u(\mathbf{x},t) = \int_0^t c^2 (t - t') M_{\mathbf{x},c(t-t')}(s(\cdot,t'))\, dt', \tag{11.60}$$

where $M_{\mathbf{x},r}(f(\cdot))$ is the mean of the function f over the spherical surface centered at $\mathbf{x}$ with radius r. We can change variables to write the solution as

$$u(\mathbf{x},t) = \int_0^{ct} r M_{\mathbf{x},r}(s(\cdot, t - \frac{r}{c}))\, dr = \int_0^{ct} \frac{1}{4\pi r} M_{\mathbf{x},r}(s(\cdot, t - \frac{r}{c}))\, 4\pi r^2\, dr. \tag{11.61}$$

This can be interpreted as an integral over volume. So this is the same as

$$u(\mathbf{x}, t) = \int_{|\mathbf{x}-\mathbf{x}'| \le ct} \frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|} s(\mathbf{x}', t - \frac{|\mathbf{x}-\mathbf{x}'|}{c})\, dV(\mathbf{x}'). \tag{11.62}$$

This says that the solution at $\mathbf{x}, t$ is the integral over a ball in space centered at $\mathbf{x}$ of radius ct. The integrand at a point on the sphere with radius r is $1/(4\pi r)$ times the source evaluated at the point at time $t - r/c$. This is because it took time r/c for the influence to travel from the point on the sphere to the center point $\mathbf{x}$.

Let us look at the limit as the speed of propagation c tends to infinity. The limit is

$$u(\mathbf{x}, t) = \int \frac{1}{4\pi|\mathbf{x}-\mathbf{x}'|} s(\mathbf{x}', t)\, dV(\mathbf{x}'). \tag{11.63}$$

This is the solution of the Poisson equation in three dimensions.

The wave equation again shows how the dimension of space plays an important role. A static source in one dimension produces a wave that increases in magnitude near the source as it spreads out in space. However in three dimensions the waves radiate away in the many directions, and they escape as rapidly as they are produced.

In three dimensions with a time varying source the only role of the propagation speed is to measure the time lag. So there is a perfectly natural static limit when c becomes infinite, in which the influence is instantaneous.

Chapter 12

Sources and Boundaries

12.1 Finite length Green's functions

This chapter considers Green's functions for differential operators defined with homogeneous boundary conditions in a bounded region. Such Green's functions solve the source problem. It will turn out that the same Green's function also gives the solution of the boundary value problem with inhomogeneous boundary conditions. This gives a remarkable unity to the discussion and connects it to the material of the preceding chapters.

Consider the heat equation

$$\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = s(x) \tag{12.1}$$

with boundary conditions $u(0,t) = 0$ and $u(L',t) = 0$ and $u(x,0) = 0$. Thus we are interested in the influence of the source. This problem could be solved by Duhamel's principle. We would expect that the long time behavior would be independent of time, since the heat would flow from the source and be absorbed at the boundary.

Say that we are interested only in the time-independent equilibrium (stationary) solution. Then the problem is

$$-\frac{d^2 u}{dx^2} = s(x) \tag{12.2}$$

with boundary conditions $u(0) = 0$ and $u(L') = 0$.

If we incorporate the boundary conditions, a calculation gives

$$u(x) = \int_0^x y(1 - \frac{x}{L'})s(y)\,dy + \int_x^{L'} x(1 - \frac{y}{L'})s(y)\,dy. \tag{12.3}$$

In other words, the Green's function is

$$G(x,y) = x(1 - \frac{y}{L'}) \tag{12.4}$$

for $x < y$ and

$$G(x, y) = y(1 - \frac{x}{L'}) \tag{12.5}$$

for $x > y$. If we think of the source point as y, then this says that the temperature as a function of x rises linearly from zero to some value as x runs from 0 to y and then decreases linearly from this value to zero as x runs from y to L'.

In terms of diffusion, this says that the particles produced by the source are eventually absorbed at the boundary. Thus this is the transient case.

However say instead that we are interested in the stationary Neumann problem with insulating boundary conditions. Then the problem is

$$-\frac{d^2u}{dx^2} = s(x) \tag{12.6}$$

with boundary conditions $du/dx(0) = 0$ and $du/dx(L') = 0$. Now we see that equilibrium is not so easy to maintain. In fact, there will be no solution unless

$$\int_0^{L'} s(y)\, dy = 0. \tag{12.7}$$

This follows directly from integrating the equation and using the boundary conditions. However it is also obvious physically. Unless the integrated input from the source is zero, there can be no equilibrium in the time dependent problem. With insulation, the temperature would either continually rise or continually drop, and there could be no stationary state. Thus we see that the existence of a Green's function is not automatic.

In diffusion this boundary condition corresponds to reflection at the boundary. The particles persist in the interior of the region. This is what is called in diffusion theory the positive recurrent case.

12.2 Finite area Green's functions

We can also ask for the Green's function for the problem

$$\nabla_{\mathbf{x}}^2 u + s(\mathbf{x}) = 0 \tag{12.8}$$

with Dirichlet boundary conditions in the two-dimensional disk of radius a. We need a function $G(\mathbf{x}, \mathbf{x}')$ that satisfies

$$-\nabla_{\mathbf{x}}^2 G(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}') \tag{12.9}$$

and that vanishes at the boundary.

We know that

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{2\pi} \log(\frac{1}{|\mathbf{x} - \mathbf{x}'|}) \tag{12.10}$$

satisfies the equation. The only trouble is the boundary condition. Therefore we must add a function that is harmonic in the disk in such a way that the boundary condition is satisfied.

The choice that works is

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{2\pi}[\log(\frac{1}{|\mathbf{x} - \mathbf{x}'|}) - \log(\frac{c}{|\mathbf{x} - \mathbf{x}''|})]. \tag{12.11}$$

Here $\mathbf{x}'$ is a point in the region, and $\mathbf{x}''$ is a suitably chosen point outside of the region. The constant $c > 0$ is also appropriately chosen. Clearly, this satisfies the equation for $\mathbf{x}$ in the region. In order to satisfy the boundary condition, we require that this be zero on the boundary. This can be accomplished by taking $c = a/|\mathbf{x}'|$ and $\mathbf{x}'' = c^2\mathbf{x}'$. So the answer is

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{2\pi}[\log(\frac{1}{|\mathbf{x} - \mathbf{x}'|}) - \log(\frac{1}{|\frac{|\mathbf{x}'|}{a}\mathbf{x} - \frac{a}{|\mathbf{x}'|}\mathbf{x}'|})]. \tag{12.12}$$

This may also be written as

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{2\pi}[\log(\frac{1}{\sqrt{r^2 - 2rr'\cos(\gamma) + r'^2}}) - \log(\frac{1}{\sqrt{r^2r'^2/a^2 - 2rr'\cos(\gamma) + a^2}})]. \tag{12.13}$$

In this formula $r = |\mathbf{x}|$ and $r' = |\mathbf{x}'|$ and γ is the angle between $\mathbf{x}$ and $\mathbf{x}'$. It is evident that when $r = a$ the Green's function vanishes.

12.3 Finite volume Green's functions

We can also ask for the Green's function for the problem

$$\nabla^2_{\mathbf{x}} u + s(\mathbf{x}) = 0 \tag{12.14}$$

with Dirichlet boundary conditions in the three-dimensional ball of radius a. We need a function $G(\mathbf{x}, \mathbf{x}')$ that satisfies

$$-\nabla^2_{\mathbf{x}} G(\mathbf{x}, \mathbf{x}') = \delta(\mathbf{x} - \mathbf{x}') \tag{12.15}$$

and that vanishes at the boundary.

