

## Appendix E

# Partial Differential Equations

In this appendix we briefly discuss some of the basic partial differential equations (PDEs) that are used in this book to illustrate the development of numerical methods, and we review the manner in which Fourier analysis can be used to gain insight into these problems.

## E.1 Classification of differential equations

First we review the classification of differential equations into elliptic, parabolic, and hyperbolic equations. Not all PDEs fall into one of these classes, by any means, but many important equations that arise in practice do. These classes of equations model different sorts of phenomena, display different behavior, and require different numerical techniques for their solution. Standard texts on partial differential equations such as Kevorkian [55] give further discussion.

### E.1.1 Second order equations

In most elementary texts the classification is given for a linear second-order differential equation in two independent variables of the form

$$au_{xx} + bu_{xy} + cu_{yy} + du_x + eu_y + fu = g.$$

The classification depends on the sign of the discriminant,

$$b^2 - 4ac \begin{cases} < 0 & \implies & \text{elliptic,} \\ = 0 & \implies & \text{parabolic,} \\ > 0 & \implies & \text{hyperbolic,} \end{cases}$$

and the names arise by analogy with conic sections. The canonical examples are the Poisson problem  $u_{xx} + u_{yy} = g$  for an elliptic problem, the heat equation  $u_t = \kappa u_{xx}$  (with  $\kappa > 0$ ) for a parabolic problem, and the wave equation  $u_{tt} = c^2 u_{xx}$  for a hyperbolic problem. In the parabolic and hyperbolic case  $t$  is used instead of  $y$  since these are typically time-dependent problems. These can all be extended to more space dimensions. These

equations describe different types of phenomena and require different techniques for their solution (both analytically and numerically), and so it is convenient to have names for classes of equations exhibiting the same general features. Other equations have some of the same features, and the classification scheme can be extended beyond the second order linear form given above. Some hint of this is given in the next few sections.

### E.1.2 Elliptic equations

The classic example of an elliptic equation is the *Poisson problem*

$$\nabla^2 u = f, \quad (\text{E.1})$$

where  $\nabla^2$  is the Laplacian operator and  $f$  is a given function of  $\vec{x} = (x, y)$  in some spatial domain  $\Omega$ . We seek a function  $u(\vec{x})$  in  $\Omega$  satisfying (E.1) together with some *boundary conditions* all along the boundary of  $\Omega$ . Elliptic equations typically model steady-state or equilibrium phenomena, and so there is no temporal dependence (however, see Section 2.16 for a counterexample). Elliptic equations may also arise in solving time-dependent problems if we are modeling some phenomena that are always in local equilibrium and equilibrate on time scales that are much faster than the time scale being modeled. For example, in “incompressible” flow the fast acoustic waves are not modeled and instead the pressure is computed by solving a Poisson problem at each time step which models the global effect of these waves.

Elliptic equations give boundary value problems where the solution at all points must be simultaneously determined based on the boundary conditions all around the domain. This typically leads to a very large sparse system of linear equations to be solved for the values of  $U$  at each grid point. If an elliptic equation must be solved in every time step of a time-dependent calculation, as in the examples above, then it is crucial that these systems be solved as efficiently as possible.

More generally, a linear elliptic equation has the form

$$Lu = f, \quad (\text{E.2})$$

where  $L$  is some *elliptic operator*. For our purposes we will consider only constant coefficient second order operators, which in  $N$  space dimensions have the form

$$L = \sum_{j,k=1}^N A_{jk} \frac{\partial^2}{\partial x_j \partial x_k} + \sum_{j=1}^N B_j \frac{\partial}{\partial x_j} + C, \quad (\text{E.3})$$

where the  $A_{jk}$ ,  $B_j$ ,  $C$  are real numbers. Note that since  $\partial^2 u / \partial x_j \partial x_k = \partial^2 u / \partial x_k \partial x_j$ , we can always choose the  $N \times N$  matrix  $A$  defined by the second order term to be symmetric. This operator is said to be elliptic if  $A$  is positive definite or negative definite, as defined in Section C.4. This means that  $v^T A v$  has the same sign for all nonzero vectors  $v \in \mathbb{R}^N$  and cannot pass through zero. This can be shown to ensure that the boundary value problem (E.2) has a unique solution. For an indication of why this is true, see Section E.3.5.

In two space dimensions writing the matrix as

$$A = \begin{bmatrix} a & b/2 \\ b/2 & c \end{bmatrix}$$

and considering when this matrix is definite, we find that the operator is elliptic if  $b^2 - 4ac < 0$ , as in the classification of the previous section.

For the Laplacian operator  $\nabla^2 u$ ,  $A$  is the  $N \times N$  identity matrix and so this is an elliptic operator. Note that in one space dimension  $\nabla^2 u$  reduces to  $u''(x)$  and the problem (E.1) is the 2-point boundary value problem considered in Chapter 2.

### E.1.3 Parabolic equations

If  $L$  is an elliptic operator with a positive definite  $A$ , then the time-dependent equation

$$u_t = Lu - f \quad (\text{E.4})$$

is well posed (see Section E.3.5) and is called *parabolic*. If  $L = \nabla^2$  is the Laplacian, then (E.4) is known as the *heat equation* or *diffusion equation* and models the diffusion of heat in a material, for example.

Now  $u(\vec{x}, t)$  varies with time and we require *initial data*  $u(\vec{x}, 0)$  for every  $\vec{x} \in \Omega$  as well as boundary conditions around the boundary at each time  $t > 0$ . If the boundary conditions are independent of time, then we might expect the heat distribution to reach a steady state in which  $u$  is independent of  $t$ . We could then solve for the steady state directly by setting  $u_t = 0$  in (E.4), which results in the elliptic equation (E.2).

Marching to steady state by solving the time-dependent equation (E.4) numerically would be one approach to solving the elliptic equation (E.2), but this is typically not the fastest method if all we require is the steady state.

