

# An Introduction to Wave Equations and Solitons

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# Section 1

## Wave Equations

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### 1.1 Introduction

This first section of these notes is intended as a very basic introduction to the theory of wave equations, concentrating on the case of a single space dimension. We will start pretty much from scratch, not assuming any prior experience with either the special terminology or the techniques used in working with these equations. On the other hand, given the nature of the audience, I will assume a fairly sophisticated general background in analysis.

An experienced applied mathematician can often tell a great deal about the behavior of solutions to a wave equation from just a cursory look at its structure. My goal in the next few sections is to disclose some of the secrets that make this possible.

What we mean by a *wave equation* will gradually be made more precise as we proceed. At first, we will just mean a certain kind of ordinary differential equation on the space  $C^\infty(\mathbf{R}^n, V)$ , where  $V$  is some finite dimensional vector space, usually  $\mathbf{R}$  or  $\mathbf{C}$ , (and generally we will take  $n = 1$ ). Thus the wave equation will look like:

$$(*) \quad u_t = f(u),$$

where  $u$  signifies a point of  $C^\infty(\mathbf{R}^n, V)$ ,  $u_t$  means  $\frac{du}{dt}$ , and  $f$  is a special kind of map of  $C^\infty(\mathbf{R}^n, V)$  to itself, namely it is a “partial differential operator”, i.e.,  $f(u)(x)$  is a smooth function  $F(u(x), u_{x_i}(x), u_{x_i x_j}(x), \dots)$  of the values of  $u$  and certain of its partial derivatives at  $x$ . (In fact, below the function  $F$  will almost always be a polynomial.) A solution of  $(*)$  is a smooth curve  $u(t)$  in  $C^\infty(\mathbf{R}^n, V)$ , such that if we write  $u(t)(x) = u(x, t)$ , then

$$\frac{\partial u}{\partial t}(x, t) = F\left(u(x), \frac{\partial u}{\partial x_i}(x, t), \frac{\partial^2 u}{\partial x_i \partial x_j}(x, t), \dots\right).$$

We will be interested in solving the so-called “Cauchy Problem” for such partial differential equations, i.e., finding a solution, in the above sense, with  $u(x, 0)$  some given element  $u_0(x)$  of  $C^\infty(\mathbf{R}^n, V)$ . So far, this should more properly be called simply an “evolution equation”. In general such equations will describe evolving phenomena which are *not* wave-like in character and, as we said above, it is only after certain additional assumptions are made concerning the function  $F$  that it is appropriate to call such an evolution equation a wave equation.

We will be interested of course in the obvious questions of existence, uniqueness, and general properties of solutions of the Cauchy problem, but even more it will be the nature and properties of certain special solutions that will concern us. In particular we will try to understand the mechanism behind the remarkable behavior of the so-called soliton solutions of certain special wave equations such as the Korteweg de Vries Equation (KdV), the Sine-Gordon Equation (SGE), the Nonlinear Schrödinger Equation (NLS), and other so-called “integrable equations”.

As well as first order ODE on  $C^\infty(\mathbf{R}^n, V)$  we could also consider second and higher order ODE, but these can be easily reduced to first order ODE by the standard trick of adding more dependent variables. For example, to study the classic wave equation in one space dimension,  $u_{tt} = c^2 u_{xx}$ , a second order ODE, we can add a new independent variable  $v$  and consider instead the first order system  $u_t = v$ ,  $v_t = c^2 u_{xx}$  (which we can put in the form (\*) by writing  $U_t = F(U)$ , with  $U = (u, v)$ ,  $F(u, v) = (v, c^2 u_{xx})$ ).

## 1.2 Travelling Waves and Plane Waves

Before discussing particular model wave equations, we will look at the kind of behavior we expect to see in solutions. There are a number of important simplifications in the description of wave propagation for the case of a single space dimension, and to develop a feeling for many of the important concepts it is best to see them first without the extra complexities that come with higher dimensions, so in what follows we will concentrate almost solely on the case  $n = 1$ .

Let's recall the basic intuitive idea of what is meant by "wave motion". Suppose that  $u(x, t)$  represents the "strength" or "amplitude" of some scalar physical quantity at the spatial point  $x$  and time  $t$ . If you like, you can think of  $u$  as representing the height of water in a canal. Then the graph of  $u^0(x) = u(x, t_0)$  gives a snapshot of  $u$  at time  $t_0$ . It is frequently the case that we can understand the evolution of  $u$  in time as representing the propagation of the shape of this graph. In other words, for  $t_1$  close to  $t_0$ , the shape of the graph of  $u^1(x) = u(x, t_1)$  near  $x_0$  will be related in some simple way to the shape of  $u^0$  near  $x_0$ .

Perhaps the purest form of this is exhibited by a so-called *travelling wave*. This is a function  $u$  of the form  $u(x, t) = f(x - ct)$  where  $f : \mathbf{R} \rightarrow V$  is a function defining the wave shape, and  $c$  is a real number defining the propagation speed of the wave. Let us define the *profile* of the wave at time  $t$  to be the graph of the function  $x \mapsto u(x, t)$ . Then the initial profile (at time  $t = 0$ ) is just the graph of  $f$ , and **at any later time  $t$ , the profile at time  $t$  is obtained by translating each point  $(x, f(x))$  of the initial profile  $ct$  units to the right to the point  $(x + ct, f(x))$** . In other words, the wave profile of a travelling wave just propagates by rigid translation with velocity  $c$ .

(We will see below that the general solution of the equation  $u_t - cu_x$  is an arbitrary travelling wave moving with velocity  $c$ , and that the general solution to the equation  $u_{tt} - c^2 u_{xx}$  is the sum (or "superposition") of two arbitrary travelling waves, both moving with speed  $|c|$ , but in opposite directions.)

There is a special kind of complex-valued travelling wave, called a *plane wave*, that plays a fundamental rôle in the theory of linear wave equations. The general form of a plane wave is  $u(x, t) = Ae^{i\phi} e^{i(kx - \omega t)}$ , where  $A$  is a positive constant called the *amplitude*,  $\phi \in [0, 2\pi)$  is called the *initial phase*, and  $k$  and  $\omega$  are two real parameters called the *wave number* and *angular frequency*. (Note that  $\frac{k}{2\pi}$  is the number of waves per unit length, while  $\frac{\omega}{2\pi}$  is the number of waves per unit time.) Rewriting  $u$  in the form  $u(x, t) = Ae^{i\phi} e^{ik(x - \frac{\omega}{k}t)}$ , we see that it is indeed a travelling wave and that its propagation velocity is  $\frac{\omega}{k}$ .

In studying a wave equation, one of the first things to look for is the travelling wave solutions (if any) that it admits. For linear wave equations (with constant coefficients) we will see that for each wave number  $k$  there is a unique angular frequency  $\omega(k)$  for which the

equation admits a plane wave solution, and the velocity  $\frac{\omega(k)}{k}$  of this plane wave as a function of  $k$  (the so-called *dispersion relation* of the equation) not only completely determines the equation, but is crucial to understanding how solutions of the equation disperse as time progresses. Moreover, the fact that there is a unique (up to a multiplicative constant) travelling wave solution  $u_k(x, t) = e^{i(kx - \omega(k)t)}$  for each wave number  $k$  will allow us to solve the equation easily by representing the general solution as a superposition of these solutions  $u_k$ ; this is the Fourier method.

**1.2.1 Remark.** For nonlinear wave equations, the travelling wave solutions are in general severely restricted. Usually only special profiles, characteristic of the particular equation, are possible for travelling wave solutions. In particular they do not normally admit any solutions of the plane wave form  $Ae^{i\phi}e^{i(kx - \omega t)}$ .

The concepts of travelling wave and plane wave still make sense when the spatial dimension  $n$  is greater than one. Given an initial “profile”  $f : \mathbf{R}^n \rightarrow V$ , and a “direction”  $\eta \in \mathbf{S}^{n-1}$ , we can define the travelling wave  $u(x, t)$  with profile  $f$  and moving with speed  $\gamma$  in the direction  $\eta$  by  $u(x, t) := f(x - \gamma t\eta)$ . Note that the graph of the function  $x \mapsto u(x, t)$  is just the graph of  $f$  translated by  $\gamma t\eta$ , so it indeed travels in the direction  $\eta$  with speed  $\gamma$ . If we choose a basis  $v_i$  for  $V$ , then we can write  $f$  as a finite sum  $f(x) = \sum_{i=1}^d f_i(x)v_i$  where  $f_i : \mathbf{R}^n \rightarrow \mathbf{C}$ , thus essentially reducing consideration to the case  $V = \mathbf{C}$ , so we will assume that  $f$  is scalar valued in what follows.

If  $\kappa \in \mathbf{S}^{n-1}$  is a direction, then the fibers of the projection  $\Pi_\kappa : x \mapsto x \cdot \kappa$  of  $\mathbf{R}^n$  onto  $\mathbf{R}$  foliates  $\mathbf{R}^n$  by the hyperplanes  $x \cdot \kappa = a$  orthogonal to  $\kappa$ . A profile,  $f : \mathbf{R}^n \rightarrow \mathbf{C}$ , that is constant on each such hyperplane is called a “plane wave profile”, and will be of the form  $f(x) = g(x \cdot \kappa)$  where  $g : \mathbf{R} \rightarrow \mathbf{C}$ . If we define  $c = \gamma\kappa \cdot \eta$ , then the corresponding travelling plane wave is  $f(x - \gamma t\eta) = g(x \cdot \kappa - ct)$ , i.e., just the travelling wave with profile  $g$  and speed  $c$  on  $\mathbf{R}$ , pulled back to  $\mathbf{R}^n$  by  $\Pi_\kappa$ .