We know that

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi}\frac{1}{|\mathbf{x} - \mathbf{x}'|} \tag{12.16}$$

satisfies the equation. The only trouble is the boundary condition. Therefore we must add a function that is harmonic in the disk in such a way that the boundary condition is satisfied.

The choice that works is

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi}[\frac{1}{|\mathbf{x} - \mathbf{x}'|} - \frac{c}{|\mathbf{x} - \mathbf{x}''|}]. \tag{12.17}$$

Here $\mathbf{x}'$ is a point in the region, and $\mathbf{x}''$ is a suitably chosen point outside of the region. The constant $c > 0$ is also appropriately chosen. Clearly, this satisfies the equation for $\mathbf{x}$ in the region. In order to satisfy the boundary condition, we

require that this be zero on the boundary. This can be accomplished by taking $c = a/|\mathbf{x}'|$ and $\mathbf{x}'' = c^2\mathbf{x}'$. So the answer is

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi}[\frac{1}{|\mathbf{x} - \mathbf{x}'|} - \frac{1}{|\frac{|\mathbf{x}'|}{a}\mathbf{x} - \frac{a}{|\mathbf{x}'|}\mathbf{x}'|}]. \tag{12.18}$$

This may also be written as

$$G(\mathbf{x}, \mathbf{x}') = \frac{1}{4\pi}[\frac{1}{\sqrt{r^2 - 2rr'\cos(\gamma) + r'^2}} - \frac{1}{\sqrt{r^2r'^2/a^2 - 2rr'\cos(\gamma) + a^2}}]. \tag{12.19}$$

12.4 Adjoints and boundary values

The Green's function may also be used to solve boundary value problems. The basic strategy is that two operators L and $L^\dagger$ are related by

$$Lu\, v - uL^\dagger v = \nabla \cdot \mathbf{b}(u, v), \tag{12.20}$$

where $\mathbf{b}(u, v)$ is bilinear in u and v. Thus

$$\int_R Lu\, v\, dV - \int_R uL^\dagger v\, dV = \int_{\partial R} \mathbf{b}(u, v) \cdot d\mathbf{A}. \tag{12.21}$$

This relates integrals involving the two operators over the region to an integral over the boundary. In the three dimensional case the boundary is a surface. In the two dimensional case the boundary is a curve. In the one dimensional case the boundary is two points, and the integral over the boundary is a sum.

Example: The simplest example is the usual integration by parts. In this case $L = d/dx$ and $L^\dagger = -d/dx$. Then

$$\frac{d}{dx}u\, v + u\frac{d}{dx}v = \frac{d}{dx}(uv). \tag{12.22}$$

The integral formula is then

$$\int_a^b \frac{d}{dx}u\, v\, dx + \int_a^b u\frac{d}{dx}v\, dx = (uv)\,|_a^b\,. \tag{12.23}$$

Example: Perhaps the most typical example is where the operators are second order. For instance, we could have $L = d^2/dx^2$ and $L^\dagger = d^2/dx^2$. Then

$$\frac{d^2}{dx^2}u\, v - u\frac{d^2}{dx^2}v = \frac{d}{dx}(\frac{du}{dx}v - u\frac{dv}{dx}). \tag{12.24}$$

The integral formula is then

$$\int_a^b \frac{d^2}{dx^2}u\, v\, dx - \int_a^b u\frac{d^2}{dx^2}v\, dx = (\frac{du}{dx}v - u\frac{dv}{dx})\,|_a^b\,. \tag{12.25}$$

Example: The same idea works in several dimensions. Say we have $L = -\nabla^2$ and $L^\dagger = -\nabla^2$. The minus signs are taken for later convenience. Then

$$-\nabla^2 u\, v + u\nabla^2 u\, v = -\nabla \cdot (\nabla u\, v - u\nabla v). \tag{12.26}$$

The integral formula is then

$$\int_R -\nabla^2 u\, v\, dV + \int_R u\nabla^2 v\, dV = -\int_{\partial R} (\nabla u\, v - u\nabla v) \cdot d\mathbf{A}. \tag{12.27}$$

Sometimes we want both L and $L^\dagger$ to be specified with homogeneous boundary conditions in such a way that the boundary term $\mathbf{b}(u, v) = 0$ when u satisfies the boundary condition for L and v satisfies the boundary condition for $L^\dagger$. Then we have the identity

$$\int_R Lu\, v\, dV = \int_R u L^\dagger v\, dV \tag{12.28}$$

for functions u and v satisfying the boundary conditions. In this case the operator $L^\dagger$ is known as the *adjoint* of the operator L.

Example: Consider the example when $L = d/dx$ and $L^\dagger = -d/dx$. The boundary condition for L is $u(a) = 0$, and the boundary condition for $L^\dagger$ is $v(b) = 0$. This is the causal boundary condition on L

Example: Consider the example when $L = d/dx$ and $L^\dagger = -d/dx$. The boundary condition for L is $u(a) = u(b)$ and for $L^\dagger$ is $v(a) = v(b)$. Then $L = -L^\dagger$. This is the periodic boundary condition.

Example: Consider the example when $L = d^2/dx^2$ and $L^\dagger = d^2/dx^2$. The boundary conditions for L are $u(a) = 0$, $u(b) = 0$ and for $L^\dagger$ are $v(a) = 0$, $v(b) = 0$. Then $L = L^\dagger$. These are the Dirichlet (absorbing) boundary conditions.

Example: Consider the example when $L = d^2/dx^2$ and $L^\dagger = d^2/dx^2$. The boundary conditions for L are $du/dx(a) = 0$, $du/dx(b) = 0$ and for $L^\dagger$ are $dv/dx(a) = 0$, $dv/dx(b) = 0$. Again $L = L^\dagger$. This are the Neumann (insulating) boundary conditions.

Example: Consider the example when $L = d^2/dx^2$ and $L^\dagger = d^2/dx^2$. The boundary conditions for L are $u(a) = u(b)$, $du/dx(a) = du/dx(b)$ and for $L^\dagger$ are $v(a) = v(b)$, $dv/dx(a) = dv/dx(b)$. Again $L = L^\dagger$. These are the periodic boundary conditions.

Example: Consider again the example when $L = d^2/dx^2$ and $L^\dagger = d^2/dx^2$. The boundary conditions for L are $u(a) = 0$, $du/dx(a) = 0$ and for $L^\dagger$ are $v(b) = 0$ and $dv/dx(b) = 0$. These are the causal boundary conditions. The operators L and $L^\dagger$ are not the same operator, since the boundary conditions are very different.

Example: Consider the example when $L = -\nabla^2$ and $L^\dagger = -\nabla^2$ acting on functions defined on a region R. The boundary conditions for L is that u vanishes on the boundary ∂R. The boundary condition for $L^\dagger$ is that v vanishes on the boundary ∂R. These are the Dirichlet boundary conditions. The operators are self-adjoint: $L = L^\dagger$.

Example: Consider the example when $L = -\nabla^2$ and $L^\dagger = -\nabla^2$ acting on functions defined on a region R. The boundary conditions for L is that $\nabla u \cdot d\mathbf{A}$ vanishes on the boundary ∂R. The boundary condition for $L^\dagger$ is that $\nabla v \cdot d\mathbf{A}$ vanishes on the boundary ∂R. These are the Neumann boundary conditions. The operators are self-adjoint: $L = L^\dagger$.