### E.1.4 Hyperbolic equations

Rather than discretizing second order hyperbolic equations such as the wave equation  $u_{tt} = c^2 u_{xx}$ , we will consider a related form of hyperbolic equations known as *first order hyperbolic systems*. The linear problem in one space dimension has the form

$$u_t + Au_x = 0, \quad (\text{E.5})$$

where  $u(x, t) \in \mathbb{R}^s$  and  $A$  is an  $s \times s$  matrix. The problem is called *hyperbolic* if  $A$  has *real* eigenvalues and is *diagonalizable*, i.e., has a complete set of linearly independent eigenvectors. These conditions allow us to view the solution in terms of propagating waves, and indeed hyperbolic systems typically arise from physical processes that give wave motion or advective transport. This is explored more in Section 10.10.

The simplest example of a hyperbolic equation is the constant-coefficient *advection equation*

$$u_t + au_x = 0, \quad (\text{E.6})$$

where  $u$  is the advection velocity. The solution is simply  $u(x, t) = u(x - at, 0)$ , so any  $u$  profile simply advects with the flow at velocity  $a$ .

As a simple example of a linear hyperbolic system, the equations of linearized acoustics arising from elasticity or gas dynamics can be written as a first order system of two equations in one space dimension as

$$\begin{bmatrix} p \\ u \end{bmatrix}_t + \begin{bmatrix} 0 & \kappa_0 \\ 1/\rho_0 & 0 \end{bmatrix} \begin{bmatrix} p \\ u \end{bmatrix}_x = 0 \quad (\text{E.7})$$

in terms of pressure and velocity perturbations, where  $\rho_0$  is the background density and  $\kappa_0$  is the “bulk modulus” of the material. Note that if we differentiate the first equation with respect to  $t$ , the second with respect to  $x$ , and then eliminate  $u_{xt} = u_{tx}$ , we obtain the second order wave equation for the pressure:

$$p_{tt} = c^2 p_{xx},$$

where

$$c = \sqrt{\kappa_0/\rho_0}$$

is the speed of sound in the material.

Often hyperbolic equations arise most naturally as first order systems, as motivated in the next section, and we consider only this formulation.

## E.2 Derivation of partial differential equations from conservation principles

Many physically relevant partial differential equations can be derived based on the principle of conservation. We can view  $u(x, t)$  as a *concentration* or *density* function for some substance or chemical that is in dilute suspension in a liquid, for example. Basic equations of the same form arise in many other applications, however. The material presented here is meant to be a brief review, and much more complete discussions are available in many sources. See, for example, [55], [61], [66], [102].

A reasonable model to consider in one space dimension is the concentration or density of a contaminant in a stream or pipe, where the variable  $x$  represents distance along the pipe. The concentration is assumed to be constant across any cross section, so that its value varies only with  $x$ . The density function  $u(x, t)$  is defined in such a way that integrating the function  $u(x, t)$  between any two points  $x_1$  and  $x_2$  gives the total mass of the substance in this section of the pipe at time  $t$ :

$$\text{Total mass between } x_1 \text{ and } x_2 \text{ at time } t = \int_{x_1}^{x_2} u(x, t) dx.$$

The density function is measured in units such as grams/meter. (Note that this  $u$  really represents the integral over the cross section of the pipe of a density function that is properly measured in grams/meter<sup>3</sup>.)

The basic form of differential equation that models many physical processes can be derived in the following way. Consider a section  $x_1 < x < x_2$  and the manner in which  $\int_{x_1}^{x_2} u(x, t) dx$  changes with time. This integral represents the total mass of the substance in this section, so if we are studying a substance that is neither created nor destroyed within this section, then the total mass within this section can change only due to the *flux* or flow of particles through the endpoints of the section at  $x_1$  and  $x_2$ . This flux is given by some function  $f$  which, in the simplest case, depends only on the value of  $u$  at the corresponding point.

### E.2.1 Advection

If the substance is simply carried along (advected) in a flow at some constant velocity  $a$ , then the flux function is

$$f(u) = au. \quad (\text{E.8})$$

The local density  $u(x, t)$  (in grams/meter, say) multiplied by the velocity (in meters/sec, say) gives the flux of material past the point  $x$  (in grams/sec).

Since the total mass in  $[x_1, x_2]$  changes only due to the flux at the endpoints, we have

$$\frac{d}{dt} \int_{x_1}^{x_2} u(x, t) dx = f(u(x_1, t)) - f(u(x_2, t)). \quad (\text{E.9})$$

The minus sign on the last term comes from the fact that  $f$  is, by definition, the flux to the right.

If we assume that  $u$  and  $f$  are smooth functions, then this equation can be rewritten as

$$\frac{d}{dt} \int_{x_1}^{x_2} u(x, t) dx = \int_{x_1}^{x_2} \frac{\partial}{\partial x} f(u(x, t)) dx$$

or, with some further modification, as

$$\int_{x_1}^{x_2} \left[ \frac{\partial}{\partial t} u(x, t) + \frac{\partial}{\partial x} f(u(x, t)) \right] dx = 0.$$

Since this integral must be zero for all values of  $x_1$  and  $x_2$ , it follows that the integrand must be identically zero. This gives, finally, the differential equation

$$\frac{\partial}{\partial t} u(x, t) + \frac{\partial}{\partial x} f(u(x, t)) = 0. \quad (\text{E.10})$$

This form of equation is called a *conservation law*.

For the case considered in Section E.2.1,  $f(u) = au$  with  $a$  constant and this equation becomes the advection equation (E.6). This equation requires initial conditions and possibly also boundary conditions in order to determine a unique solution. The simplest case is the *Cauchy problem* on  $-\infty < x < \infty$  (with no boundary), also called the pure initial value problem. Then we need only to specify initial data

$$u(x, 0) = \eta(x). \quad (\text{E.11})$$

Physically, we would expect the initial profile of  $\eta$  to simply be carried along with the flow at speed  $a$ , so we should find

$$u(x, t) = \eta(x - at). \quad (\text{E.12})$$

It is easy to verify that this function satisfies the advection equation (E.6) and is the solution of the PDE.

The curves

$$x = x_0 + at$$

through each point  $x_0$  at time 0 are called the *characteristics* of the equation. If we set

$$U(t) = u(x_0 + at, t)$$

then

$$\begin{aligned} U'(t) &= au_x(x_0 + at, t) + u_t(x_0 + at, t) \\ &= 0 \end{aligned}$$

using (E.6). Along these curves the PDE reduces to a simple ordinary differential equation (ODE)  $U' = 0$  and the solution must be constant along each such curve, as is also seen from the solution (E.12).