The exponential plane wave  $u(x, t) = e^{i(kx - \omega t)}$  that we used for the case  $n = 1$  has the profile  $u(y, 0) = e^{iky}$ . If we use this same profile for  $n > 1$ , i.e., define  $g(y) = e^{iky}$ , then our travelling waves will have the form  $e^{ik(x \cdot \kappa - ct)} = e^{i(kx \cdot \kappa - \omega t)}$  where, as above,  $\omega = kc$ . If we define  $\xi = k\kappa$  and recall that  $\kappa$  was a unit vector, then our travelling wave is  $u_{\xi, \omega}(x, t) = e^{i(x \cdot \xi - \omega t)}$ , where now the wave number is  $\|\xi\|$ , and the speed,  $c$ , is related to the angular frequency  $\omega$  by  $c = \frac{\omega}{\|\xi\|}$ . At any point,  $x$ ,  $u_{\xi, \omega}(x, t)$  is periodic in  $t$  with frequency  $\frac{\omega}{2\pi}$ , and fixing  $t$ ,  $u_{\xi, \omega}(x, t)$  is periodic with period  $\frac{\|\xi\|}{2\pi}$  along any line parallel to  $\xi$ . We shall see that for  $n > 1$  too, there is a dispersion relation associated to any linear wave equation, and the Fourier magic still works; i.e., for each  $\xi$  there will be a unique frequency  $\omega(\xi)$  such that  $u_\xi(x, y) = u_{\xi, \omega(\xi)}(x, t)$  is a solution of the wave equation, and we will again be able to represent the general solution as a superposition of these special travelling wave solutions.

### 1.3 Some Model Equations

In this section we will introduce some of the more important model wave equations (and classes of wave equations) that will be studied in more detail in later sections

**1.3—Example 1.** Perhaps the most familiar wave equation is  $u_{tt} - c^2\Delta u = 0$ , and I will refer to it as “The Classic Wave Equation”. Here  $\Delta$  is the Laplace operator, and the operator  $\frac{\partial^2}{\partial t^2} - \Delta$  is called the wave operator, or D’Alembertian operator. We can reduce

this to the first-order form considered above by replacing the one-component vector  $u$  by a two-component vector  $(u, v)$  that satisfies the PDE  $(u, v)_t = (v, c^2 \Delta u)$ , i.e., the wave shape  $u$  and velocity  $v$  satisfy the system of two linear PDE  $u_t = v$  and  $v_t = c^2 \Delta u$ . As we shall see next, in one space dimension it is extremely easy to solve the Cauchy problem for the Classic Wave Equation explicitly.

Namely, in one space dimension we can factor the wave operator,  $\frac{\partial^2}{\partial t^2} - c^2 \frac{\partial^2}{\partial x^2}$ , as the product  $(\frac{\partial}{\partial t} - c \frac{\partial}{\partial x})(\frac{\partial}{\partial t} + c \frac{\partial}{\partial x})$ . This suggests that we transform to so-called “characteristic coordinates”,  $\xi = x - ct$  and  $\eta = x + ct$ , in which the wave equation becomes simply  $\frac{\partial^2 u}{\partial \xi \partial \eta} = 0$ . This clearly has the general solution  $u(\xi, \eta) = F(\xi) + G(\eta)$ , so transforming back to “laboratory coordinates”  $x, t$ , the general solution is  $u(x, t) = F(x - ct) + G(x + ct)$ . If the initial shape of the wave is  $u(x, 0) = u_0(x)$  and its initial velocity is  $u_t(x, 0) = v_0(x) = v_0(x)$ , then an easy algebraic computation gives the following very explicit formula:

$$u(x, t) = \frac{1}{2}[u_0(x - ct) + u_0(x + ct)] + \frac{1}{2c} \int_{x-ct}^{x+ct} v_0(\xi) d\xi,$$

known as “D’Alembert’s Solution” of the Cauchy Problem for the Wave Equation in one space dimension. Note the geometric interpretation in the important “plucked string” case,  $v_0 = 0$ ; the initial profile  $u_0$  breaks up into the sum of two travelling waves, both with the same profile  $u_0/2$ , and one travels to the right with speed  $c$  and the other to the left with speed  $c$ . (We shall see later that something similar happens when  $n > 1$ . One can again decompose the initial shape, but now into a *continuous* superposition of shapes  $u_\kappa$ , one for each “direction”  $\kappa$  on the unit sphere  $\mathbf{S}^{n-1}$ , and each  $u_\kappa$  then moves as a travelling wave with the speed  $c$  in the direction  $\xi$ .)

▷ **1.3—Exercise 1.** Derive D’Alembert’s solution. (Hint:  $u_0(x) = F(x) + G(x)$ , so  $u'_0(x) = F'(x) + G'(x)$ , while  $v_0(x) = u_t(x, 0) = -cF'(x) + cG'(x)$ .)

**1.3.1 Remark.** There are a number of important consequences that follow easily from the form of the D’Alembert solution:

- a) The solution is well-defined for initial conditions  $(u_0, v_0)$  in the space of distributions, and gives a flow on this much larger space.
- b) The quantity  $\int_{-\infty}^{\infty} |u_t|^2 + |u_x|^2 dx$  is a “constant of the motion”. More precisely, if this integral is finite at one time for a solution  $u(x, t)$ , then it is finite and has the same value at any other time.

▷ **1.3—Exercise 2.** Prove this.

(Hint:  $|u_t(x, t)|^2 + |u_x(x, t)|^2 = 2|F'(x + ct)|^2 + 2|G'(x - ct)|^2$ .)

- c) The “domain of dependence” of a point  $(x, t)$  of space-time consists of the interval  $[x - ct, x + ct]$ . That is, the value of any solution  $u$  at  $(x, t)$  depends only on the values  $u_0$  and  $v_0$  in the interval  $[x - ct, x + ct]$ . Another way to say this is that the “region of influence” of a point  $x_0$  consists of the interior of the “light-cone” with vertex at  $x_0$ , i.e., all points  $(x, t)$  satisfying  $x_0 - ct < x < x_0 + ct$ . (These are the points having  $x_0$  in their domain of dependence.) Still a third way of stating this is that the Classical Wave Equation has signal propagation speed  $c$ , meaning that the value of a solution at  $(x, t)$  depends only on the values of  $u_0$  and  $v_0$  at points  $x_0$  from which a signal propagating with speed  $c$  could reach  $x$  in time  $t$  (i.e., points inside the sphere of radius  $ct$  about  $x$ .)

**1.3—Example 2.** The “Linear Advection Equation”,  $u_t - cu_x = 0$ . Using again the trick of transforming to the coordinates,  $\xi = x - ct$ ,  $\eta = x + ct$ , now the equation becomes  $\frac{\partial u}{\partial \xi} = 0$ , and hence the general solution is  $u(\xi) = \text{constant}$ , and the solution to the Cauchy Problem is  $u(x, t) = u_0(x - ct)$ . As before we see that if  $u_0$  is any distribution then  $u(t) = u_0(x - ct)$  gives a well-defined curve in the space of distributions that satisfies  $u_t - cu_x = 0$ , so that we really have a flow on the space of distributions whose generating vector field is  $c\frac{\partial}{\partial x}$ . Since  $c\frac{\partial}{\partial x}$  is a skew-adjoint operator on  $L^2(\mathbf{R})$ , it follows that this flow restricts to a one-parameter group of isometries of  $L^2(\mathbf{R})$ , i.e.,  $\int_{-\infty}^{\infty} u(x, t)^2 dx$  is a constant of the motion.

▷ **1.3—Exercise 3.** Prove directly that  $\frac{d}{dt} \int_{-\infty}^{\infty} u(x, t)^2 dx$  is zero. (Hint: It suffices to show this when  $u_0$  is smooth and has compact support, since these are dense in  $L^2$ . Now for such functions we can rewrite the integral as  $\int_{-\infty}^{\infty} \frac{\partial}{\partial t} u(x, t)^2 dx$  and the result will follow if we can show that  $\frac{\partial}{\partial t} u(x, t)^2$  can be written for each  $t$  in the form  $\frac{d}{dx} h(x)$ , where  $h$  is smooth and has compact support.)

**1.3.2 Remark.** Clearly the domain of dependence of  $(x, t)$  is now just the single point  $x - ct$ , the region of influence of  $x_0$  is the line  $x = x_0 + ct$ , and the signal propagation speed is again  $c$ . The main difference with Example 1 is that the Linear Advection Equation describes wave moving in one direction with velocity  $c$ , while The Classic Wave Equation describes wave moving in both directions with velocity  $c$ .

▷ **1.3—Exercise 4.** (Duhamel’s Principle.) The homogeneous Linear Advection Equation describes waves moving to the right in a *non-dispersive* and *non-dissipative* one-dimensional linear elastic medium when there are no external forces acting on it. (The italicised terms will be explained later.) If there is an external force, then the appropriate wave equation will be an inhomogeneous version of the equation,  $u_t - cu_x = F(x, t)$ . Show that the Cauchy Problem now has the solution  $u(x, t) = u_0(x - ct) + \int_0^t F(x - ct + c\xi, \xi) d\xi$ .

**1.3—Example 3.** General Linear Evolution Equation,  $u_t + P(\frac{\partial}{\partial x})u = 0$ . Here  $P(\xi)$  is a polynomial with complex coefficients. For example, if  $P(\xi) = -c\xi$  then we get back the Linear Advection Equation. We will outline the theory of these equations in a separate subsection below where as we shall see, they can analyzed easily and thoroughly using the Fourier Transform. It will turn out that to qualify as a wave equation, the odd coefficients of the polynomial  $P$  should be real and the even coefficients pure imaginary, or more simply,  $P(i\xi)$  should be imaginary valued on the real axis. This is the condition for  $P(\frac{\partial}{\partial x})$  to be a skew-adjoint operator on  $L^2(\mathbf{R})$ .