In some circumstances the operators L and $L^\dagger$ both have inverses. In this case they determine Green's functions G and $G^\dagger$.

Theorem 12.1 *The Green's functions G and $G^\dagger$ for the adjoint operators L and $L^\dagger$ satisfy*

$$G(\mathbf{x}, \mathbf{x}') = G^\dagger(\mathbf{x}', \mathbf{x}). \tag{12.29}$$

Proof: Take the adjoint identity in the special case when $u(\mathbf{x}) = \int G(\mathbf{x}, \mathbf{x}') s(\mathbf{x}')\, dV(\mathbf{x}')$ and $v(\mathbf{x}) = \int G^\dagger(\mathbf{x}, \mathbf{x}'') t(\mathbf{x}'')\, dV(\mathbf{x}'')$. Then it says that

$$\int s(\mathbf{x}) \int G^\dagger(\mathbf{x}, \mathbf{x}'') t(\mathbf{x}'')\, dV(\mathbf{x}'')\, dV(\mathbf{x}) = \int \int G(\mathbf{x}, \mathbf{x}') s(\mathbf{x}') dV(\mathbf{x}') t(\mathbf{x})\, dV(\mathbf{x}). \tag{12.30}$$

By changing variables of integration we can write this instead as

$$\int \int G^\dagger(\mathbf{x}', \mathbf{x}) s(\mathbf{x}') t(\mathbf{x})\, dV(\mathbf{x}')\, dV(\mathbf{x}) = \int \int G(\mathbf{x}, \mathbf{x}') s(\mathbf{x}') t(\mathbf{x}) dV(\mathbf{x}')\, dV(\mathbf{x}). \tag{12.31}$$

The only way this can happen for arbitrary functions $s(\mathbf{x}')$ and $t(\mathbf{x})$ is that $G^\dagger(\mathbf{x}', \mathbf{x}) = G(\mathbf{x}, \mathbf{x}')$.

The Green's function $G^\dagger$ is the adjoint of the Green's function G. This formula shows that the adjoint is an analog of the transpose operation for matrices. Note that if the operator is self-adjoint, that is, $L = L^\dagger$, then the Green's function will be also be self-adjoint. This translates into the symmetry property $G(\mathbf{x}', \mathbf{x}) = G(\mathbf{x}, \mathbf{x}')$.

Example: Consider the example when $L = d/dx$ and $L^\dagger = -d/dx$. Then for causal boundary conditions u is required to vanish at a and v is required to vanish at b. The two Green's functions are given by $u(x) = \int_a^x s(x)\, dx$ and $v(x) = \int_x^b t(x)\, dx$.

Example: Consider the example when $L = d^2/dx^2$ and $L^\dagger = d^2/dx^2$. Then for Dirichlet boundary conditions u and v are both required to vanish at the boundary. The two operators and their Green's functions are the same. The Green's function is piecewise linear with a slope discontinuity on the diagonal and vanishes at the end points. It is symmetric under interchange of its arguments.

Example: Consider again the example when $L = d^2/dx^2$ and $L^\dagger = d^2/dx^2$. Then the causal boundary conditions are when u and du/dx are required to vanish at a and v and dv/dx are required to vanish at b. Then the two operators and their Green's functions are quite different. They are both given by integrating twice, but with different constants of integration.

The following theorem is the central result of this chapter.

Theorem 12.2 *Let u be a function and let $Lu = s$ in the region R. Then u is determined by s and by its boundary values on the boundary ∂R by*

$$u(\mathbf{x}) = \int_R G(\mathbf{x}, \mathbf{x}') s(\mathbf{x}') \, dV(\mathbf{x}') - \int_{\partial R} \mathbf{b}(u(\mathbf{x}'), G(\mathbf{x}, \mathbf{x}')) \cdot d\mathbf{A}(\mathbf{x}'). \tag{12.32}$$

Proof: This formula comes from making the special choice $v(\mathbf{x}') = G^\dagger(\mathbf{x}', \mathbf{x}) = G(\mathbf{x}, \mathbf{x}')$ and taking u to be a function that is not required to satisfy homogeneous boundary conditions. Since $L^\dagger_{\mathbf{x}'} G^\dagger(\mathbf{x}', \mathbf{x}) = \delta(\mathbf{x}' - \mathbf{x})$, the general formula gives

$$\int_R G(\mathbf{x}, \mathbf{x}') s(\mathbf{x}') \, dV(\mathbf{x}') - u(\mathbf{x}) = \int_{\partial R} \mathbf{b}(u(\mathbf{x}), G(\mathbf{x}, \mathbf{x}')) \cdot d\mathbf{A}(\mathbf{x}'). \tag{12.33}$$

This formula expresses the value of the solution u at the point $\mathbf{x}$ in terms of the source s within the region and an integral over the boundary of the region of an expression involving u and its normal derivative. This fundamental result shows that the Green's function not only solves the source problem, but also the boundary value problem.

12.5 The Dirichlet problem for the Laplace operator

The Dirichlet problem for the Laplace operator is the classic example. Let $L = -\nabla^2$ with Dirichlet boundary conditions. The boundary identity is

$$(-\nabla^2) u \, v - u \, (-\nabla^2) v = -\nabla \cdot (\nabla u \, v - u \nabla v). \tag{12.34}$$

The Green's function vanishes at the boundary. Therefore, if we take $v(\mathbf{x}') = G(\mathbf{x}, \mathbf{x}')$ and u to be a solution of the Laplace equation, we obtain

$$u(\mathbf{x}) = -\int_{\partial R} u(\mathbf{x}') \nabla_{\mathbf{x}'} G(\mathbf{x}, \mathbf{x}') \cdot d\mathbf{A}(\mathbf{x}'). \tag{12.35}$$

Thus

$$-\nabla_{\mathbf{x}'} G(\mathbf{x}, \mathbf{x}') \cdot d\mathbf{A}(\mathbf{x}') \tag{12.36}$$

is a kind of Poisson kernel for the bounded region R. If we can figure out the Green's function $G(\mathbf{x}, \mathbf{x}')$ for the region, we can also figure out this Poisson kernel, which will act as a kind of approximate delta function as $\mathbf{x}$ approaches the boundary.

We can work this out for the disk of radius a in two dimension. The Poisson kernel is

$$\frac{1}{2\pi} \frac{\partial}{\partial r'} [\log(\sqrt{r^2 - 2rr'\cos(\gamma) + r'^2}) - \log(\sqrt{r^2 r'^2/a^2 - 2rr'\cos(\gamma) + a^2})] r' \, d\theta. \tag{12.37}$$

Here $\gamma = \theta' - \theta$. When we differentiate and set $r' = a$, we get

$$p(r, \gamma)\, d\theta' = \frac{1}{2\pi} \frac{a^2 - r^2}{r^2 - 2ar\cos(\gamma) + a^2}\, d\theta'. \tag{12.38}$$

This is the usual Poisson kernel for the disk of radius a.

We can also get the formula for the Poisson kernel for the ball of radius a in three dimensions. This is

$$-\frac{1}{4\pi}\frac{\partial}{\partial r'}\Big[\frac{1}{\sqrt{r^2 - 2rr'\cos(\gamma) + r'^2}} - \frac{1}{\sqrt{r^2 r'^2/a^2 - 2rr'\cos(\gamma) + a^2}}\Big] r'^2 \sin(\theta')\, d\theta'\, d\phi'. \tag{12.39}$$

Here $\cos(\gamma) = \sin(\theta)\sin(\theta')\cos(\phi' - \phi) + \cos(\theta)\cos(\theta')$. When we differentiate and set $r' = a$, we get

$$p(r, \gamma)\sin(\theta')\, d\theta'\, d\phi' = \frac{1}{4\pi} \frac{a(a^2 - r^2)}{(r^2 - 2ar\cos(\gamma) + a^2)^{\frac{3}{2}}}\, \sin(\theta')\, d\theta'\, d\phi'. \tag{12.40}$$

This is the usual Poisson kernel for the ball of radius a.