### E.2.2 Diffusion

Now suppose that the fluid in the pipe is not flowing and has zero velocity. Then according to the above equation,  $u_t = 0$  and the initial profile  $\eta(x)$  does not change with time. However, if  $\eta$  is not constant in space then in fact it will tend to slowly change due to molecular diffusion. The velocity  $a$  should really be thought of as a *mean velocity*, the average velocity that the roughly  $10^{23}$  molecules in a given drop of fluid have. But individual molecules are bouncing around in different directions and so molecules of the substance we are tracking will tend to get spread around in the ambient fluid, just as a drop of ink spreads in water. There will tend to be a net motion from regions where the density is large to regions where it is smaller, and in fact it can be shown that the flux (in one dimension) is proportional to  $-u_x$ . The flux at a point  $x$  now depends on the value of  $u_x$  at this point, rather than on the value of  $u$ , so we write

$$f(u_x) = -\kappa u_x, \quad (\text{E.13})$$

where  $\kappa$  is the *diffusion coefficient*. The relation (E.13) is known as *Fick's law*. Using this flux in (E.10) gives

$$u_t = \kappa u_{xx}, \quad (\text{E.14})$$

which is known as the *diffusion equation*.

This equation is also called the *heat equation* since heat diffuses in much the same way. In this case  $u(x, t)$  represents the density of thermal energy, which is proportional to the temperature. The proportionality factor is the *heat capacity* of the material, which we'll take to be the value 1 (with suitable units) so that  $u$  can also be viewed as the temperature. The one-dimensional equation models the conduction of heat in a rod. The heat conduction coefficient  $\kappa$  depends on the material and how well it conducts heat. The relation (E.13) is known as *Fourier's law of heat conduction*, which states more generally that the flux of thermal energy is proportional to the temperature gradient.

In some problems the diffusion coefficient may vary with  $x$ , for example, in a rod made of a composite of different materials. Then  $f = -\kappa(x)u_x$  and the equation becomes

$$u_t = (\kappa(x)u_x)_x.$$

Returning to the example of fluid flow, more generally there would be both advection and diffusion occurring simultaneously. Then the flux is  $f(u, u_x) = au - \kappa u_x$ , giving the *advection-diffusion* equation

$$u_t + au_x = \kappa u_{xx}. \quad (\text{E.15})$$

The diffusion and advection-diffusion equations are examples of the general class of PDEs called *parabolic*.

### E.2.3 Source terms

In some situations  $\int_{x_1}^{x_2} u(x, t) dx$  changes due to effects other than flux through the end-points of the section, if there is some source or sink of the substance within the section. Denote the density function for such a source by  $\psi(x, t)$ . (Negative values of  $\psi$  correspond to a sink rather than a source.) Then the equation becomes

$$\frac{d}{dt} \int_{x_1}^{x_2} u(x, t) dx = - \int_{x_1}^{x_2} \frac{\partial}{\partial x} f(u(x, t)) dx + \int_{x_1}^{x_2} \psi(x, t) dx.$$

This leads to the PDE

$$u_t(x, t) + f(u(x, t))_x = \psi(x, t). \quad (\text{E.16})$$

For example, if we have heat conduction in a rod together with an external source of heat energy distributed along the rod with density  $\psi$ , then we have

$$u_t = \kappa u_{xx} + \psi.$$

In some cases the strength of the source may depend on the value of  $u$ . For example, if the rod is immersed in a liquid that is held at constant temperature  $u_0$ , then the flux of heat into the rod at the point  $(x, t)$  is proportional to  $u_0 - u(x, t)$  and the equation becomes

$$u_t(x, t) = \kappa u_{xx}(x, t) + \alpha(u_0 - u(x, t)).$$

### E.2.4 Reaction-diffusion equations

One common form of source term arises from chemical kinetics. If the components of  $u \in \mathbb{R}^s$  represent concentrations of  $s$  different species reacting with one another, then the kinetics equations have the form  $u_t = \mathbb{R}(u)$ , as described in Section 7.4.1. This assumes the different species are well mixed at all times and so the concentrations vary only with time. If there are spatial variations in concentrations, then these equations may be combined with diffusion of each species. This would lead to a system of *reaction-diffusion equations* of the form

$$u_t = \kappa u_{xx} + \mathbb{R}(u). \quad (\text{E.17})$$

The diffusion coefficient could be different for each species, in which case  $\kappa$  would be a diagonal matrix instead of a scalar. This generalizes to more space dimensions by replacing  $u_{xx}$  by  $\nabla^2 u$ , the Laplacian of  $u$ .

Advection terms might also be present if the reactions are taking place in a flowing fluid. More generally the reaction-diffusion equations may be coupled with nonlinear equations of fluid dynamics, which may themselves contain both hyperbolic terms and parabolic viscous terms.

## E.3 Fourier analysis of linear partial differential equations

For *linear* PDEs, Fourier analysis is often used to obtain solutions or perform theoretical analysis. This is because the functions  $e^{i\xi x} = \cos(\xi x) + i \sin(\xi x)$  are essentially<sup>1</sup>

<sup>1</sup>On a periodic domain. For the Cauchy problem these functions are not  $L^2$  functions and so strictly speaking are not called eigenfunctions, but this is unimportant for our purposes.

*eigenfunctions* of the differentiation operator  $\partial_x = \frac{\partial}{\partial x}$ . Differentiating this function gives a scalar multiple of the function, and hence simple differential equations (linear constant coefficient ones, at least) are simplified and can be reduced to algebraic equations.

Fourier analysis is equally important in the study of finite difference methods for *linear* PDEs for the same reason: these same functions are eigenfunctions of translation invariant finite difference operators. This is exploited in Sections 9.6 and 10.5, where von Neumann stability analysis of finite difference methods is discussed. An understanding of Fourier analysis of PDEs is also required in Section 10.9, where finite difference methods are analyzed by studying “modified equations.”