**1.3—Example 4.** The General Conservation Law,  $u_t = (F(u))_x$ . Here  $F(u)$  can any smooth function of  $u$  and certain of its partial derivatives with respect to  $x$ . For example, if  $P(\xi) = a_1\xi + \dots + a_n\xi^n$ , we can get the linear evolution equation  $u_t = P(\frac{\partial}{\partial x})u$  by taking  $F(u) = a_1u + \dots + a_n\frac{\partial^{n-1}u}{\partial x^{n-1}}$ , and  $F(u) = -(\frac{1}{2}u^2 + \delta^2u_{xx})$  gives the KdV equation  $u_t + uu_x + \delta^2u_{xxx} = 0$  that we consider just below. Note that if  $F(u(x, t))$  vanishes at infinity then integration gives  $\frac{d}{dt} \int_{-\infty}^{\infty} u(x, t) dx = 0$ , i.e.,  $\int_{-\infty}^{\infty} u(x, t) dx$  is a “constant of the motion”, and this is where the name “Conservation Law” comes from. We will be concerned mainly with the case that  $F(u)$  is a zero-order operator, i.e.,  $F(u)(x) = F(u(x))$ , where  $F$  is a smooth function on  $\mathbf{R}$ . In this case, if we let  $f = F'$ , then we can write our Conservation Law in the form  $u_t = f(u)u_x$ . In particular, taking  $f(\xi) = c$  (i.e.,  $F(\xi) = c\xi$ ) gives

the Linear Advection Equation  $u_t = cu_x$ , while  $F(\xi) = -\frac{1}{2}\xi^2$  gives the important Inviscid Burgers Equation,  $u_t + uu_x = 0$ .

There is a very beautiful and highly developed theory of such Conservation Laws, and again we will devote a separate subsection to outlining some of the basic results from this theory. Recall that for the Linear Advection Equation we have an explicit solution for the Cauchy Problem, namely  $u(x, t) = u_0(x - ct)$ , which we can also write as  $u(x, t) = u_0(x - f(u(x, t))t)$ , where  $f(\xi) = c$ . If we are incredibly optimistic we might hope that we could more generally solve the Cauchy Problem for  $u_t = f(u)u_x$  by solving  $u(x, t) = u_0(x - f(u(x, t))t)$  as an implicit equation for  $u(x, t)$ . This would mean that we could generalize our algorithm for finding the profile of  $u$  at time  $t$  from the initial profile as follows: translate each point  $(\xi, u_0(\xi))$  of the graph of  $u_0$  to the right by an amount  $f(u_0(\xi))t$  to get the graph of  $x \mapsto u(x, t)$ . This would of course give us a simple method for solving any such Cauchy Problems, and **the amazing thing is that this bold idea actually works**. However, one must be careful. As we shall see, this algorithm (which goes under the name “the method of characteristics”) contains the seeds of its own eventual failure. For a general initial condition  $u_0$  and function  $f$ , we shall see that we can predict a positive time  $T_B$  (the so-called “breaking time”) after which the solution given by the method of characteristics can no longer exist as a smooth, single-valued function.

**1.3—Example 5.** The Korteweg-de Vries (KdV) Equation,  $u_t + uu_x + \delta^2 u_{xxx} = 0$ . If we re-scale the independent variables by  $t \rightarrow \beta t$  and  $x \rightarrow \gamma x$ , then the KdV equation becomes:

$$u_t + \left(\frac{\beta}{\gamma}\right)uu_x + \left(\frac{\beta}{\gamma^3}\right)\delta^2 u_{xxx} = 0,$$

so by appropriate choice of  $\beta$  and  $\gamma$  we can obtain any equation of the form  $u_t + \lambda uu_x + \mu u_{xxx} = 0$ , and any such equation is referred to as “the KdV equation”. A commonly used choice that is convenient for many purposes is  $u_t + 6uu_x + u_{xxx} = 0$ , although the form  $u_t - 6uu_x + u_{xxx} = 0$  (obtained by replacing  $u$  by  $-u$ ) is equally common. We will use both these forms. This is surely one of the most important and most studied of all evolution equations. It is over a century since it was shown to govern wave motion in a shallow channel, but less than forty years since the remarkable phenomenon of soliton interactions was discovered in studying certain of its solutions. Shortly thereafter the so-called Inverse Scattering Transform (IST) for solving the KdV equation was discovered and the equation was eventually shown to be an infinite dimensional completely integrable Hamiltonian system. This equation, and its remarkable properties will be one of our main objects of study.

**1.3—Example 6.** The Sine-Gordon Equation (SGE),  $u_{tt} - u_{xx} = \sin(u)$ . This equation is considerably older than KdV. It was discovered in the late eighteen hundreds to be the master equation for the study of “pseudospherical” surfaces, i.e., surfaces of Gaussian curvature  $K$  equal to  $-1$  immersed in  $\mathbf{R}^3$ , and for that reason it was intensively studied (and its solitons discovered, but not recognized as such) long before KdV was even known. However it was only in the course of trying to find other equations that could be solved by the IST that it was realized that SGE was also a integrable equation.

**1.3—Example 7.** The Nonlinear Schrödinger Equation,  $iu_t + u_{xx} + u|u|^2 = 0$ . This is of more recent origin. It was the third evolution equation shown to have soliton behavior and to be integrable, and recently has been intensively studied because it describes the

propagation of pulses of laser light in optical fibers. The latter technology that is rapidly becoming the primary means for long-distance, high bandwidth communication, which in turn is the foundation of the Internet and the World Wide Web.

## 1.4 Linear Wave Equations—Dispersion and Dissipation

Evolution equations that are not only linear but also translation invariant (i.e., have constant coefficients) can be solved explicitly using Fourier methods. They are interesting both for their own sake, and also because they can serve as a tool for studying nonlinear equations.

The general linear evolution equation has the form  $u_t + P(\frac{\partial}{\partial x})u = 0$ , where to begin with we can assume that the polynomial  $P$  has coefficients that are smooth complex-valued functions of  $x$  and  $t$ :  $P(\frac{\partial}{\partial x})u = \sum_{i=1}^r a_i(x, t) \frac{\partial^i u}{\partial x^i}$ . For each  $(x_0, t_0)$ , we have a space-time translation operator  $T_{(x_0, t_0)}$  acting on smooth functions of  $x$  and  $t$  by  $T_{(x_0, t_0)}u(x, t) = u(x - x_0, t - t_0)$ . We say that the operator  $P(\frac{\partial}{\partial x})$  is *translation invariant* if it commutes with all the  $T_{(x_0, t_0)}$ .

▷ **1.4—Exercise 1.** Show that the necessary and sufficient condition for  $P(\frac{\partial}{\partial x})$  to be translation invariant is that the coefficients  $a_i$  of  $P$  should be constant complex numbers.

### 1.4.1 Invariance Principles.

There are at least two good reasons to assume that our equation is translation invariant. First, the eminently practical one that in this case we will be able to use Fourier transform techniques to solve the initial value problem explicitly, and investigate in detail the nature of its solutions.

But there is frequently an even more important philosophical reason for postulating translation invariance. Assume that we are trying to model the dynamics of some fundamental physical field quantity  $u$  by an evolution equation of the above type. Thus  $x$  will denote the “place where”, and  $t$  the “time when” the quantity has the value  $u(x, t)$ . Now, if our proposed physical law is indeed “fundamental”, its validity should not depend on where or when it is applied—it will be the same on Alpha Centauri as on Earth, and the same in a million years as it is today—we can even take that as part of the definition of what we mean by fundamental. The way to give a precise mathematical formulation of this principle of space-time symmetry or homogeneity is to demand that our equation should be invariant under some transitive group acting on space and time.

But, like most philosophical discussions, this only begs a deeper question. How does it happen that the space-time we live in appears to admit a simply-transitive abelian group action under which the physical laws are invariant? On the level of Newtonian physics (or Special Relativity) this is simply taken as axiomatic. General Relativity gives an answer that is both more sophisticated and more satisfying. The basic symmetry principle postulated is the Principle of Equivalence. This demands that the truly Fundamental Laws of Physics should be invariant under the (obviously transitive) group of *all* diffeomorphisms of space-time. Of course there are very few laws that are *that* fundamental—but Einstein’s Field Equations for a (pseudo-)Riemannian metric on space-time is one of them, and the physical evidence for its correctness is pretty overwhelming. In a neighborhood of any point of space-



time we can then coordinatize space-time by using geodesic coordinates (i.e., by identifying space-time with its tangent space at that point using the Riemannian exponential map). To use Einstein’s lovely metaphor, we get into an elevator and cut the rope. In these natural coordinates, the space-time appears flat to second order, and the translation group that comes from the linear structure of the tangent space is an approximate symmetry group.

I will not try here to answer the still far deeper philosophical mystery of *why* our physical world seems to be governed by laws that exhibit such remarkable symmetry. This is closely related to what Eugene Wigner called “The Unreasonable Effectiveness of Mathematics in the Natural Sciences” in a famous article by that name [W]. (For another view of this topic see [H].) But I cannot help wondering if the so-called “Anthropic Principle” is not at least part of the answer. Perhaps only a Universe governed by such symmetry principles manifests the high degree of stability that is conducive to the evolution of the kind of self-cognizant, intelligent life that would worry about this point. In other words: mathematicians, physicists, and philosophers can exist to wonder about why such fundamental laws govern, only in those universes where they do in fact govern.

In any case, we shall henceforth assume that  $P$  does in fact have constant complex numbers as coefficients. If we substitute the Ansatz  $u(x, t) = e^{i(kx - \omega t)}$  into our linear equation,  $u_t + P(\frac{\partial}{\partial x})u = 0$ , then we find the relation  $-i\omega u + P(ik)u = 0$ , or  $\omega = \omega(k) := \frac{1}{i}P(ik)$ . For  $u(x, t)$  to be a plane wave solution, we need the angular frequency,  $\omega$ , to be real. Thus, we will have a (unique) plane wave solution for each real wave number  $k$  just when  $\frac{1}{i}P(ik)$  is real (or  $P(ik)$  is imaginary) for  $k$  on the real axis. This just translates into the condition that the odd coefficients of  $P$  should be real and the even coefficients pure imaginary. Let us assume this in what follows. As we shall see, one consequence will be that we can solve the initial value problem for any initial condition  $u_0$  in  $L^2$ , and the solution is a superposition of these plane wave solutions—clearly a strong reason to consider this case as describing honest “wave equations”, whatever that term should mean. Then we will follow up by taking a look at what happens when we relax this condition.

The relation  $\omega(k) := \frac{1}{i}P(ik)$  relating the angular frequency  $\omega$  and wave number  $k$  of a plane wave solution of a linear wave equation is called the *dispersion relation* for the equation. The propagation velocity of the plane wave solution with wave number  $k$  is called the *phase velocity* at wave number  $k$ , and is given by the formula  $\frac{\omega(k)}{k} = \frac{1}{ik}P(ik)$  (which is also sometimes referred to as the dispersion relation for the equation). It is important to observe that the dispersion relation is not only determined by the polynomial  $P$  that defines the evolution equation, but it conversely determines  $P$ .