12.6 The Dirichlet problem for diffusion

This section will treat diffusion in a bounded region R of Euclidean space. The particle is assumed to start at a point in the region and then diffuse until it reaches the boundary ∂R. Then it vanishes. Thus this is the transient case.

The operator

$$Lu = \frac{1}{2}\sigma(\mathbf{x})^2 \nabla^2 u + \mathbf{a}(\mathbf{x}) \nabla u \tag{12.41}$$

is the backward operator for diffusion. The adjoint is the forward operator

$$L^\dagger v = \frac{1}{2}\nabla^2(\sigma(\mathbf{x})^2 v) - \nabla \cdot (\mathbf{a}(\mathbf{x}) v). \tag{12.42}$$

The backward equation is

$$\frac{\partial u}{\partial t} = Lu \tag{12.43}$$

The forward equation is

$$\frac{\partial v}{\partial t} = L^\dagger v. \tag{12.44}$$

Consider a diffusing particle that starts at a point $\mathbf{x}$. Let $p(\mathbf{x}, \mathbf{x}', t)$ be the probability density for the position at time t as a function of $\mathbf{x}'$. This quantity satisfies the backward equation as a function of the initial variable $\mathbf{x}$ and time t, and it satisfies the forward equation as a function of the final variable $\mathbf{x}'$ and time t. It describes the probability that the diffusing particle at time t has not yet reached the boundary and is near the point $\mathbf{y}$.

The Green's function for diffusion is

$$G(\mathbf{x}, \mathbf{x}') = \int_0^\infty p(\mathbf{x}, \mathbf{x}', \tau)\, d\tau. \tag{12.45}$$

It describes the expected time that the particle starting at $\mathbf{x}$ spends near $\mathbf{x}'$ before reaching the boundary. It inverts the backward operator as a function of the initial variable, and it inverts the forward operator as a function of the final variable.

If we collect a reward at a rate $f(\mathbf{x}')$ when the particle has not yet reached the boundary and is at $\mathbf{x}'$, then the expected total reward when the particle starts at $\mathbf{x}$ is

$$u(\mathbf{x}) = \int_R G(\mathbf{x}, \mathbf{x}') f(\mathbf{x}') \, dV(\mathbf{x}'). \tag{12.46}$$

The boundary value problem also has such an interpretation. The fundamental identity is

$$Lu\, v - u\, L^\dagger v = \nabla \cdot \mathbf{b}(u, v), \tag{12.47}$$

where the boundary term is

$$\mathbf{b}(u, v) = (\frac{1}{2}\sigma(\mathbf{x})^2 \nabla u)\, v - u(\frac{1}{2}\nabla(\sigma(\mathbf{x})^2 v) - \mathbf{a}(\mathbf{x})v). \tag{12.48}$$

The boundary condition defining the Green's functions are that the functions vanish on the boundary of the region. If we take $v(\mathbf{x}') = G(\mathbf{x}, \mathbf{x}')$ and u to be a solution of $Lu = 0$, then we obtain

$$u(\mathbf{x}) = \int_{\partial R} u(\mathbf{x}')[\frac{1}{2}\nabla_{\mathbf{x}'}(\sigma(\mathbf{x}')^2 G(\mathbf{x}, \mathbf{x}')) - \mathbf{a}(\mathbf{x}) G(\mathbf{x}, \mathbf{x}')] \cdot d\mathbf{A}(\mathbf{x}'). \tag{12.49}$$

The interpretation of this formula is that particles start diffusing at the point $\mathbf{x}$. They diffuse until they hit the boundary at some final point $\mathbf{x}'$. There they receive an award of size $u(\mathbf{x}')$. The solution $u(\mathbf{x})$ is the average size of the reward as a function of the initial point. It is given by the average of the reward $u(\mathbf{x}')$ at the final point $\mathbf{x}'$ on the boundary weighted by the probability of a particle impacting the boundary at that final point. This is the integral in the last expression.

12.7 The initial value problem

The considerations of this chapter shed light on Duhamel's principle. The idea is to take the region to be a region in space-time. For instance, it could be a semi-infinite rectangle with $a \le x \le b$ and $0 \le t$. Consider for instance the heat operator

$$L = \frac{\partial}{\partial t} - \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2} \tag{12.50}$$

with adjoint

$$L^\dagger = -\frac{\partial}{\partial t} - \frac{\sigma^2}{2}\frac{\partial^2}{\partial x^2} \tag{12.51}$$

The time boundary condition on L is that $u = 0$ when $t = 0$, while the time boundary condition on $L^\dagger$ is that $v = 0$ when $t' = \infty$. We assume the space boundary conditions are such that the functions vanish at $x = a$ and $x = b$.

The Green's function is $G(x,t;x',t')$, and the boundary condition in time says that $G(x,t;x',t') = 0$ for $t' > t$. The solution of the source problem $Lu = s$ is

$$u(x,t) = \int_0^\infty \int_a^b G(x,t;x',t') s(x',t') \, dx' \, dt'. \tag{12.52}$$

The fundamental identity is

$$Lu\, v - u\, L^\dagger v = \frac{d}{dx}\frac{\sigma^2}{2}(-\frac{du}{dx}\, v + u\, \frac{dv}{dx}) + \frac{\partial}{\partial t}(uv). \tag{12.53}$$

The right hand side is a kind of divergence in space-time Assume that u and v vanish at $x = a$ and $x = b$. Assume in addition that v vanishes at $t = \infty$. The identity in integrated form is then

$$\int_0^\infty \int_a^b Lu\, v \, dx' \, dt' - \int_0^\infty \int_a^b u\, L^\dagger v \, dx' \, dt' = -\int_a^b u(x',0) v(x',0) \, dx'. \tag{12.54}$$

Consider a solution of $Lu = 0$. Take $v(x',t') = G(x,t;x',t')$. The fundamental identity gives

$$u(x,t) = \int_a^b G(x,t;x',0) u(x',0) \, dx'. \tag{12.55}$$

This explains again why the solution of the initial value problem is given by the same Green's function as the solution of the source problem in space-time.

The second order case is similar. Again take a rectangle in space-time. Consider the wave operator

$$L = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} \tag{12.56}$$

with adjoint

$$L^\dagger = \frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}. \tag{12.57}$$

Both operators satisfy Dirichlet boundary conditions in the space variables. The time boundary condition on L is that $u = 0$ and $\partial u/\partial t = 0$ when $t = 0$, while the time boundary condition on $L^\dagger$ is that $v = 0$ and $\partial v/\partial t = 0$ when $t' = \infty$. The Green's function satisfies $G(x,t;x',t') = 0$ for $t' > t$. The solution of the source problem $Lu = s$ is

$$u(x,t) = \int_0^\infty \int_a^b G(x,t;x',t') s(x',t') \, dx' \, dt'. \tag{12.58}$$

The fundamental identity is

$$Lu\, v - u\, L^\dagger v = \frac{d}{dx}(-\frac{du}{dx}\, v + u\, \frac{dv}{dx}) + \frac{\partial}{\partial t}\frac{1}{c^2}(\frac{\partial u}{\partial t} v - u\frac{\partial v}{\partial t}). \tag{12.59}$$

Consider a solution of $Lu = 0$ vanishing at $x = a$ and at $x = b$. Take $v(x', t') = G(x, t; x', t')$ and integrate in time from 0 to ∞ and over space. This gives

$$u(x,t) = \frac{1}{c^2}\int_a^b G(x,t;x',0)\frac{\partial u(x',0)}{\partial t'}\,dx' - \frac{1}{c^2}\int_a^b \frac{\partial G(x,t;x',0)}{\partial t'}u(x',0)\,dx'. \tag{12.60}$$

Again the solution of the initial value problem is given by the Green's function, but in a more complicated way.