### E.3.1 Fourier transforms

Recall that a function  $v(x)$  is in the space  $L^2$  if it has a finite 2-norm, defined by

$$\|v\|_2 = \left( \int_{-\infty}^{\infty} |v(x)|^2 dx \right)^{1/2}.$$

If  $v \in L^2$ , then we can define its Fourier transform  $\hat{v}(\xi)$  by

$$\hat{v}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} v(x) e^{-i\xi x} dx. \quad (\text{E.18})$$

The function  $\hat{v}(\xi)$  is also in  $L^2$  and in fact it has exactly the same 2-norm as  $v$ ,

$$\|\hat{v}\|_2 = \|v\|_2. \quad (\text{E.19})$$

This is known as *Parseval's relation*.

We can express the original function  $v(x)$  as a linear combination of the set of functions  $e^{i\xi x}$  for different values of  $\xi$ , which together form a basis for the infinite dimensional function space  $L^2$ . The Fourier transform  $\hat{v}(\xi)$  gives the coefficients in the expression

$$v(x) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{v}(\xi) e^{i\xi x} d\xi, \quad (\text{E.20})$$

which is known as the *inverse Fourier transform*. This is analogous to writing a vector as a linear combination of basis vectors.

### E.3.2 The advection equation

We already know the solution (E.12) to the advection equation (E.6), but to illustrate the role of Fourier analysis we will solve the advection equation  $u_t + au_x = 0$  using Fourier transforms. We will transform in  $x$  only and denote the transform of  $u(x, t)$  (a function of  $x$  at each fixed  $t$ ) by  $\hat{u}(\xi, t)$ :

$$\hat{u}(\xi, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} u(x, t) e^{-i\xi x} dx. \quad (\text{E.21})$$

Then

$$u(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(\xi, t) e^{i\xi x} d\xi \quad (\text{E.22})$$

and differentiating this with respect to  $t$  and  $x$  gives



$$u_t(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}_t(\xi, t) e^{i\xi x} dx,$$

$$u_x(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{u}(\xi, t) i\xi e^{i\xi x} dx.$$

From this we see that the Fourier transform of  $u_t(x, t)$  is  $\hat{u}_t(\xi, t)$  and the Fourier transform of  $u_x(x, t)$  is  $i\xi \hat{u}(\xi, t)$ . Fourier transforming the advection equation by computing

$$\frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} (u_t + au_x) e^{-i\xi x} dx = 0$$

thus gives

$$\hat{u}_t(\xi, t) + ai\xi \hat{u}(\xi, t) = 0$$

or

$$\hat{u}_t = -i\xi a \hat{u}.$$

This is a time-dependent ODE for the evolution of  $\hat{u}(\xi, t)$  in time. There are two important points to notice:

- Since differentiation with respect to  $x$  has become multiplication by  $i\xi$  after Fourier transforming, the original PDE involving derivatives with respect to  $x$  and  $t$  has become an ODE in  $t$  alone.
- The ODEs for different values of  $\xi$  are decoupled from one another. We have to solve an infinite number of ODEs, one for each value of  $\xi$ , but they are decoupled scalar equations rather than a coupled system.

It is easy to solve these ODEs. We need initial data  $\hat{u}(\xi, 0)$  at time  $t = 0$  for each value of  $\xi$ , but this comes from Fourier transforming the initial data  $u(x, 0) = \eta(x)$ ,

$$\hat{u}(\xi, 0) = \hat{\eta}(\xi) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \eta(x) e^{-i\xi x} dx.$$

Solving the ODEs then gives

$$\hat{u}(\xi, t) = e^{-i\xi at} \hat{\eta}(\xi). \quad (\text{E.23})$$

We can now Fourier transform back using (E.22) to get the desired solution  $u(x, t)$ :

$$\begin{aligned} u(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-i\xi at} \hat{\eta}(\xi) e^{i\xi x} d\xi \\ &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\eta}(\xi) e^{i\xi(x-at)} d\xi \\ &= \eta(x - at). \end{aligned}$$

This last equality comes from noting that we are simply evaluating the inverse Fourier transform of  $\hat{\eta}$  at the point  $x - at$ . We see that we have recovered the standard solution (E.12) of the advection equation in this manner.

We can also calculate the “Green’s function” for the advection equation, the solution to  $u_t + au_x = 0$  with special initial data  $\eta(x) = \delta(x - \bar{x})$ . The solution is clearly

$$G(x, t; \bar{x}) = \delta(x - \bar{x} - at). \quad (\text{E.24})$$

The general solution for arbitrary  $\eta(x)$  can be written as a linear combination of these Green's functions, weighted by the data:

$$\begin{aligned} u(x, t) &= \int_{-\infty}^{\infty} \eta(\bar{x}) G(x, t; \bar{x}) d\bar{x} \\ &= \int_{-\infty}^{\infty} \eta(\bar{x}) \delta(x - \bar{x} - at) d\bar{x} \\ &= \eta(x - at). \end{aligned} \quad (\text{E.25})$$

### E.3.3 The heat equation

Now consider the heat equation,

$$u_t = \kappa u_{xx}. \quad (\text{E.26})$$

Since the Fourier transform of  $u_{xx}(x, t)$  is  $(i\xi)^2 \hat{u}(\xi, t) = -\xi^2 \hat{u}(\xi, t)$ , Fourier transforming (E.26) gives the ODE

$$\hat{u}_t(\xi, t) = -\kappa \xi^2 \hat{u}(\xi, t). \quad (\text{E.27})$$

Again we have initial data  $\hat{u}(\xi, 0) = \hat{\eta}(\xi)$  from the given initial data on  $u$ . Now solving the ODE gives

$$\hat{u}(\xi, t) = e^{-\kappa \xi^2 t} \hat{\eta}(\xi). \quad (\text{E.28})$$

Note that this has a very different character than (E.23), the Fourier transform obtained from the advection equation. For the advection equation,  $\hat{u}(\xi, t) = e^{ia\xi t} \hat{\eta}(\xi)$  and  $|\hat{u}(\xi, t)| = |\hat{\eta}(\xi)|$  for all  $t$ . Each Fourier component maintains its original amplitude and is modified only in phase, leading to a traveling wave behavior in the solution.