Now let  $u_0$  be any initial wave profile in  $L^2$ , so that  $u_0(x) = \int \hat{u}_0(k)e^{ikx} dk$ , where  $\hat{u}_0(k) = \frac{1}{2\pi} \int u_0(x)e^{-ikx} dk$  is the Fourier Transform of  $u$ . Defining  $\hat{u}(k, t) = e^{-P(ik)t}\hat{u}_0(k)$ , we see that  $\hat{u}(k, t)e^{ikx} = \hat{u}_0(k)e^{ik(x - \frac{\omega(k)}{k}t)}$  is a plane wave solution to our equation with initial condition  $\hat{u}_0(k)e^{ikx}$ . We now define  $u(x, t)$  (formally) to be the superposition of these plane waves:  $u(x, t) \sim \int \hat{u}(k, t)e^{ikx} dk$ . So far we have not really used the fact that  $P(ik)$  is imaginary for  $k$  real, and this  $u(x, t)$  would still be a formal solution without that assumption. The way we shall use the condition on  $P$  is to notice that it implies  $|e^{-P(ik)t}| = 1$ . Thus,  $|\hat{u}(k, t)| = |\hat{u}_0(k)|$ , so  $\hat{u}(k, t)$  is in  $L^2$  for all  $t$ , and in fact it has the same norm as  $\hat{u}_0$ . It then follows from Plancherel’s Theorem that  $u(x, t)$  is in  $L^2$  for all  $t$ , and has the same norm as  $u_0$ . It is now elementary to see that our formal solution  $u(x, t)$  is in fact an honest solution of the Cauchy Problem for our evolution equation, and in fact defines a one-parameter group of unitary transformations of  $L^2$ . (Another way to

see this is to note that since  $\frac{\partial}{\partial x}$  is a skew-adjoint operator on  $L^2$ , so is any odd power or  $i$  times any even power, so that  $P(\frac{\partial}{\partial x})$ , is skew-adjoint and hence  $\exp(-P(\frac{\partial}{\partial x})t)$  is a one-parameter group of unitary transformations of  $L^2$ . But a rigorous proof that  $\frac{\partial}{\partial x}$  is a skew-adjoint operator (and not just formally skew-adjoint) involves essentially the same Fourier analysis.)

We next look at what can happen if we drop the condition that the odd coefficients of  $P$  are real and the even coefficients pure imaginary.

Consider first the special case of the Heat (or Diffusion) Equation,  $u_t - \alpha u_{xx} = 0$ , with  $\alpha > 0$ . Here  $P(x) = -\alpha X^2$ , so  $|e^{-P(ik)t}| = |e^{-k^2 t}|$ . Thus, when  $t > 0$ ,  $|e^{-P(ik)t}| < 1$ , and  $|\hat{u}(k, t)| < |\hat{u}_0(k)|$ , so again  $u(k, t)$  is in  $L^2$  for all  $t$ , but now  $\|u(x, t)\|_{L^2} < \|u_0(x)\|_{L^2}$ . Thus our solution is not a unitary flow on  $L^2$ , but rather a contracting, positive semi-group. In fact, it is easy to see that for each initial condition  $u_0 \in L^2$ , the solution tends to zero in  $L^2$  exponentially fast as  $t \rightarrow \infty$ , and in fact it tends to zero uniformly too. This so-called *dissipative* behavior is clearly not very “wave-like” in nature, and the Heat Equation is not considered to be a wave equation. On the other hand, the fact that the propagator  $|e^{-P(ik)t}|$  is so rapidly decreasing implies very strong regularity for the solution  $u(x, t)$  as a function of  $x$  as soon as  $t > 0$ .

▷ **1.4—Exercise 2.** Show that for any initial condition  $u_0$  in  $L^2$ , the solution  $u(x, t)$  of the Heat Equation is an analytic function of  $x$  for any  $t > 0$ . (Hint: If you know the Paley-Wiener Theorem, this is of course an immediate consequence, but it is easy to prove directly.)

What happens for  $t < 0$ ? In this case  $|e^{-P(ik)t}| = |e^{-k^2 t}|$  is not an essentially bounded function of  $k$ , and indeed grows more rapidly than any polynomial, so that multiplication by it does not map  $L^2$  into itself. or any of the Sobolev spaces. In fact, it is immediate from the above exercise, that if  $u_0 \in L^2$  is *not* analytic, then there cannot be an  $L^2$  solution  $u(x, t)$  of the Heat Equation with initial condition  $u_0$  on any non-trivial interval  $(-T, 0]$ .

It is not hard to extend this analysis for the Heat Equation to any monomial  $P$ :  $P(X) = a_n X^n$ , where  $a_n = \alpha + i\beta$ . Then  $|e^{-P(ik)t}| = |e^{i^n \alpha t}| |e^{i^{n+1} \beta t}|$ . If  $n = 2m$  is even, this becomes  $|e^{(-1)^m \alpha t}|$ , while if  $n = 2m + 1$  is odd, it becomes  $|e^{(-1)^{(m+1)} \beta t}|$ . If  $\alpha$  (respectively  $\beta$ ) is zero, we are back to our earlier case that gives a unitary flow on  $L^2$ . If not, then we get essentially back to the dissipative semi-flow behavior of the heat equation. Whether the semi-flow is defined for  $t > 0$  or  $t < 0$  depends on the parity of  $m$  and the sign of  $\alpha$  (repectively  $\beta$ ).

▷ **1.4—Exercise 3.** Work out the details.

We will now return to our assumption that  $P(D)$  is a skew-adjoint operator, i.e., the odd coefficients of  $P(X)$  are real and the even coefficients pure imaginary. We next note that this seemingly ad hoc condition is actually equivalent to a group invariance principle, similar to translation invariance.

### 1.4.2 Symmetry Principles in General—and CPT in Particular.

One of the most important ways to single out important and interesting model equations for study is to look for equations that satisfy various symmetry or invariance principles. Suppose our equation is of the form  $\mathcal{E} = 0$  where  $\mathcal{E}$  is some differential operator on a linear space  $\mathcal{F}$  of smooth functions, and we have some group  $G$  that acts on  $\mathcal{F}$ . Then we say that

the equation is  $G$ -invariant (or that  $G$  is a symmetry group for the equation) if the operator  $\mathcal{E}$  commutes with the elements of  $G$ . Of course it follows that if  $u \in \mathcal{F}$  is a solution of  $\mathcal{E} = 0$ , then so is  $gu$  for all  $g$  in  $G$ .

As we have already noted, the evolution equation  $u_t + P(D)u = 0$  is clearly invariant under time translations, and is invariant under spatial translations if and only if the coefficients of the polynomial  $P(X)$  are constant. Most of the equations of physical interest have further symmetries, i.e., are invariant under larger groups, reflecting the invariance of the underlying physics under these groups. For example, the equations of pre-relativistic physics are Galilean invariant, while those of relativistic physics are Lorentz invariant. We will consider here a certain important discrete symmetry that so far has proved to be universal in physics.

We denote by  $\mathbf{T}$  the “time-reversal” map  $(x, t) \rightarrow (x, -t)$ , and by  $\mathbf{P}$  the analogous “parity” or spatial reflection map  $(x, t) \rightarrow (-x, t)$ . These involutions act as linear operators on functions on space-time by  $u(x, t) \rightarrow u(x, -t)$  and  $u(x, t) \rightarrow u(-x, t)$  respectively. There is a third important involution, that does not act on space-time, but directly on complex-valued functions; namely the conjugation operator  $\mathbf{C}$ , mapping  $u(x, t)$  to its complex conjugate  $u(x, t)^*$ . Clearly  $\mathbf{C}$ ,  $\mathbf{P}$ , and  $\mathbf{T}$  commute, so their composition  $\mathbf{CPT}$  is also an involution  $u(x, t) \rightarrow u(-x, -t)^*$  acting on complex-valued functions defined on space-time. We note that  $\mathbf{CPT}$  maps the function  $u(x, t) = e^{i(kx - \omega t)}$  (with real wave number  $k$ ) to the function  $u(x, t) = e^{i(kx - \omega^* t)}$ , so it fixes such a  $u$  if and only if  $u$  is a plane wave.

▷ **1.4—Exercise 4.** Prove that  $u_t + P(D)u = 0$  is  $\mathbf{CPT}$ -invariant if and only if  $P(D)$  is skew-adjoint, i.e., if and only if  $P(i\xi)$  is pure imaginary for all real  $\xi$ . Check that the KdV, NLS, and Sine-Gordon equation are also  $\mathbf{CPT}$ -invariant.

### 1.4.3 Examples of Linear Evolution Equations.

**1.4—Example 1.** Choosing  $P(\xi) = c\xi$ , gives the Linear Advection Equation  $u_t + cu_x = 0$ . The dispersion relation is  $\frac{\omega(k)}{k} = \frac{P(ik)}{ik} = c$ , i.e., all plane wave solutions have the same phase velocity  $c$ . For this example we see that  $\hat{u}(k, t)e^{ikx} = \hat{u}_0(k)e^{ik(x-ct)}$ , and since  $\int \hat{u}_0(k)e^{ikx} dk = u_0(x)$ , it follows that  $u(x, t) = \int \hat{u}(k, t)e^{ik(x-ct)} dk = u_0(x - ct)$ , giving an independent proof of this explicit solution to the Cauchy Problem in this case.

The next obvious case to consider is  $P(\xi) = c\xi + d\xi^3$ , giving the dispersion relation  $\frac{\omega(k)}{k} = \frac{P(ik)}{ik} = c(1 - (d/c)k^2)$ , and the wave equation  $u_t + cu_x + du_{xxx} = 0$ . This is sometimes referred to as the “weak dispersion” wave equation. Note that the phase velocity at wave number  $k$  is a constant,  $c$ , plus a constant times  $k^2$ . It is natural therefore to transform to coordinates moving with velocity  $c$ , i.e., make the substitution  $x \mapsto x - ct$ , and the wave equation becomes  $u_t + du_{xxx} = 0$ . Moreover, by rescaling the independent variable  $x$  we can get rid of the coefficient  $d$ . This leads us to our next example.