This gives a new perspective on the d'Alembert formula for the solution of the wave equation. The source problem is

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right)u = s(x,t). \tag{12.61}$$

with initial condition that $u = 0$ and $\partial u/\partial t = 0$ when $t = 0$. The solution is

$$u(x,t) = \frac{c}{2}\int_0^t \int_{|x-x'|\le c(t-t')} s(x',t')\,dx'\,dt'. \tag{12.62}$$

Thus the Green's function is

$$G(x,t;x',t') = \frac{c}{2}H(t-t')1_{[-c(t-t'),c(t-t')]}(x-x'). \tag{12.63}$$

Here we use the notation 1_S for the function that is 1 on S and 0 on the complement of S. In particular $H(\tau) = 1_{[0,\infty)}(\tau)$. Therefore we can write

$$u(x,t) = \int_0^\infty \int_{-\infty}^\infty G(x,t;x',t')s(x',t')\,dx'\,dt'. \tag{12.64}$$

Now consider instead the initial value problem

$$\left(\frac{1}{c^2}\frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2}\right)u = 0 \tag{12.65}$$

with initial conditions $u(x, 0) = f(x)$ and $\partial u/\partial t(x, 0) = g(x)$. Take $v(x', t') = G(x, t; x', t')$ and use the fundamental identity. This gives

$$u(x,t) = \frac{1}{c^2}\int_{-\infty}^\infty G(x,t;x',t')g(x')\,dx' - \frac{1}{c^2}\frac{\partial}{\partial t'}\int_{-\infty}^\infty G(x,t;x',t')f(x')\,dx' \tag{12.66}$$

evaluated at $t' = 0$. When we plug in the expression for the Green's function and set $t' = 0$, we get

$$u(x,t) = \frac{1}{2c}\int_{x-ct}^{x+ct} g(x')\,dx' + \frac{1}{2}[f(x+ct) + f(x-ct)]]. \tag{12.67}$$

This is exactly the d'Alembert solution.

The conclusion is that the source problem and the initial value problem are closely related. One can think of the wave as due to a source or due to the initial conditions. There is some choice in viewpoint, since these initial conditions may be the result of emission from a source that acted at a yet earlier time.

12.8 Adjoints and spectral theory

There is a somewhat more general kind of adjoint that is useful. This involves also a given weight function $w > 0$. The two operators L and L^* are now related by

$$Lu\, v\, w - uL^* v\, w = \nabla \cdot \mathbf{b}(u, v), \tag{12.68}$$

where $\mathbf{b}(u, v)$ is bilinear in u and v (and also depends on w). Thus

$$\int_R Lu\, v\, w\, dV - \int_R uL^* v\, w\, dV = \int_{\partial R} \mathbf{b}(u, v) \cdot d\mathbf{A}. \tag{12.69}$$

This relates integrals involving the weight function. The operator L^* is now the adjoint with respect to this weight function w. We require that u and v be restricted so that the boundary integral on the right vanishes. Then we have

$$\int_R Lu\, v\, w\, dV = \int_R uL^* v\, w\, dV. \tag{12.70}$$

We shall be particularly interested in the case when $L = L^*$. In this case the operator is said to be self-adjoint with respect to the weight function.

The relation with the old notion of adjoint is that $L^* v = \frac{1}{w} L^\dagger(wv)$. So the condition of self-adjointness is that $L^\dagger(wv) = wLv$.

Example: Perhaps the most basic example is the operator d^2/dx^2 on the interval from a to b. If we take Dirichlet boundary conditions this is self-adjoint with respect to the weight function 1.

Example: The operator d^2/dx^2 on the interval from a to b with Neumann boundary conditions is also self-adjoint with respect to 1.

Example: An example with a non-trivial weight function is the radial part of the Laplace operator in two dimensions. In this case $L = (1/r)d/dr\, r\, d/dr$. The weight function is r. The identity is

$$Lu\, v\, r - u\, Lv\, r = \frac{d}{dr}[r(\frac{du}{dr} v - u \frac{dv}{dr})]. \tag{12.71}$$

Take the region to be the interval from 0 to a. Then we can make this a self-adjoint operator by requiring that the functions in its domain vanish at a. The integral identity is then

$$\int_0^a Lu\, v\, r\, dr = \int_0^a u\, Lv\, r\, dr. \tag{12.72}$$

Example: Another example is $\partial^2/\partial\theta^2$ on the circle. This is obviously self-adjoint with respect to the weight function 1; due to the periodicity there is effectively no boundary.

Example: Consider the radial part of the Laplace operator in three dimensions. In this case $L = (1/r^2)d/dr\, r^2\, d/dr$. The weight function is r^2. The identity is

$$Lu\, v\, r^2 - u\, Lv\, r^2 = \frac{d}{dr}[r^2(\frac{du}{dr} v - u \frac{dv}{dr})]. \tag{12.73}$$

Take the region to be the interval from 0 to a. Then we can make this a self-adjoint operator by requiring that the functions in its domain vanish at a.

Example: Yet another example is the angular part of the Laplace operator in three dimensions. The region is the sphere, and the weight function is $\sin(\theta)$. This is again self-adjoint.

An eigenvalue for an operator is a number λ for which there is a function u (not the zero function) with

$$Lu = \lambda u. \tag{12.74}$$

Theorem 12.3 *Let L be self-adjoint with respect to the weight function w. Suppose λ and μ are eigenvalues of L, with $Lu = \lambda u$ and $Lv = \mu v$. Then if $\lambda \neq \mu$, the eigenfunctions u and v are orthogonal in the sense that*

$$\int_R u\, v\, w\, dV = 0. \tag{12.75}$$

This raises the possibility of expanding an arbitrary function in a series in eigenfunctions of the operator L. We have seen that this can be done in various simple cases, such as the second derivative operator with Dirichlet or Neumann boundary conditions. Other examples we have seen are the operators governing circular and spherical harmonics.