For the heat equation, however,  $|\hat{u}(\xi, t)|$  decays in time exponentially fast. The decay rate depends on  $\kappa$ , the diffusion coefficient, and also on  $\xi$ , the wave number. Highly oscillatory components (with  $\xi^2$  large) decay much faster than those with low wave numbers. This results in a *smoothing* of the solution as time evolves. (See Figure 9.3.)

The fact that the solution contains components that decay at very different rates leads us to expect numerical difficulties with stiffness, similar to those discussed for ODEs in Chapter 8. In Section 9.4 we will see that this is indeed the case and that implicit methods must generally be used to efficiently solve the heat equation.

A single Fourier mode decaying exponentially in time is one special solution to the heat equation. Another class of special solutions that is useful to know about arises from Gaussian initial data. The Fourier transform of a Gaussian is another Gaussian. Take

$$\eta(x) = e^{-\beta x^2} \quad (\text{E.29})$$

for some  $\beta$ . Then

$$\begin{aligned} \hat{\eta}(\xi) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\beta x^2} e^{i\xi x} dx \\ &= \frac{1}{\sqrt{2\beta}} e^{-\xi^2/4\beta}. \end{aligned} \quad (\text{E.30})$$

Then (E.22) combined with (E.28) gives the solution

$$\begin{aligned} u(x, t) &= \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} e^{-\kappa \xi^2 t} \hat{\eta}(\xi) e^{i\xi x} d\xi \\ &= \frac{1}{2\sqrt{\pi\beta}} \int_{-\infty}^{\infty} e^{-\xi^2(\kappa t + 1/4\beta)} e^{i\xi x} d\xi. \end{aligned} \quad (\text{E.31})$$

This is just the inverse Fourier transform of another Gaussian, with  $e^{-\xi^2/4C}$  in place of  $e^{-\xi^2/4\beta}$ , where  $C = 1/(4\kappa t + 1/\beta)$ , and so

$$\begin{aligned} u(x, t) &= \sqrt{\frac{C}{\beta}} e^{-Cx^2} \\ &= \frac{1}{\sqrt{4\beta\kappa t + 1}} e^{-x^2/(4\kappa t + 1/\beta)}. \end{aligned} \quad (\text{E.32})$$

As  $t$  increases this Gaussian becomes more spread out and the magnitude decreases, as we expect from diffusion. You can check that (E.32) solves the heat equation directly by differentiating.

Note what happens if we shift the initial data to a different location,

$$\eta(x) = e^{-\beta(x-\bar{x})^2}. \quad (\text{E.33})$$

Then the solution simply shifts too,

$$u(x, t) = \frac{1}{\sqrt{4\beta\kappa t + 1}} e^{-(x-\bar{x})^2/(4\kappa t + 1/\beta)}. \quad (\text{E.34})$$

As a special case we can find the Green's function for the heat equation. Scale the data (E.33) by  $\sqrt{\beta/\pi}$  so that it has integral equal to 1 and represents a smeared out version of the delta function, setting

$$v_\beta(x, 0; \bar{x}) = \sqrt{\frac{\beta}{\pi}} e^{-\beta(x-\bar{x})^2}. \quad (\text{E.35})$$

The solution to (E.26) with this data is then

$$v_\beta(x, t; \bar{x}) = \frac{1}{\sqrt{4\pi\kappa t + \pi/\beta}} e^{-(x-\bar{x})^2/(4\kappa t + 1/\beta)}. \quad (\text{E.36})$$

Now let  $\beta \rightarrow 0$  so the initial data approaches a delta function. The solution  $v_\beta(x, t; \bar{x})$  then approaches the Green's function for (E.26),

$$G(x, t; \bar{x}) = \frac{1}{\sqrt{4\pi\kappa t}} e^{-(x-\bar{x})^2/(4\kappa t)}. \quad (\text{E.37})$$

Delta function initial data spreads out into a decaying Gaussian. Note that initial data concentrated at a single point (an idealization of a very tiny drop of ink in water, say)

spreads out immediately to have a nonzero value for all  $x$ . More generally if we look at the solution for general initial data by integrating  $\eta(\bar{x})$  against the Green's function, we see that the data at each  $\bar{x}$  immediately have an effect everywhere. Thus information propagates infinitely quickly in the heat equation. This is quite different from the advection equation, where the data at  $\bar{x}$  affect the solution at only one point  $\bar{x} + at$  at a later time  $t$ .

Of course physically information cannot propagate at infinite speed, and the discrepancy with the behavior of the heat equation simply shows that the heat equation is only a model of reality, and one that is not exactly correct. But note that away from the point  $\bar{x}$  the effect decays very rapidly and so this is often a very accurate model of reality.

### E.3.4 The backward heat equation

Note that the diffusion coefficient  $\kappa$  is required to be positive (because heat flows from warm to cool regions, not the other way around). Mathematically we could consider trying to solve the equation (E.26) with  $\kappa < 0$  but this equation turns out to be *ill-posed*<sup>2</sup>. One way to interpret this physically is to view it as solving the heat equation with coefficient  $-\kappa > 0$  backward in time, starting at some final heat distribution and working backward to the heat distribution at earlier times. Intuitively this can be seen to be ill-posed because many different sets of initial data can give rise to very similar solutions at later times since any high-frequency components in initial data for the heat equation are very rapidly smoothed out. We can formally solve the backward heat equation in Fourier space with the expression (E.28), but for  $\kappa < 0$  each Fourier mode is growing exponentially in time instead of decaying. Exponential growth in itself doesn't make the problem ill posed—many well-posed equations have exponentially growing solutions—but the problem with (E.28) is that the growth rate depends on the wave number  $\xi$  and increases without bound with  $\xi$ . We can make an infinitesimal high-frequency perturbation to the initial data that will make an order 1 change in the solution at some fixed time  $t$ . Hence the solution to the backward heat equation does not depend continuously on the data.