**1.4—Example 2.**  $P(\xi) = \xi^3$ , gives the equation  $u_t + u_{xxx} = 0$ . Now the dispersion relation is non-trivial; plane wave solutions with wave number  $k$  move with phase velocity  $\frac{\omega(k)}{k} = \frac{P(ik)}{ik} = -k^2$ , so the Fourier components  $\hat{u}_0(k)e^{ik(x+k^2t)}$  of  $u(x, t)$  with a large wave number  $k$  move faster than those with smaller wave number, causing an initially compact wave profile to gradually disperse as these Fourier modes move apart and start to interfere destructively.

It is not hard in this example to write a formula for  $u(x, t)$  explicitly in terms of  $u_0$ ,

instead of  $\hat{u}_0$ , namely:

$$u(x, t) = \frac{1}{\sqrt{\pi} \sqrt[3]{3t}} \int_{-\infty}^{\infty} \text{Ai} \left( \frac{x - \xi}{\sqrt[3]{3t}} \right) u_0(\xi) d\xi.$$

Here Ai is the Airy function, a bounded solution of  $w'' - zw = 0$  that can be defined explicitly by:

$$\text{Ai}(z) = \frac{1}{\sqrt{\pi}} \int_0^{\infty} \cos \left( \frac{t^3}{3} + tz \right) dt,$$

and it follows from this that  $v(x, t) = \frac{1}{\sqrt{\pi} \sqrt[3]{3t}} \text{Ai} \left( \frac{x}{\sqrt[3]{3t}} \right)$  satisfies  $v_t + v_{xxx} = 0$ , and  $\lim_{t \rightarrow 0} v(x, t) = \delta(x)$ .

**1.4.4 Remark.** More generally, for a wave equation  $u_t + P(\frac{\partial}{\partial x})u = 0$ , the solution,  $p(x, t)$ , of the Cauchy Problem with  $p(x, 0) = \delta(x)$  is called the Fundamental Solution or Propagator for the equation. It follows that the solution to the Cauchy problem for a general initial condition is given by convolution with  $p$ , i.e.,  $u(x, t) = \int_{-\infty}^{\infty} p(x - \xi, t)u_0(\xi) d\xi$ .

▷ **1.4—Exercise 5.** (General Duhamel Principle) Suppose  $p$  is the fundamental solution for the homogeneous wave equation  $u_t + P(\frac{\partial}{\partial x})u = 0$ . Show that the solution to the Cauchy Problem for the corresponding inhomogeneous equation  $u_t + P(\frac{\partial}{\partial x})u = F(x, t)$  is given by  $\int_{-\infty}^{\infty} p(x - \xi, t)u_0(\xi) d\xi + \int_0^t d\tau \int_{-\infty}^{\infty} p(x - \xi, t - \tau)F(\xi, \tau) d\xi$ .

Before leaving linear wave equations we should say something about the important concept of *group velocity*. We consider an initial wave packet,  $u_0$ , that is synthesized from a relatively narrow band of wave numbers,  $k$ , i.e.,  $u_0(x) = \int_{k_0 - \epsilon}^{k_0 + \epsilon} \hat{u}_0(k)e^{ikx} dk$ . Thus the corresponding frequencies  $\omega(k)$  will also be restricted to a narrow band around  $\omega(k_0)$ , and since all the plane wave Fourier modes are moving at approximately the velocity  $\frac{\omega(k_0)}{k_0}$ , the solution  $u(x, t)$  of the Cauchy Problem will tend to disperse rather slowly and keep an approximately constant profile  $f$ , at least for a short initial period. One might expect that the velocity at which this approximate wave profile moves would be  $\frac{\omega(k_0)}{k_0}$ , the central phase velocity, but as we shall now see, it turns out to be  $\omega'(k_0)$ . To see this we expand  $(kx - \omega(k)t)$  in a Taylor series about  $k_0$ :

$$(kx - \omega(k)t) = (k_0x - \omega(k_0)t) + (k - k_0)(x - \omega'(k_0)t) + O((k - k_0)^2),$$

and substitute this in the formula  $u(x, t) = \int_{k_0 - \epsilon}^{k_0 + \epsilon} \hat{u}_0(k)e^{i(kx - \omega(k)t)} dk$  for the solution. Assuming  $\epsilon$  is small enough that the higher order terms in this expansion can be ignored in the interval  $[k_0 - \epsilon, k_0 + \epsilon]$  we get the approximation  $u(x, t) \approx f(x - \omega'(k_0)t)e^{i(k_0x - \omega(k_0)t)}$ , where  $f(x) = \int_{k_0 - \epsilon}^{k_0 + \epsilon} \hat{u}_0(k)e^{i(k - k_0)x} = u_0(x)e^{-ik_0x} dk$ . Thus, to this approximation, the solution  $u(x, t)$  is just the plane wave solution of the wave equation having wave number  $k_0$ , but amplitude modulated by a traveling wave with profile  $f$  and moving at the group velocity  $\omega'(k_0)$ .

▷ **1.4—Exercise 6.** Consider the solution  $u(x, t)$  to a linear wave equation that is the superposition of two plane wave solutions, the first with wave number  $k_0$  and the second with wave number  $k_0 + \Delta k$ , that is close to  $k_0$ . Let  $\Delta\omega = \omega(k_0 + \Delta k) - \omega(k_0)$ . Show that  $u(x, t)$  is (exactly!) the first plane wave solution amplitude modulated by a travelling wave of profile  $f(x) = 1 + e^{i\Delta kx}$  and velocity  $\frac{\Delta\omega}{\Delta k}$ . (So that in this case there is no real dispersion.)

**1.4.5 Remark.** In many important physical applications (e.g., light travelling in a transparent medium such as an optical fiber)  $\omega'' < 0$ , i.e., the dispersion curve is convex upwards, so that the phase velocity exceeds the group velocity, and high frequency plane waves are slower than low frequency plane waves. Thus, wavelets enter the envelope of a group from the left, and first grow and then diminish in amplitude as they pass through the group and exit to the right. This is called *normal dispersion*, the opposite case  $\omega'' > 0$  being referred to as *anomalous dispersion*.

### 1.4—Example 3. De Broglie Waves.

Schrödinger's Equation for a particle in one dimension,  $\psi_t = i\frac{\hbar}{2m}\psi_{xx} + \frac{1}{\hbar}u\psi$ , provides an excellent model for comparing phase and group velocity. Here  $\hbar = 6.626 \times 10^{-34}$  Joule seconds is Planck's quantum of action,  $\hbar = h/2\pi$ , and  $u$  is the potential function, i.e.,  $-u'(x)$  gives the force acting on the particle when its location is  $x$ . We will only consider the case of a free particle, i.e., one not acted on by any force, so we take  $u = 0$ , and Schrödinger's Equation reduces to  $\psi_t + P(\frac{\partial}{\partial x})\psi = 0$ , where  $P(\xi) = \frac{\hbar}{i}\frac{\xi^2}{2m}$ . The dispersion relation therefor gives  $v_\phi(k) = \frac{\omega(k)}{k} = \frac{P(ik)}{ik} = \frac{\hbar k}{2m}$  as the phase velocity of a plane wave solution of wave number  $k$ , (a so-called de Broglie wave), and thus the group velocity is  $v_g(k) = \omega'(k) = \frac{\hbar k}{m}$ . Now the classical velocity of a particle of momentum  $p$  is  $\frac{p}{m}$ , and this implies the relation  $p = \hbar k$  between momentum and wave number. Since the wave-length  $\lambda$  is related to the wave number by  $\lambda = \frac{2\pi}{k}$ , this gives the formula  $\lambda = \frac{h}{p}$  for the so-called de Broglie wave-length of a particle of momentum  $p$ . (This was the original de Broglie hypothesis, associating a wave-length to a particle.) Note that the energy  $E$  of a particle of momentum  $p$  is  $\frac{p^2}{2m}$ , so  $E(k) = \frac{(\hbar k)^2}{2m} = \hbar\omega(k)$ , the classic quantum mechanics formula relating energy and frequency.

For this wave equation it is easy and interesting to find explicitly the evolution of a Gaussian wave-packet that is initially centered at  $x_0$  and has wave number centered at  $k_0$ —in fact this is given as an exercise in almost every first text on quantum mechanics. For the Fourier Transform of the initial wave function  $\psi_0$ , we take  $\hat{\psi}_0(k) = G(k - k_0, \sigma_p)$ , where

$$G(k, \sigma) = \frac{1}{(2\pi)^{\frac{1}{4}}\sqrt{\sigma}} \exp\left(-\frac{k^2}{4\sigma^2}\right)$$

is the  $L^2$  normalized Gaussian centered at the origin and having “width”  $\sigma$ . Then, as we saw above,  $\psi(x, t)$ , the wave function at time  $t$ , has Fourier Transform  $\hat{\psi}(k, t)$  given by  $\hat{\psi}_0(k)e^{-P(ik)t}$ , and  $\psi(x, t) = \int \hat{\psi}(k, t)e^{ikx} dk$ . Using the fact that the Fourier Transform of a Gaussian is another Gaussian, we find easily that  $\psi(x, t) = A(x, t)e^{i\phi(x, t)}$ , where the amplitude  $A$  is given by  $A(x, t) = G(x - v_g t, \sigma_x(t))$ . Here, as above,  $v_g = v_g(k_0) = \frac{\hbar k_0}{m}$  is the group velocity, and the spatial width  $\sigma_x(t)$  is given by  $\sigma_x(t) = \frac{\hbar}{2\sigma_p}\left(1 + \frac{4\sigma_p^4 t^2}{\hbar^2 m^2}\right)$ . We recall that the square of the amplitude  $A(x, t)$  is just the probability density at time  $t$  of finding the particle at  $x$ . Thus, we see that this is a Gaussian whose mean (which is the expected position of the particle) moves with the velocity of the classical particle. Note that we have a completely explicit formula for the width  $\sigma_x(t)$  of the wave packet as a function of time, so the broadening effect of dispersion is apparent. Also note that the Heisenberg's Uncertainty Principle,  $\sigma_x(t)\sigma_p \geq \frac{\hbar}{2}$  is actually an equality at time zero, and it is the broadening of dispersion that makes it a strict inequality at later times.