There is a very general theorem to this effect. This is the spectral theorem. This theorem applies to an operator L that has a Green's function G and that is self-adjoint with respect to w. The adjoint of the Green's function is $G^*(x, y) = \frac{1}{w(x)} G(y, x) w(y)$. The condition that the Green's function is self-adjoint with respect to the weight function is that

$$w(x)G(x, y) = w(y)G(y, x). \tag{12.76}$$

A Green's function is said to satisfy the Hilbert-Schmidt condition if

$$M^2 = \int \int G^*(y, x)G(x, y)\, dx\, dy < \infty. \tag{12.77}$$

One special case of the spectral theorem uses the hypothesis that $G = G^*$ is self-adjoint and satisfies the Hilbert-Schmidt condition. Under this hypotheses, there is a basis of eigenvectors of G with corresponding eigenvalues $\mu_1, \mu_2, \mu_3, \ldots$ such that

$$\sum_{n=1}^{\infty} \mu_n^2 = M^2. \tag{12.78}$$

Since G is the inverse of L, it follows that L has eigenvalues $\lambda_1, \lambda_2, \lambda_3, \ldots$ that are the reciprocals of the eigenvalues of G. In particular,

$$\sum_{n=1}^{\infty} \frac{1}{\lambda_n^2} = M^2. \tag{12.79}$$

Example: Take the example of the Dirichlet problem for the interval from 0 to 1. The weight function is 1. The Green's function is equal to $x(1 - y)$ for

$x < y$ and to $y(1-x)$ for $x > y$. Since $d^2/dx^2 \sin(\pi n x) = -\pi^2 n^2 \sin(\pi n x)$, the identity gives

$$\sum_{n=1}^{\infty} \frac{1}{\pi^4} \frac{1}{n^4} = \frac{1}{90}. \tag{12.80}$$

The condition of self-adjointness and the spectral theorem are a mathematical miracle, but what is the physical meaning of self-adjointness? The example of diffusion sheds some light.

Let $\rho(\mathbf{x}) > 0$ and let

$$Lu = \frac{1}{\rho(\mathbf{x})} \nabla \cdot (\frac{\sigma(\mathbf{x})^2}{2} \rho(\mathbf{x}) \nabla u). \tag{12.81}$$

Then we have the identity

$$Lu\, v\, \rho(\mathbf{x}) - u\, Lv\, \rho(\mathbf{x}) = \nabla \cdot [\frac{\sigma(\mathbf{x})^2}{2} \rho(\mathbf{x}) (\nabla u\, v - u\, \nabla v)]. \tag{12.82}$$

This shows that L is self-adjoint with respect to ρ when Dirichlet (or Neumann) boundary conditions are imposed.

This example works because L has a special form with the ρ in both numerator and denominator. We can write this as

$$Lu = \frac{\sigma(\mathbf{x})^2}{2} \nabla^2 u + \mathbf{a}(\mathbf{x}) \cdot \nabla u. \tag{12.83}$$

where

$$\mathbf{a}(\mathbf{x}) \rho(\mathbf{x}) - \nabla (\frac{\sigma(\mathbf{x})^2}{2} \rho(\mathbf{x})) = 0. \tag{12.84}$$

This is the detailed balance condition that says that the current due to drift is exactly balanced by the current due to diffusion at each point. This is a rather special situation in diffusion, especially in dimensions greater than one. Given a drift vector field $\mathbf{a}(\mathbf{x})$ the existence of such a ρ is not at all automatic; it is necessary that $2\mathbf{a}(\mathbf{x})/\sigma(\mathbf{x})^2$ be a gradient.

12.9 Conclusion

This course has dealt with a variety of partial differential equations. Most of them have been linear and fall into the hyperbolic, parabolic, elliptic classification.

Hyperbolic equations describe waves moving through space as a function of time. They move with a maximum speed.

Parabolic equations describe dissipative processes where a function of space spreads out over time. The typical examples are the diffusion of particles and the spread of heat.

Elliptic equations may be thought of as describing the equilibrium at large time of a parabolic equation. There are many circumstances when this equilibrium exists. However if there is a source, then there must be a place where the solution can dissipate at a rate that matches the production at the source.

For linear partial differential equation the solution is specified by a specified inhomogeneous source and by inhomogeneous initial or boundary conditions. The influence of the source is given by the Green's function. This also describes the influence of the initial or boundary conditions.

An initial condition may be thought of as a boundary condition, where the boundary is of a region in space-time. An equation that is first order in time requires one initial condition, while an equation that is second order in time requires two initial conditions. Usually these are causal boundary conditions, in that they are imposed at time zero and not at infinite time.

When the boundary is of a region in space, then the boundary conditions are of a different character. An equation that is second order in the space variables usually requires a single boundary condition on each side. This condition will specify the function or specify its derivative, but usually not both.

Consider the contrast for second order equations: for the time variable there are two boundary conditions at time zero and none at time infinity, while for the space variable there is one boundary condition on each side. The number of boundary conditions are the same, but they are arranged differently. This is more than physical intuition; the mathematical analysis of how solutions depend on the boundary conditions confirms that this is the proper way to set up the problems.

Some equations may be analyzed in more detail by using spectral theory. The simplest examples are equations that are invariant under translations or under rotations. The appropriate spectral decompositions are then given by the Fourier transform or by circular or spherical harmonics.

For non-linear equations there is no good spectral theory, and even Green's function methods do not apply. There are new effects where the solutions organize themselves to form some special pattern, such as a shock wave or a travelling reaction-diffusion wave. This is the research frontier in partial differential equations.

Appendix A

Partial Derivatives

A.1 Notation for partial derivatives

Say that we have variables that are related by a function f. Thus we could have

$$s = f(u, v). \tag{A.1}$$

Then we can define new functions

$$\frac{\partial s}{\partial u} = f'_{|1}(u, v) \tag{A.2}$$

and

$$\frac{\partial s}{\partial v} = f'_{|2}(u, v). \tag{A.3}$$

The functions $f'_{|1}$ is defined by fixing the the second input and taking the derivative with respect to the first input to f. Similarly, the function $f'_{|2}$ is defined by fixing the first input and taking the derivative with respect to the second input.

Now say that we have another relation

$$s = g(u, w). \tag{A.4}$$

Then we can define new functions

$$\frac{\partial s}{\partial u} = g'_{|1}(u, w) \tag{A.5}$$

and

$$\frac{\partial s}{\partial w} = g'_{|2}(u, w). \tag{A.6}$$

These are different answers. The first moral that we can draw is this:

The notation $\partial s/\partial u$ is ambiguous.

A better notation would be something like the following. Say that $s = f(u, v) = g(u, w)$. Then the derivative along curves of constant v is

$$\frac{\partial s}{\partial u} \mid_{v=\text{const}} = f'_{|1}(u, v) \tag{A.7}$$

and along curves of constant w is

$$\frac{\partial s}{\partial u} \mid_{w=\text{const}} = g'_{|1}(u, w). \tag{A.8}$$

This device allows the use of variables to indicate partial derivatives in a way that avoids ambiguity. In fact, people who apply partial derivatives in practice often use just such a notation.

The meaning of $\partial s/\partial u$ depends on what other variable is held constant.

A.2 The chain rule

Say that we have

$$s = f(u, v) \tag{A.9}$$

and also

$$u = h(p, q) \tag{A.10}$$

and

$$v = k(p, q). \tag{A.11}$$

Then

$$s = f(h(p, q), k(p, q)) \tag{A.12}$$

defines s as a function of p and q. The *chain rule* says that we can calculate the partial derivaties

$$\frac{\partial s}{\partial p} = \frac{\partial s}{\partial u}\frac{\partial u}{\partial p} + \frac{\partial s}{\partial v}\frac{\partial v}{\partial p} \tag{A.13}$$

and

$$\frac{\partial s}{\partial q} = \frac{\partial s}{\partial u}\frac{\partial u}{\partial q} + \frac{\partial s}{\partial v}\frac{\partial v}{\partial q}. \tag{A.14}$$

Confusion results when we have a situation like the following one. Say that we have

$$s = f(u, v) \tag{A.15}$$

and also

$$u = h(p, v). \tag{A.16}$$

Then

$$s = f(h(p, v), v)) \tag{A.17}$$

defines s as a function of p and v. The chain rule gives

$$\frac{\partial s}{\partial v} = \frac{\partial s}{\partial u}\frac{\partial u}{\partial v} + \frac{\partial s}{\partial v}. \tag{A.18}$$

The same $\partial s/\partial v$ occurs with two different meanings.