### E.3.5 More general parabolic equations

Consider a second order parabolic equation  $u_t = Lu$  in  $N$  space dimensions as defined in Section E.1.3. For simplicity, just consider the second order part of the system, so

$$L = \sum_{j,k=1}^N A_{jk} \frac{\partial^2}{\partial x_j \partial x_k}, \quad (\text{E.38})$$

where the  $N \times N$  coefficient matrix  $A$  is symmetric positive definite. Let  $\xi = (\xi_1, \dots, \xi_N)$  be a wave number vector, one for each space dimension, so that a general Fourier mode has the form  $e^{i\xi \cdot x}$ , where  $x = (x_1, \dots, x_N)$ . Let  $\hat{u}(\xi, t)$  be the Fourier transform of  $u(x, t)$  in all space dimensions, defined by

$$\hat{u}(\xi, t) = \frac{1}{\sqrt{2\pi}} \int u(x, t) e^{-i\xi \cdot x} dx, \quad (\text{E.39})$$

<sup>2</sup>A problem is said to be *well posed* (in the sense of Hadamard) if it has a unique solution for every valid set of data and if the solution depends continuously on the data.

where the integral is now over all of  $N$ -dimensional space. Then it can be verified that the parabolic equation  $u_t = Lu$  transforms to

$$\hat{u}_t(\xi, t) = -\xi^T A \xi \hat{u}(\xi, t). \quad (\text{E.40})$$

The requirement that  $A$  be positive definite is just what is needed to ensure that all Fourier modes decay, giving a well-posed problem. If  $\xi^T A \xi < 0$  for some vector  $\xi$ , then it is also negative for any scalar multiple  $\alpha \xi$  of this wave vector, and there would be exponential growth of some Fourier modes with arbitrarily large growth rate  $\alpha^2 \xi^T A \xi$ . As observed for the backward heat equation, this would give an ill-posed problem. (For the heat equation with  $N = 1$ , the matrix  $A$  is just the scalar coefficient  $\kappa$ .)

### E.3.6 Dispersive waves

Now consider the equation

$$u_t = u_{xxx}. \quad (\text{E.41})$$

Fourier transforming now leads to the ODE

$$\hat{u}_t(\xi, t) = -i\xi^3 \hat{u}(\xi, t),$$

so

$$\hat{u}(\xi, t) = e^{-i\xi^3 t} \hat{\eta}(\xi).$$

This has a character similar to advection problems in that  $|\hat{u}(\xi, t)| = |\hat{\eta}(\xi)|$  for all time and each Fourier component maintains its original amplitude. However, when we recombine with the inverse Fourier transform we obtain

$$u(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\eta}(\xi) e^{i\xi(x-\xi^2 t)} d\xi, \quad (\text{E.42})$$

which shows that the Fourier component with wave number  $\xi$  is propagating with velocity  $\xi^2$ . In the advection equation all Fourier components propagate with the same speed  $a$ , and hence the shape of the initial data is preserved with time. The solution is the initial data shifted over a distance  $at$ .

With (E.41), the shape of the initial data in general will not be preserved, unless the data is simply a single Fourier mode. This behavior is called *dispersive* since the Fourier components disperse relative to one another. Smooth data typically lead to oscillatory solutions since the cancellation of high wave number modes that smoothness depends on will be lost as these modes shift relative to one another. See, for example, Whitham [102] for an extensive discussion of dispersive waves.

Extending this analysis to an equation of the form

$$u_t + au_x + bu_{xxx} = 0, \quad (\text{E.43})$$

we find that the solution can be written as

$$u(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\eta}(\xi) e^{i\xi(x-(a-b\xi^2)t)} d\xi,$$

where  $\hat{\eta}(\xi)$  is the Fourier transform of the initial data  $\eta(x)$ . Each Fourier mode  $e^{i\xi x}$  propagates at velocity  $a - b\xi^2$ , called the phase velocity of this wave number. In general the initial data  $\eta(x)$  is a linear combination of infinitely many different Fourier modes. For  $b \neq 0$  these modes propagate at different speeds relative to one another. Their peaks and troughs will be shifted relative to other modes and they will no longer add up to a shifted version of the original data. The waves are called dispersive since the different modes do not move in tandem. Moreover, we will see below that the “energy” associated with different wave numbers also disperses.

### E.3.7 Even- versus odd-order derivatives

Note that odd-order derivatives  $\partial_x, \partial_x^3, \dots$  (as in the advection equation or the dispersive equation (E.41)) have pure imaginary eigenvalues  $i\xi, -i\xi^3, \dots$ , which results in Fourier components that propagate with their magnitude preserved. Even-order derivatives, such as the  $\partial_x^2$  in the heat equation, have real eigenvalues ( $-\xi^2$  for the heat equation), which results in exponential decay of the eigencomponents. Another such equation is

$$u_t = -u_{xxxx},$$

in which case  $\hat{u}(\xi, t) = e^{-\xi^4 t} \hat{\eta}(\xi)$ . Solutions to this equation behave much like solutions to the heat equation but with even more rapid damping of oscillatory data.

Another interesting example is

$$u_t = -u_{xx} - u_{xxxx}, \quad (\text{E.44})$$

for which

$$\hat{u}(\xi, t) = e^{(\xi^2 - \xi^4)t} \hat{\eta}(\xi). \quad (\text{E.45})$$

Note that the  $u_{xx}$  term has the “wrong” sign—it looks like a backward heat equation and there is exponential growth of some wave numbers. But for  $|\xi| > 1$  the fourth order diffusion dominates and  $\hat{u}(\xi, t) \rightarrow 0$  exponentially fast. For all  $\xi$  we have  $|\hat{u}(\xi, t)| \leq e^{t/4} |\hat{\eta}(\xi)|$  (since  $\xi^2 - \xi^4 \leq 1/4$  for all  $\xi$ ) and the equation is well posed.

The Kuramoto–Sivashinsky equation (11.13) involves terms of this form, and the exponential growth of some wave numbers leads to chaotic behavior and interesting pattern formation.

### E.3.8 The Schrödinger equation

The discussion of the previous section supposed that  $u(x, t)$  is a real-valued function. The vacuum Schrödinger equation for a complex wave function  $\psi(x, t)$  has the form (dropping some physical constants)

$$i\psi_t(x, t) = -\psi_{xx}(x, t). \quad (\text{E.46})$$

This involves a second derivative, but note the crucial fact that  $\psi_t$  is multiplied by  $i$ . Fourier transforming thus gives

$$i\hat{\psi}_t(\xi, t) = \xi^2 \hat{\psi}(\xi, t),$$

so

$$\hat{\psi}(\xi, t) = e^{-i\xi^2 t} \hat{\psi}(\xi, 0)$$

and

$$\psi(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\psi}(\xi, 0) e^{i\xi(x-(a-\xi)t)} d\xi.$$

Hence the Schrödinger equation has dispersive wavelike solutions in spite of the even-order derivative.