**1.4.6 Remark.** For a non-free particle (i.e., when the potential  $u$  is *not* a constant function) the Schrödinger Equation,  $\psi_t = i\frac{\hbar}{2m}\psi_{xx} + \frac{1}{i\hbar}u\psi$ , no longer has coefficients that are constant in  $x$ , so we don't expect solutions that are exponential in both  $x$  and  $t$  (i.e., plane waves or de Broglie waves). But the equation is still linear, and it is still invariant under time translations, so do we expect to be able to expand the general solution into a superposition of functions of the form  $\psi_E(x, t) = \phi(x)e^{-i\frac{E}{\hbar}t}$ . (We have adopted the physics convention, replacing the frequency,  $\omega$ , by  $\frac{E}{\hbar}$ , where  $E$  is the energy associated to that frequency.) If we substitute this into the Schrödinger equation, then we see that the “energy eigenfunction” (or “stationary wave function”)  $\phi$  must satisfy the so-called time-independent Schrödinger Equation,  $(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + u)\phi = E\phi$ . Note that this is just a second-order linear ODE, so for each choice of  $E$  it will have a two-dimensional linear space of solutions. This linear equation will show up with a strange twist when we solve the nonlinear KdV equation,  $u_t - 6uu_x + u_{xxx} = 0$ , by the remarkable Inverse Scattering Method. Namely, we will see that if the one-parameter family of potentials  $u(t)(x) = u(x, t)$  evolves so as to satisfy the KdV equation, then the corresponding family of Schrödinger operators,  $(-\frac{\hbar^2}{2m}\frac{d^2}{dx^2} + u)$ , are unitarily equivalent, a fact that will play a key rôle in the Inverse Scattering Method. (Note that the “time”,  $t$ , in the time-dependent Schrödinger Equation is not related in any way to the  $t$  in the KdV equation.)

**1.4.7 Remark.** We next explain how to generalize the Fourier methods above for solving linear PDE to the case  $n > 1$ . For simplicity, we will only consider the case of scalar equations—i.e., we will assume that  $u$  is a complex-valued function (rather than one taking values in some complex vector space  $V$ ), but the more general vector-valued case can be handled similarly, (see the exercise below). As we saw earlier, the analog of plane waves in more space dimensions are travelling waves of the form  $u_{\xi, \omega}(x, t) = e^{i(x \cdot \xi - \omega t)}$ , where  $\xi \in \mathbf{R}^n$ . Now  $\frac{\xi}{\|\xi\|} \in \mathbf{S}^{n-1}$  is the direction of the plane wave motion, the wave number is  $\|\xi\|$ , and the speed,  $c$ , is related to the angular frequency  $\omega$  (which must be real) by  $c = \frac{\omega}{\|\xi\|}$ .

Suppose we have a constant coefficient linear wave equation,  $u_t + P(D)u = 0$ . Here  $P(X) = \sum_{|\alpha| \leq r} A_\alpha X^\alpha$  is a complex polynomial in  $X = (X_1, \dots, X_n)$ , and we are using standard “multi-index notation”. Thus,  $\alpha$  denotes an  $n$ -tuple of non-negative integers,  $|\alpha| = \alpha_1 + \dots + \alpha_n$ ,  $X^\alpha = X_1^{\alpha_1} \dots X_n^{\alpha_n}$ ,  $D = (\frac{\partial}{\partial x_1}, \dots, \frac{\partial}{\partial x_n})$ , and  $D^\alpha = \frac{\partial^{|\alpha|}}{\partial x_1^{\alpha_1} \dots \partial x_n^{\alpha_n}}$ . Note that  $D^\alpha u_{\xi, \omega} = (i\xi)^\alpha u_{\xi, \omega}$ , and hence  $P(D)u_{\xi, \omega} = P(i\xi)u_{\xi, \omega}$ , where  $P(i\xi)$  is the so-called total symbol of  $P(D)$ , i.e.,  $\sum_{|\alpha| \leq r} i^{|\alpha|} \xi^\alpha A_\alpha$ . On the other hand,  $\frac{\partial}{\partial t} u_{\xi, \omega} = -i\omega u_{\xi, \omega}$ , so  $u_{\xi, \omega}$  is a solution of  $u_t + P(D)u = 0$  if and only if  $\omega = \omega(\xi) = \frac{1}{i}P(i\xi)$ , and this is now the dispersion relation. Since  $\omega$  must be real, if we want to have a plane wave solution for each  $\xi$ , the condition as before is that  $P(i\xi)$  must be pure imaginary for all  $\xi \in \mathbf{R}^n$ . This clearly is the case if and only if  $A_\alpha$  is real for  $|\alpha|$  odd, and imaginary for  $|\alpha|$  even, and this is also equivalent to requiring that  $P(D)$  be a skew-adjoint operator on  $L^2(\mathbf{R}^n, \mathbf{C})$ . If  $u_0(x) = \int \hat{u}(\xi)e^{ix \cdot \xi} d\xi$  in  $L^2(\mathbf{R}^n)$  is given, then  $u(x, t) = \int \hat{u}(\xi)u_{\xi, \omega(\xi)}(x, t) d\xi$  solves the given wave equation and  $u(x, 0) = u_0(x)$ . As in the case  $n = 1$ , the transformation  $U(t)$  mapping  $u_0$  to  $u(t) = u(x, t)$  defines a one-parameter group of unitary transformations acting on  $L^2(\mathbf{R}^n, \mathbf{C})$  with  $P(D)$  as its infinitesimal generator, i.e.,  $U(t) = \exp(tP(D))$ .

▷ **1.4—Exercise 7.** Analyze the vector-valued wave equation  $u_t + P(D)u = 0$ , with  $u$  now a  $\mathbf{C}^d$ -valued function. Again,  $P(X) = \sum_{|\alpha| \leq r} A_\alpha X^\alpha$ , the coefficients  $A_\alpha$  now lying in the space of linear operators on  $\mathbf{C}^d$  (or  $d \times d$  complex matrices). Show that for  $P(D)$  to be a

skew-adjoint operator on  $L^2(\mathbf{R}^n, \mathbf{C}^d)$  generating a one-parameter group of unitary operators  $U(t)$ , the total symbol  $P(i\xi) = \sum_{|\alpha| \leq r} i^{|\alpha|} \xi^\alpha A_\alpha$  must be skew-adjoint operator on  $\mathbf{C}^d$  for all  $\xi$  in  $\mathbf{R}^n$ , and this in turn means that  $A_\alpha$  is self-adjoint for  $|\alpha|$  odd and skew-adjoint for  $|\alpha|$  even. Check this is equivalent to the **CPT**-invariance of  $u_t + P(D)u = 0$ . Write an explicit formula for  $U(t)u_0$  using vector-valued Fourier transforms.

**1.4—Example 4.** Finally we take a quick look at the classic linear wave equation,  $u_{tt} - c^2 \Delta u = 0$  with more spatial dimensions. If we substitute the plane wave Ansatz  $u(x, t) = u_{\xi, \omega}(x, t) = e^{i(x \cdot \xi - \omega t)}$  into this equation, we find that  $(\omega^2 - c^2 \|\xi\|^2)u = 0$ , so  $\omega(k) = c \|\xi\|$ , or  $\frac{\omega(k)}{\|\xi\|} = c$ . Thus, all the plane wave solutions travel at the same speed,  $c$ , but now they can travel with this speed in infinitely many different directions  $\xi$ , instead of just the two possible directions (“right” and “left”) when  $n = 1$ . If we now take a Gaussian initial condition  $u(x, 0)$  (and say assume that  $u_t(x, 0) = 0$ ) and analyze it into its Fourier components, we see that because the various components all move with speed  $c$  but in different directions, the original Gaussian wave packet will spread out and become dispersed.

Both a plucked piano string and the waves from a pebble dropped in a pond satisfy the classic wave equation. But in the first case we observe two travelling waves race off in opposite directions, maintaining their original shape as they go, while in the second we see a circular wave pattern moving out from the central source, gradually losing amplitude as the energy spreads out over a larger and larger circle.

▷ **1.4—Exercise 8.** Show that  $u_{tt} - c^2 \Delta u = 0$  is Lorentz invariant, conformally invariant, and **CPT**-invariant

## 1.5 Conservation Laws

Let  $u(x, t)$  denote the density of some physical quantity at the point  $x$  and time  $t$ , and  $\vec{\phi}(x, t)$  its flux, i.e.,  $\vec{\phi}(x, t) \cdot \vec{n} dA$  is the rate of flow of the quantity across a surface element  $dA$  with unit normal  $\vec{n}$ . Finally, let  $g(x, t)$  denote the rate at which the quantity is being created at  $x$  at time  $t$ . Then, essentially by the meanings of these definitions, given any region  $V$  with smooth boundary  $\partial V$ ,

$$\frac{d}{dt} \int_V u(x, t) dV = \int_V g(x, t) dV - \int_{\partial V} \vec{\phi}(x, t) \cdot \vec{n} dA,$$

which is the general form of a conservation law in integrated form. (Note that in the one space dimensional case this becomes  $\int_a^b u(x, t) dx = \int_a^b g(x, t) dx - [\phi(b, t) - \phi(a, t)]$ .) If  $u$  is  $C^1$ , then by Gauss’s Theorem,

$$\int_V \left( \frac{\partial u(x, t)}{\partial t} + \nabla \cdot \vec{\phi}(x, t) \right) dV = \int_V g(x, t) dV,$$

so, dividing by the volume of  $V$ , and letting  $V$  shrink down on a point  $x$  we get the corresponding differential form of the conservation law,

$$\frac{\partial u(x, t)}{\partial t} + \nabla \cdot \vec{\phi}(x, t) = g(x, t),$$

or in one space dimension,  $u_t + \phi_x = g$ . We will be mainly concerned with the case  $g = 0$ , and we note that in this case it follows that if  $\phi$  vanishes at infinity, then  $\int_{-\infty}^{\infty} u(x, t) dt$  is independent of  $t$  (which explains why this is called a conservation law).