This can be fixed by keeping track of the functional relationships. Or one can adopt the more explicit notation. This would give

$$\frac{\partial s}{\partial v} \mid_{p=\text{const}} = \frac{\partial s}{\partial u} \mid_{v=\text{const}} \frac{\partial u}{\partial v} \mid_{p=\text{const}} + \frac{\partial s}{\partial v} \mid_{u=\text{const}} . \tag{A.19}$$

A.3 Evaluation

Up to this point we have maintained the distinction between variables like s, u, v, p, q that characterize physical quantities and functions like f, g, and h that define relationships between numbers. However in partial differential equations there is often a subtle blending of the two notations.

Say that we have variables that are related by a function f. Thus we could have

$$s = f(u, v). \tag{A.20}$$

Then we can define new functions

$$\frac{\partial s}{\partial u} = f'_{|1}(u, v) \tag{A.21}$$

and

$$\frac{\partial s}{\partial v} = f'_{|2}(u, v). \tag{A.22}$$

Say that we want to indicate the values $f(a, b)$ and $f'_{|1}(a, b)$ and $f'_{|2}(a, b)$ at certain input values a and b. Then we can write these values as

$$s(u = a, v = b) = f(a, b). \tag{A.23}$$

Also

$$\frac{\partial s}{\partial u}(u = a, v = b) = f'_{|1}(a, b) \tag{A.24}$$

and

$$\frac{\partial s}{\partial v}(u = a, v = b) = f'_{|2}(a, b). \tag{A.25}$$

The principle is that the function values are indicated by the variables such as s and u and v that are related by the functions and by assigning values to certain of the variables.

Notice that an expression like $u = a$ is not an equality. Rather, it is an assignment that can be read "the point where u has the value a" or "the result of assigning the value a to u."

Say that we have

$$s = f(u, v) \tag{A.26}$$

and also

$$u = h(p, q) \tag{A.27}$$

and

$$v = k(p, q). \tag{A.28}$$

Say that we want to take the value of the composite function at values c and d. We may write this as

$$s(p = c, q = d) = f(h(c, d), k(c, d)). \tag{A.29}$$

The principle is again that the function value is indicated by the variables s and p and q that are related by the function.

It is the custom often to use a somewhat careless notation that depends on the context. Say that we have variables that are related by a function f. Thus we could have

$$s = f(u, v). \tag{A.30}$$

The careless notation is to write the value $f(a, b)$ at numerical input values as

$$s(a, b) = f(a, b). \tag{A.31}$$

Notice that this depends on the contextual information that s is being regarded as a function of u and v.

Say that we have

$$s = f(u, v) \tag{A.32}$$

and also

$$u = h(p, q) \tag{A.33}$$

and

$$v = k(p, q). \tag{A.34}$$

Say that we want to take the value of the composite function at values c and d. We may write this as

$$s(c, d) = f(h(c, d), k(c, d)). \tag{A.35}$$

The meaning of the left hand side is quite different, since now s is being regarded as a function of p and q.

This notational confusion is very common in partial differential equations. It is standard to write something like $u = f(x, t)$, where x and t are space and time variables in the alternate form $u(x, t)$. Then the value $u(x = x_0, t = t_0) = f(x_0, t_0)$ is written $u(x_0, t_0)$.

If $x = g(t)$, then $u = f(g(t), t)$, and the alternate form for this is $u(t)$. Perhaps it would be better to write something like $u(x = g(t), t = t)$. The value $u(x = g(t_0), t = t_0) = f(g(t_0), t_0)$ is just written $u(t_0)$.

As an example, consider the chain rule in the form

$$\frac{du}{dt} = \frac{\partial u}{\partial t} + \frac{\partial u}{\partial x}\frac{dx}{dt}. \tag{A.36}$$

Let $x_0 = g(t_0)$. Again the value $u(x = x_0, t = t_0)$ is written as $u(t_0)$. Furthermore, the value of the derivative

$$\frac{du}{dt}(t = t_0) = \frac{\partial u}{\partial t}(x = x_0, t = t_0) + \frac{\partial u}{\partial x}(x = x_0, t = t_0)\frac{dx}{dt}(t = t_0). \tag{A.37}$$

is written

$$\frac{du}{dt}(t_0) = \frac{\partial u}{\partial t}(x_0, t_0) + \frac{\partial u}{\partial x}(x_0, t_0)\frac{dx}{dt}(t_0). \tag{A.38}$$

A.4 Matrix notation

These lectures have not made use of matrix notation. However matrix notation gives an illuminating perspective on the chain rule.

Sometimes it is natural to keep track of the dependencies using indices. Thus, for example, we might have

$$s_i = f_i(u_1, u_2) \tag{A.39}$$

for $i = 1, 2$, where

$$u_k = g_k(p_1, p_2) \tag{A.40}$$

for $k = 1, 2$. Here f_1, f_2, g_1, and g_2 are given functions. The chain rule says in this case that

$$\frac{\partial s_i}{\partial p_j} = \frac{\partial s_i}{\partial u_1}\frac{\partial u_1}{\partial p_j} + \frac{\partial s_i}{\partial u_2}\frac{\partial u_2}{\partial p_j} \tag{A.41}$$

for $j = 1, 2$. In terms of the functions this says that if

$$h_i(p_1, p_2) = f_i(g_1(p_1, p_2), g_2(p_1, p_2)), \tag{A.42}$$

then

$$h'_{i|j}(p_1, p_2) = f'_{i|1}(u_1, u_2)g'_{1|j}(p_1, p_2) + f'_{i|2}(u_1, u_2)g'_{2|j}(p_1, p_2) \tag{A.43}$$

Here we are using a notation like $g'_{1|2}$ to denote the function obtained from g_1 by differentiating with respect to the second input. One sees that it is rather clumsy to be precise about all the functional relationships.

These equations can be written in a much more compact form using matrix language. Thus for instance if $s = f(u)$, where s and u both have two components, then

$$\frac{\partial s}{\partial u} = f'(u) \tag{A.44}$$

is a two by two matrix. The chain rule in terms of variables is the matrix product

$$\frac{\partial s}{\partial p} = \frac{\partial s}{\partial u}\frac{\partial u}{\partial p}. \tag{A.45}$$

The chain rule may also be expressed in terms of the functions f and g and h related by $h(p) = f(g(p)$. This is again a matrix product

$$h'(p) = f'(g(p))\, g'(p). \tag{A.46}$$

Appendix B

Mean square convergence

B.1 Convergence of Fourier series

This appendix deals with the convergence of Fourier series and Fourier integrals. The main message is that convergence questions become rather simple in the setting of mean square convergence.

Consider a Fourier series for a function f with period L. This has the form

$$f(x) = c_0 + \sum_{n=1}^{\infty} 2a_n \cos(k_n x) + \sum_{n=1}^{\infty} 2b_n \cos(k_n x). \tag{B.1}$$

Here $k_n = 2\pi n/L$. The coefficients are given by

$$a_n = \frac{1}{L} \int_{-L/2}^{L/2} \cos(k_n y) f(y)\, dy \tag{B.2}$$

and

$$b_n = \frac{1}{L} \int_{-L/2}^{L/2} \sin(k_n y) f(y)\, dy \tag{B.3}$$

The following theorem is easy to prove by using the orthogonality relations for the trigonometric functions.