### E.3.9 The dispersion relation

Consider a general real-valued PDE of the form

$$u_t + a_1 u_x + a_3 u_{xxx} + a_5 u_{xxxxx} + \cdots = 0 \quad (\text{E.47})$$

that contains only odd-order derivative in  $x$ . The Fourier transform  $\hat{u}(\xi, t)$  satisfies

$$\hat{u}_t(\xi, t) + a_1 i \xi \hat{u}(\xi, t) - a_3 i \xi^3 \hat{u}(\xi, t) + a_5 i \xi^5 \hat{u}(\xi, t) + \cdots = 0,$$

and hence

$$\hat{u}(\xi, t) = e^{-i\omega t} \hat{\eta}(\xi),$$

where

$$\omega = \omega(\xi) = a_1 \xi - a_3 \xi^3 + a_5 \xi^5 - \cdots. \quad (\text{E.48})$$

The solution can thus be written as

$$u(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\eta}(\xi) e^{i(\xi x - \omega(\xi)t)} d\xi. \quad (\text{E.49})$$

The relation (E.48) between  $\xi$  and  $\omega$  is called the *dispersion relation* for the PDE. Once we've gone through this full Fourier analysis a couple times we realize that since the different wave numbers  $\xi$  decouple, the dispersion relation for a linear PDE can be found simply by substituting a single Fourier mode of the form

$$u(x, t) = e^{-i\omega t} e^{i\xi x} \quad (\text{E.50})$$

into the PDE and canceling the common terms to find the relation between  $\omega$  and  $\xi$ . This is similar to what is done when applying von Neumann analysis for analyzing finite difference methods (see Section 9.6). In fact, there is a close relation between determining the dispersion relation and doing von Neumann analysis, and the dispersion relation for a finite difference method can be defined by an approach similar to von Neumann analysis by setting  $U_j^n = e^{-i\omega n k} e^{i\xi j h}$ , i.e., using  $e^{-i\omega k}$  in place of  $g$ .

Note that this same analysis can be done for equations that involve even-order derivatives, such as

$$u_t + a_1 u_x + a_2 u_{xx} + a_3 u_{xxx} + a_4 u_{xxxx} + \cdots = 0,$$

but then we find that

$$\omega(\xi) = a_1 \xi + i a_2 \xi^2 - a_3 \xi^3 - i a_4 \xi^4 - \cdots.$$

The even-order derivatives give imaginary terms in  $\omega(\xi)$  so that

$$e^{-i\omega t} = e^{(a_2\xi^2 - a_4\xi^4 + \dots)t} e^{i(a_1\xi - a_3\xi^3 + \dots)t}.$$

The first term gives exponential growth or decay, as we expect from Section E.3.3, rather than dispersive behavior. For this reason we call the PDE (purely) dispersive only if  $\omega(\xi)$  is real for all  $\xi \in \mathbb{R}$ . Informally we also speak of an equation like  $u_t = u_{xx} + u_{xxx}$  as having both a diffusive and a dispersive term.

In the purely dispersive case (E.47) the single Fourier mode (E.50) can be written as

$$u(x, t) = e^{i\xi(x - (\omega/\xi)t)}$$

and so a pure mode of this form propagates at velocity  $\omega/\xi$ . This is called the *phase velocity* for this wave number,

$$c_p(\xi) = \frac{\omega(\xi)}{\xi}. \quad (\text{E.51})$$

Most physical problems have data  $\eta(x)$  that is not simply sinusoidal for all  $x \in (-\infty, \infty)$  but instead is concentrated in some restricted region, e.g., a Gaussian pulse as in (E.29),

$$\eta(x) = e^{-\beta x^2}. \quad (\text{E.52})$$

The Fourier transform of this function is a Gaussian in  $\xi$ , (E.30),

$$\hat{\eta}(\xi) = \frac{1}{\sqrt{2\beta}} e^{-\xi^2/4\beta}. \quad (\text{E.53})$$

Note that for  $\beta$  small,  $\eta(x)$  is a broad and smooth Gaussian with a Fourier transform that is sharply peaked near  $\xi = 0$ . In this case  $\eta(x)$  consists primarily of low wave number smooth components. For  $\beta$  large  $\eta(x)$  is sharply peaked while the transform is broad. More high wave number components are needed to represent the rapid spatial variation of  $\eta(x)$  in this case.

If we solve the dispersive equation with data of this form, then the different modes propagate at different phase velocities and will no longer sum to a Gaussian, and the solution evolves as shown in Figure E.1, forming “dispersive ripples.” Note that for large times it is apparent that the wave length of the ripples is changing through this wave and that the energy associated with the low wave numbers is apparently moving faster than the energy associated with larger wave numbers. The propagation velocity of this energy is not, however, the phase velocity  $c_p(\xi)$ . Instead it is given by the *group velocity*

$$c_g(\xi) = \frac{d\omega(\xi)}{d\xi}. \quad (\text{E.54})$$

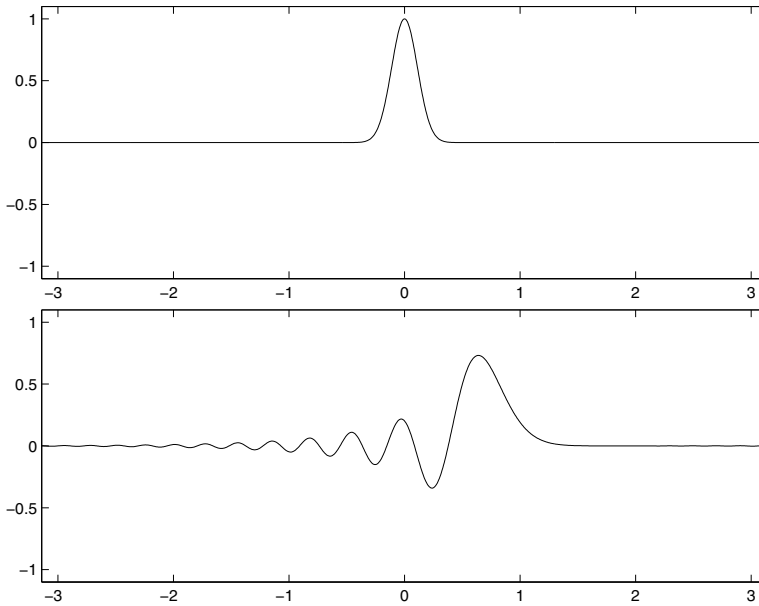
For the advection equation  $u_t + au_x = 0$  the dispersion relation is  $\omega(\xi) = a\xi$  and the group velocity agrees with the phase velocity (since all waves propagate at the same velocity  $a$ ), but more generally the two do not agree. For the dispersive equation (E.43),  $\omega(\xi) = a\xi - b\xi^3$  and we find that