As it stands, this is a single equation for two “unknown” functions  $u$  and  $\phi$ , and is underdetermined. Usually however we have some so-called “constitutive equation” expressing  $\phi$  in terms of  $u$ . In the most general case,  $\phi(x, t)$  will be a function not only of  $u(x, t)$  but also of certain partial derivatives of  $u$  with respect to  $x$ , however we will only consider the case of constitutive equations of the form  $\phi(x, t) = F(u(x, t))$ , where  $F$  is a smooth function on  $\mathbf{R}$  whose derivative  $F'$  will be denoted by  $f$ . Thus our conservation law finally takes the form:

$$(CL) \quad u_t + f(u)u_x = 0.$$

We will usually assume that  $f'(u) \geq 0$ , so that  $f$  is a non-decreasing function. This is satisfied in most of the important applications.

**1.5—Example 1.** Take  $F(u) = cu$ , so  $f(u) = c$  and we get once again the Linear Advection Equation  $u_t - cu_x = 0$ . The Method of Characteristics below will give yet another proof that the solution to the Cauchy Problem is  $u(x, t) = u_0(x - ct)$ .

**1.5—Example 2.** Take  $F(u) = \frac{1}{2}u^2$ , so  $f(u) = u$  and we get the important Inviscid Burgers Equation,  $u_t + uu_x = 0$ .

We will next explain how to solve the Cauchy Problem for such a Conservation Law using the so-called Method of Characteristics. We look for smooth curves  $(x(s), t(s))$  in the  $(x, t)$ -plane along which the solution to the Cauchy Problem is constant. Suppose that  $(x(s_0), t(s_0)) = (x_0, 0)$ , so that the constant value of  $u(x, t)$  along this so-called characteristic curve is  $u_0(x_0)$ . Then  $0 = \frac{d}{ds}u((x(s), t(s))) = u_x x' + u_t t'$ , and hence

$$\frac{dx}{dt} = \frac{x'(s)}{t'(s)} = -\frac{u_t}{u_x} = f(u(x(s), t(s))) = f(u_0(x_0)),$$

so the characteristic curve is a straight line of slope  $f(u_0(x_0))$ , i.e.,  $u$  has the constant value  $u_0(x_0)$  along the line  $\Gamma_{x_0} : x = x_0 + f(u_0(x_0))t$ . Note the following geometric interpretation of this last result: **to find the wave profile at time  $t$  (i.e., the graph of the map  $x \mapsto u(x, t)$ ), translate each point  $(x_0, u_0(x_0))$  of the initial profile to the right by the amount  $f(u_0(x_0))t$ .** (This is what we promised to show in Example 1.3.4.) The analytic statement of this geometric fact is that the solution  $u(x, t)$  to our Cauchy Problem must satisfy the implicit equation  $u(x, t) = u_0(x - tf(u(x, t)))$ . Of course the above is heuristic—how do we know that a solution exists?—but it isn’t hard to work backwards and make the argument rigorous.

The idea is to first define “characteristic coordinates”  $(\xi, \tau)$  in a suitable strip  $0 \leq t < T_B$  of the  $(x, t)$ -plane. We define  $\tau(x, t) = t$  and  $\xi(x, t) = x_0$  along the characteristic  $\Gamma_{x_0}$ , so  $t(\xi, \tau) = \tau$  and  $x(\xi, \tau) = \xi + f(u_0(\xi))\tau$ . But of course, for this to make sense, we must show that there is a unique  $\Gamma_{x_0}$  passing through each point  $(x, t)$  in the strip  $t < T_B$ .

The easiest case is  $f' = 0$ , say  $f = c$ , giving the Linear Advection Equation,  $u_t + cu_x = 0$ . In this case, all characteristics have the same slope,  $1/c$ , so that no two characteristics intersect, and there is clearly exactly one characteristic through each point, and we can define  $T_B = \infty$ .



From now on we will assume that the equation is “truly nonlinear”, in the sense that  $f'(u) > d > 0$ , so that  $f$  is a strictly increasing function.

If  $u'_0$  is everywhere positive, then  $u_0(x)$  is strictly increasing, and hence so is  $f(u_0(x))$ . In this case we can again take  $T_B = \infty$ . For, since the slope of the characteristic  $\Gamma_{x_0}$  issuing from  $(x_0, 0)$  is  $\frac{1}{f(u_0(x))}$ , it follows that if  $x_0 < x_1$  then  $\Gamma_{x_1}$  has smaller slope than  $\Gamma_{x_0}$ , and hence these two characteristics cannot intersect for  $t > 0$ , so again every point  $(x, t)$  in the upper half-plane lies on at most one characteristic  $\Gamma_{x_0}$ .

Finally the interesting general case: suppose  $u'_0$  is somewhere negative. In this case we define  $T_B$  to be the infimum of  $[-u'_0(x)f'(u_0(x))]^{-1}$ , where the inf is taken over all  $x$  with  $u'_0(x) < 0$ . For reasons that will appear shortly, we call  $T_B$  the *breaking time*. As we shall see,  $T_B$  is the largest  $T$  for which the Cauchy Problem for (CL) has a solution with  $u(x, 0) = u_0(x)$  in the strip  $0 \leq t < T$  of the  $(x, t)$ -plane. It is easy to construct examples for which  $T_B = 0$ ; this will happen if and only if there exists a sequence  $\{x_n\}$  with  $u'_0(x_n) \rightarrow -\infty$ . In the following we will assume that  $T_B$  is positive, and that in fact there is a point  $x_0$  where  $T_B = \frac{-1}{u'_0(x_0)f'(u_0(x_0))}$ . In this case, we will call  $\Gamma_{x_0}$  a *breaking characteristic*.

Now choose any point  $x_0$  where  $u'_0(x_0)$  is negative. For  $x_1$  slightly greater than  $x_0$ , the slope of  $\Gamma_{x_1}$  will be greater than the slope of  $\Gamma_{x_0}$ , and it follows that these two characteristics will meet at the point  $(x, t)$  where  $x_1 + f(u_0(x_1))t = x = x_0 + f(u_0(x_0))t$ , namely when  $t = -\frac{x_1 - x_0}{f(u_0(x_1)) - f(u_0(x_0))}$ .

▷ **1.5—Exercise 1.** Show that  $T_B$  is the least  $t$  for which any two characteristics intersect at some point  $(x, t)$  with  $t \geq 0$ .

▷ **1.5—Exercise 2.** Show that there is always at least one characteristic curve passing through any point  $(x, t)$  in the strip  $0 \leq t < T_B$  (and give a counterexample if  $u'_0$  is not required to be continuous).

Thus the characteristic coordinates  $(\xi, \tau)$  are well-defined in the strip  $0 \leq t < T_B$  of the  $(x, t)$ -plane. Note that since  $x = \xi + f(u_0(\xi))\tau$ ,  $\frac{\partial x}{\partial \xi} = 1 + f'(u_0(\xi))u'_0(\xi)\tau$ , and  $\frac{\partial x}{\partial \tau} = f(u_0(\xi))$ , while  $\frac{\partial t}{\partial \xi} = 0$  and  $\frac{\partial t}{\partial \tau} = 1$ . It follows that the Jacobian of  $(x, t)$  with respect to  $(\xi, \tau)$  is  $\frac{\partial x}{\partial \xi} = 1 + f'(u_0(\xi))u'_0(\xi)\tau$ , which is positive in  $0 \leq t < T_B$ , so that  $(\xi, \tau)$  are smooth coordinates in this strip. On the other hand, if  $\Gamma_{x_0}$  is a breaking characteristic, then the Jacobian approaches zero along  $\Gamma_{x_0}$  as  $t$  approaches  $T_B$ , confirming that the characteristic coordinates cannot be extended to any larger strip.

By our heuristics above, we know that the solution of the Cauchy Problem for (CL) with initial value  $u_0$  should be given in characteristic coordinates by the explicit formula  $u(\xi, \tau) = u_0(\xi)$ , and so we define a smooth function  $u$  in  $0 \leq t < T_B$  by this formula. Since the map from  $(x, t)$  to  $(\xi, \tau)$  is a diffeomorphism, this also defines  $u$  as a smooth function of  $x$  and  $t$ , but it will be simpler to do most calculations in characteristic coordinates. In any case, since a point  $(x, t)$  on the characteristic  $\Gamma_\xi$  satisfies  $x = \xi + f(u_0(\xi))t$ , we see that  $u = u(x, t)$  is the solution of the implicit equation  $u = u_0(x - tf(u))$ . It is obvious that  $u(x, 0) = u_0(x)$ , and we shall see next that  $u(x, t)$  satisfies (CL).

▷ **1.5—Exercise 3.** Use the chain-rule:  $u_x = u_\xi \frac{\partial \xi}{\partial x}$  and  $u_t = u_\xi \frac{\partial \xi}{\partial t}$  to compute the partial

derivatives  $u_x$  and  $u_t$  as functions of  $\xi$  and  $\tau$ :

$$u_t(\xi, \tau) = -\frac{u'_0(\xi)f(u_0(\xi))}{1 + u'_0(\xi)f'(u_0(\xi))\tau}$$

and

$$u_x(\xi, \tau) = \frac{u'_0(\xi)}{1 + u'_0(\xi)f'(u_0(\xi))\tau}$$

and deduce from this that  $u$  actually satisfies the equation (CL) in  $0 \leq t < T_B$ .

▷ **1.5—Exercise 4.** Show that, along a breaking characteristic  $\Gamma_{x_0}$ , the value of  $u_x$  at the point  $x = x_0 + f(u_0(x_0))t$  is given by  $\frac{u'_0(x_0)T_B}{T_B - t}$ . (Note that this is just the slope of the wave profile at time  $t$  over the point  $x$ .)

We can now get a qualitative but very precise picture of how  $u$  develops a singularity as  $t$  approaches the breaking time  $T_B$ , a process usually referred to as *shock formation or steepening and breaking of the wave profile*.