Theorem B.1 *Let f be periodic with period L. Then*

$$\frac{1}{L} \int_{-L/2}^{L/2} |f(x)|^2\, dx = |c_0|^2 + \sum_{n=1}^{\infty} 2|a_n|^2 + \sum_{n=1}^{\infty} 2|b_n|^2. \tag{B.4}$$

This is a remarkable identity, because it relates a measure of the size of the function to a sum involving all the Fourier coefficients. It is tempting to think that this identity might be the key to understanding convergence of Fourier series, and this is indeed the case. However there are some subtle issues, and these need to be addressed.

The first point is to notice that if the coefficients are absolutely summable, that is, $\sum_n |a_n| < \infty$ and $\sum_n |b_n| < \infty$, then the Fourier series converges absolutely and uniformly in x. It follows that the function f must be a continuous function. So one can only expect convergence in this sense for continuous functions.

If the coefficients are absolutely summable, then they are square summable, that is $\sum_n |a_n|^2 < \infty$ and $\sum_n |b_n|^2 < \infty$. However the converse is not necessarily true. So being square summable is a more general condition. Nevertheless, there is a remarkable result that brings simplicity to the whole picture. The basic fact is given in the following theorem.

Theorem B.2 *Let f be a function that is square integrable, that is,*

$$\int_{L/2}^{L/2} |f(x)|^2 \, dx < \infty. \tag{B.5}$$

Let

$$S_N(x) = c_0 + \sum_{n=1}^{N} 2a_n \cos(k_n x) + \sum_{n=1}^{N} 2b_n \cos(k_n x) \tag{B.6}$$

be the Nth partial sum of the Fourier series. Then S_N converges to f in the mean square sense, that is,

$$\int_{L/2}^{L/2} |f(x) - S_N(x)|^2 \, dx \to 0 \tag{B.7}$$

as $N \to \infty$.

There is no requirement that the function f be continuous. This is a general and clean result, and it is the landmark fact about convergence of Fourier series.

All of this discussion applies equally well when the Fourier series is written in complex form. The reader is advised to rewrite the results for this case.

B.2 Convergence of Fourier transforms

Consider a Fourier transform representation of the form

$$f(x) = \int_0^\infty 2a(k) \cos(kx) \, \frac{dk}{2\pi} + \int_0^\infty 2b(k) \cos(kx) \frac{dk}{2\pi}. \tag{B.8}$$

Here

$$a(k) = \int_{-\infty}^{\infty} \cos(ky) f(y) \, dy \tag{B.9}$$

and

$$b(k) = \int_{-\infty}^{\infty} \sin(ky) f(y) \, dy \tag{B.10}$$

for $k \geq 0$.

If the Fourier coefficients are absolutely integrable, so that $\int_{-\infty}^{\infty} |a(k)|\,dk < \infty$ and $\int_{-\infty}^{\infty} |a(k)|\,dk < \infty$, then it follows that the function f is continuous. So again this is more restrictive than is desirable. Furthermore, it is not initially clear that the Fourier coefficients $a(k)$ and $b(k)$ even exist unless the function f is absolutely integrable.

To understand the meaning of these equations, it is useful to compare them with the case of a periodic function. However the comparison is easier with a somewhat different definition of the coefficients. Let

$$a(k_n) = La_n \tag{B.11}$$

and

$$b(k_n) = Lb_n \tag{B.12}$$

and similarly $c(0) = Lc_0$. Then the formulas are

$$f(x) = c(0)\,\frac{\Delta k}{2\pi} + \sum_{n=1}^{\infty} 2a(k_n)\cos(k_n x)\,\frac{\Delta k}{2\pi} + \sum_{n=1}^{\infty} 2b(k_n)\cos(k_n x)\frac{\Delta k}{2\pi}. \tag{B.13}$$

Here $k_n = 2\pi n/L$ and $\Delta k_n = 2\pi/L$. The coefficients are given by

$$a(k_n) = \int_{-L/2}^{L/2} \cos(k_n y) f(y)\,dy \tag{B.14}$$

and

$$b(k_n) = \int_{-L/2}^{L/2} \sin(k_n y) f(y)\,dy \tag{B.15}$$

We also have the identity

$$\int_{-L/2}^{L/2} f(x)|^2\,dx = |c(0)|^2\,\frac{\Delta k}{2\pi} + \sum_{n=1}^{\infty} 2|a(k_n)|^2\,\frac{\Delta k}{2\pi} + \sum_{n=1}^{\infty} 2|b(k_n)|^2\,\frac{\Delta k}{2\pi}. \tag{B.16}$$

The hope is that as $L \to \infty$ and $\Delta k = 2\pi/L \to 0$ the sums over frequencies are replaced by integrals over frequencies. The following theorems justify this hope in a particular precise sense.

Theorem B.3 *Let f be a function that is square integrable, that is, such that $\int_{-\infty}^{\infty} |f(x)|^2\,dx < \infty$. Let*

$$a_L(k) = \int_{-L/2}^{L/2} \cos(ky) f(y)\,dy \tag{B.17}$$

and

$$b_L(k) = \int_{-L/2}^{L/2} \sin(ky) f(y)\,dy \tag{B.18}$$

for $k \geq 0$ be the frequency coefficients computed for an interval of length L. Then there exist coefficients $a(k)$ and $b(k)$ so that

$$\int_0^\infty |a(k) - a_L(k)|^2 \, dx \to 0 \tag{B.19}$$

and

$$\int_0^\infty |b(k) - b_L(k)|^2 \, dx \to 0 \tag{B.20}$$

as $L \to \infty$.

The theorem just stated says that if the function f is square integrable, then it has corresponding frequency coefficients. Notice that a function may be square integrable without being absolutely integrable. For instance, the function might decay at $\pm\infty$ like a multiple of $1/x$. The integral of the function would not converge, but the square of the function would decay like a constant times $1/x^2$ and so there would be no problem with convergence of the integral of the square at infinity.

Theorem B.4 *Let f be a function that is square integrable, that is,*

$$\int_{-\infty}^\infty |f(x)|^2 \, dx < \infty. \tag{B.21}$$

Then

$$\int_{-\infty}^\infty |f(x)|^2 \, dx = \int_0^\infty 2|a(k)|^2 \, \frac{dk}{2\pi} + \int_0^\infty 2|b(k)|^2 \, \frac{dk}{2\pi}. \tag{B.22}$$

The preceding theorem says that the size of a function is reflected in a precise way in the size of its Fourier transform coefficients.

Theorem B.5 *Let f be a function that is square integrable, that is,*

$$\int_{-\infty}^\infty |f(x)|^2 \, dx < \infty. \tag{B.23}$$

Let

$$S_N(x) = \int_0^N 2a(k) \cos(kx) \, \frac{dk}{2\pi} + \int_0^N 2b(k) \cos(kx) \frac{dk}{2\pi} \tag{B.24}$$

be the contribution from frequencies up to N. Then S_N converges to f in the mean square sense, that is,

$$\int_{-\infty}^\infty |f(x) - S_N(x)|^2 \, dx \to 0 \tag{B.25}$$

as $N \to \infty$.

Notice that this theorem does not require the function f to be continuous. The convergence in the theorem takes place in a mean square sense, and this is sufficiently flexibile to allow quite general functions.

The moral of the story is that if one wants a simple picture of the relation between the function and its Fourier coefficients, then absolute convergence is not the proper perspective. If instead one takes convergence in the mean square sense, then there is a clean equivalence between the space representation and the frequency representation.

Again the reader should translate all this into complex form.