$$c_g(\xi) = a - 3b\xi^2,$$

whereas

$$c_p(\xi) = a - b\xi^2.$$





**Figure E.1.** *Gaussian initial data propagating with dispersion.*

### E.3.10 Wave packets

The notion and importance of group velocity is easiest to appreciate by considering a “wave packet” with data of the form

$$\eta(x) = e^{i\xi_0 x} e^{-\beta x^2} \quad (\text{E.55})$$

or the real part of such a wave,

$$\eta(x) = \cos(\xi_0 x) e^{-\beta x^2}. \quad (\text{E.56})$$

This is a single Fourier mode modulated by a Gaussian, as shown in Figure E.2.

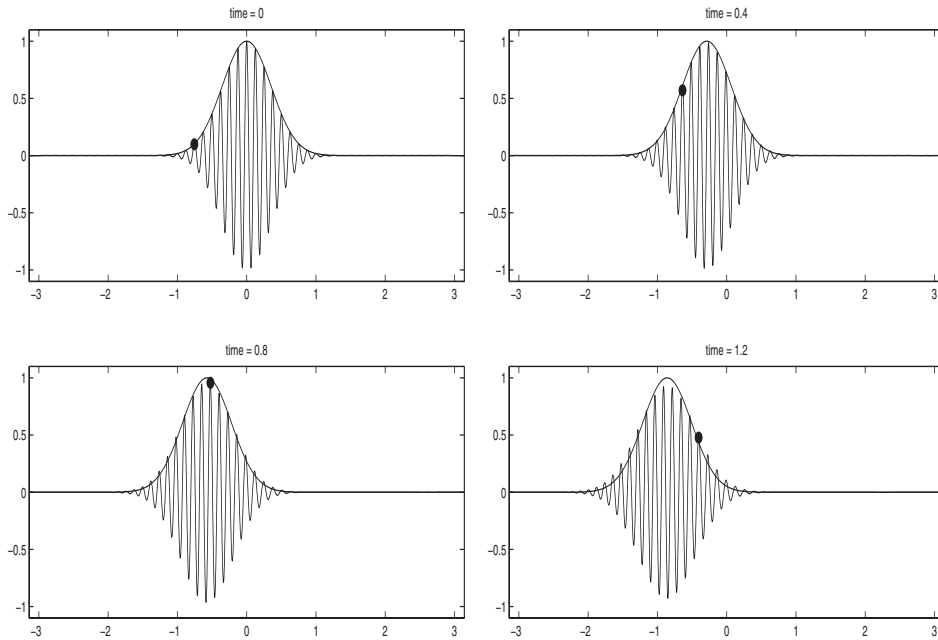
The Fourier transform of (E.55) is

$$\hat{\eta}(\xi) = \frac{1}{\sqrt{2\beta}} e^{-(\xi - \xi_0)^2 / 4\beta}, \quad (\text{E.57})$$

a Gaussian centered about  $\xi - \xi_0$ . If the packet is fairly broad ( $\beta$  small), then the Fourier transform is concentrated near  $\xi = \xi_0$  and hence the propagation properties of the wave packet are well approximated in terms of the phase velocity  $c_p(\xi)$  and the group velocity  $c_g(\xi)$ . The wave crests propagate at the speed  $c_p(\xi_0)$ , while the envelope of the packet propagates at the group velocity  $c_g(\xi_0)$ .

To get some idea of why the packet propagates at the group velocity, consider the expression (E.49),

$$u(x, t) = \frac{1}{\sqrt{2\pi}} \int_{-\infty}^{\infty} \hat{\eta}(\xi) e^{i(\xi x - \omega(\xi)t)} d\xi.$$



**Figure E.2.** The oscillatory wave packet satisfies the dispersive equation  $u_t + au_x + bu_{xxx} = 0$ . Also shown is a black dot attached to one wave crest, translating at the phase velocity  $c_p(\xi_0)$ , and a Gaussian that is translating at the group velocity  $c_g(\xi_0)$ . Shown for a case in which  $c_g(\xi_0) < 0 < c_p(\xi_0)$ .

For a concentrated packet, we expect  $u(x, t)$  to be very close to zero for most  $x$ , except near some point  $ct$ , where  $c$  is the propagation velocity of the packet. To estimate  $c$  we will ask where this integral could give something nonzero. At each fixed  $x$  the integral is a Gaussian in  $\xi$  (the function  $\hat{\eta}(\xi)$ ) multiplied by an oscillatory function of  $\xi$  (the exponential factor). Integrating this product will give essentially zero at a particular  $x$  provided the oscillatory part is oscillating rapidly enough in  $\xi$  that it averages out to zero, although it is modulated by the Gaussian  $\hat{\eta}(\xi)$ . This happens provided the function  $\xi x - \omega(\xi)t$  appearing as the phase in the exponential is rapidly varying as a function of  $\xi$  at this  $x$ . Conversely, we expect the integral to be significantly different from zero only near points  $x$  where this phase function is stationary, i.e., where

$$\frac{d}{d\xi}(\xi x - \omega(\xi)t) = 0.$$

This occurs at

$$x = \omega'(\xi)t,$$

showing that the wave packet propagates at the group velocity  $c_g = \omega'(\xi)$ . This approach to studying oscillatory integrals is called the “method of stationary phase” and is useful in other applications as well. See, for example, [55], [102] for more on dispersive waves.