Namely, let  $\Gamma_{x_0}$  be a breaking characteristic and consider an interval  $I$  around  $x_0$  where  $u_0$  is decreasing. Let's follow the evolution of that part of the wave profile that is originally over  $I$ . Recall our algorithm for evolving the wave profile: each point  $(x, u_0(x))$  of the initial profile moves to the right with a constant velocity  $f(u_0(x))$ , so at time  $t$  it is at  $(x + f(u_0(x))t, u_0(x))$ . Thus, the higher part of the wave profile, to the left, will move faster than the lower part to the right, so the profile will bunch up and become steeper, until it eventually becomes vertical or “breaks” at time  $T_B$  when the slope of the profile actually becomes infinite over the point  $x_0 + f(u_0(x_0))T_B$ . (In fact, the above exercise shows that the slope goes to  $-\infty$  like a constant times  $\frac{1}{t - T_B}$ .) Note that the values of  $u$  remain bounded as  $t$  approaches  $T_B$ . In fact, it is clearly possible to continue the wave profile past  $t = T_B$ , using the same algorithm. However, for  $t > T_B$  there will be values  $x^*$  where the vertical line  $x = x^*$  meets the wave profile at time  $t$  in two distinct points (corresponding to two characteristics intersecting at the point  $(x^*, t)$ ), so the profile is no longer the graph of a single-valued function.

**1.5.1 Remark.** Despite the fact that  $u_x$  blows up along a breaking characteristic as  $t \rightarrow T_B$ , surprisingly the total variation of the function  $x \mapsto u(x, t)$  not only doesn't blow up as  $t$  approaches  $T_B$ , it is actually a constant of the motion, i.e.,  $\int |u_x(x, t)| dx = \int |u'_0(\xi)| d\xi$ . To see this, note that  $\frac{\partial x}{\partial \xi} = 1 + f'(u_0(\xi))u'_0(\xi)t$  is clearly positive for  $t < T_B$ , so that  $|u_x(x, t)| dx = |u_x(\xi, \tau)| \frac{\partial x}{\partial \xi} d\xi = |u_x(\xi, \tau)| (1 + f'(u_0(\xi))u'_0(\xi)\tau) d\xi$  and use the above formula for  $u_x(\xi, \tau)$ . Thus, although  $|u_x|$  gets very large as  $t$  approaches  $T_B$ , it is only large on a set of small measure.

For certain purposes it is interesting to know how higher derivatives  $u_{xx}, u_{xxx}, \dots$  behave as  $t$  approaches  $T_B$  along a breaking characteristic, (in particular, in the next section we will want to compare  $u_{xxx}$  with  $uu_x$ ). These higher partial derivatives can be estimated in terms of powers of  $u_x$  using  $\frac{\partial}{\partial x} = \frac{\partial}{\partial \xi} \left( \frac{\partial x}{\partial \xi} \right)^{-1}$ , and  $\frac{\partial x}{\partial \xi} = 1 + f'(u_0(\xi))u'_0(\xi)\tau$ .

▷ **1.5—Exercise 5.** Show that along a breaking characteristic  $\Gamma_{x_0}$ , as  $t \rightarrow T_B$ ,  $u_{xx} = O(u_x^3) = O((t - T_B)^{-3})$ . Similarly, show that  $u_{xxx} = O(u_x^5) = O((t - T_B)^{-5})$ .

For more details on the formation of singularities in conservation laws and other PDEs see [J] and [La2]. Below we will consider what happens after the breaking time  $T_B$ . Although

we can no longer have a smooth solution, it turns out that there may still be physically meaningful solutions of the integrated form of the conservation law. But first we consider an interesting example.

### 1.5—Example 3. Traffic Flow on a Highway.

We imagine an ideal, straight, infinitely long highway, modeled by the real line. To simplify the analysis, we assume that there are no entrance or exit ramps, and we will smooth out the discrete nature of the cars and model the traffic density and flux by approximating continuous statistical averages. We choose an arbitrary origin, and we let  $u(x, t)$  denote the density of cars at the point  $x$  at time  $t$  (in units of cars per kilometer), and we let  $\phi(x, t)$  denote the flux of cars, i.e., the rate at which cars are passing the point  $x$  at time  $t$  (in units of cars per second). We will also want to consider the speed of the traffic at  $x$  at time  $t$ , which we will denote by  $v(x, t)$  and measure it in kilometers per second. We have the obvious relation  $\phi = vu$ . If we choose any two points  $a$  and  $b$  along the highway, then clearly we have the conservation law in integrated form,  $\frac{d}{dt} \int_a^b u(x, t) dx + \phi(b, t) - \phi(a, t) = 0$ ; i.e., the rate of change of the total number of cars between  $a$  and  $b$  plus the rate at which cars are coming in at  $b$  minus the rate at which they are leaving at  $a$  must be zero (since no cars are leaving between  $a$  and  $b$ ). Assuming  $u$  is smooth, and letting  $a$  and  $b$  approach  $x$  we get the differential form of the conservation law,  $u_t + \phi_x = 0$ .

To proceed further we will need a constitutive relation, relating  $u$  and  $\phi$ . It is natural to try to model this using the intuitively observed “law” of traffic flow that the denser the traffic, the slower drivers will travel. For simplicity, we assume that there is a maximum velocity  $v_{max}$  (the “speed limit”) and a maximum density  $u_{max}$  and we assume that the speed at which drivers travel is  $v_{max}$  on an empty road (i.e., when  $u = 0$ ), 0 when traffic is bumper to bumper, (i.e., when  $u = u_{max}$ ) and linear in between. This leads to the relation  $v(u) = v_{max}(1 - u/u_{max})$ , and then using  $\phi = vu$  we derive the constitutive relation,  $\phi(u) = F(u) = uv(u)$ . The conservation law then takes the form  $u_t + F'(u)u_x = u_t + (v(u) + uv'(u))u_x = 0$ , or  $u_t + v_{max}(1 - 2u/u_{max})u_x = 0$ .

Of course, traffic engineers use much more realistic models that take into account on and off ramps, and use more sophisticated constitutive relations, but already with this model one can see interesting phenomena such as the development of a “shock wave” as oncoming traffic meets traffic stopped at a red light. We illustrate this below, after first introducing the simplest kind of non-smooth solutions of conservation laws

#### 1.5.2 Shock Wave Solutions and the Rankine-Hugoniot Jump Condition.

Let  $x_s(t)$  denote a smooth curve  $C$  in the closed upper-half  $(x, t)$ -plane, defined for all  $t \geq 0$ , and so dividing the upper-half plane into two open regions,  $R^-$  to the left and  $R^+$  to the right. Let  $u(x, t)$  be a smooth solution of the conservation law  $u_t + \phi_x$  in the union of these two regions. We assume that the restrictions  $u|_{R^-}$  and  $u|_{R^+}$  each extend continuously to the boundary curve  $C$ , although these two extensions do not necessarily agree. Given a point  $p = (x_s(t), t)$  on  $C$ , the difference between the limits  $u(x_s^+, t)$  of  $u$  at  $p$  from the right and the limit  $u(x_s^-, t)$  from the left defines the “jump”  $[u](x_s, t) = u(x_s^+, t) - u(x_s^-, t)$  across  $C$  at this point. Since  $\phi$  is given by a constitutive equation  $\phi(x, t) = F(u(x, t))$ , we also have a corresponding jump  $[\phi](x_s, t) = \phi(x_s^+, t) - \phi(x_s^-, t)$  in  $\phi$  as we cross  $C$ . We will call such a piecewise smooth solution  $u$  of the conservation law a *shock wave* solution of the conservation law with *shock path*  $C$  if in addition to satisfying the equation in each of  $R^-$  and  $R^+$ , it also satisfies the integrated form of the conservation law, i.e., for all

$a < b$ ,  $\frac{d}{dt} \int_a^b u(x, t) dx + \phi(b, t) - \phi(a, t) = 0$ . By choosing  $a < x_s(t) < b$  and breaking the above integral into a sum corresponding to the sub-intervals  $[a, x_s(t)]$  and  $[x_s(t), b]$  (and then letting  $a$  and  $b$  approach  $x_s(t)$ ), we can easily derive the following:

**Rankine-Hugoniot Jump Condition.** *Let  $u$  be a shock wave solution of the conservation law  $u_t + \phi_x$  with shock path  $C$  given by  $(x_s(t), t)$ . Then  $x_s(t)$  satisfies the following ordinary differential equation, known as the Rankine-Hugoniot Jump Condition:*

$$\frac{dx_s(t)}{dt} = \frac{[\phi](x_s, t)}{[u](x_s, t)}.$$

▷ **1.5—Exercise 6.** A Shock Wave Solution of the Inviscid Burgers Equation. Let's try to solve the Inviscid Burgers Equation,  $u_t + uu_x = 0$ , with the initial condition  $u_0(x) = 1$  for  $x < 0$  and  $u_0(x) = 0$  for  $x \geq 0$ . It is easy to see that there are pairs of characteristics that meet after an arbitrarily short time, so  $T_B = 0$ , and this can have no smooth solution. Show that  $u(x, t) = 1$  for  $x < t/2$  and  $u(x, t) = 0$  for  $x > t/2$  is a shock wave solution with shock path  $x_s(t) = t/2$ .

▷ **1.5—Exercise 7.** A Shock Wave at a Red Light. Consider highway traffic that is backing up as it runs into a red light. Assume that the oncoming traffic has a constant density  $u_1$ , and at time  $t = 0$  it runs into the stopped traffic which has density  $u_{max}$  beginning at  $x = 0$  and extending to the right. Show that the shock curve is given by  $x_s(t) = -v_{max}(\frac{u_1}{u_{max}})t$  and the density is  $u_1$  to the left, and  $u_{max}$  to the right. In other words, traffic is backing up at the speed  $v_{max}(\frac{u_1}{u_{max}})$ .

## 1.6 Split-Stepping

We now return to the KdV equation, say in the form  $u_t = -uu_x - u_{xxx}$ . If we drop the nonlinear term, we have left the dispersive wave equation  $u_t = -u_{xxx}$ , that we considered in the section on linear wave equations. Recall that we can solve its Cauchy Problem, either by using the Fourier Transform or by convolution with an explicit fundamental solution that we wrote in terms of the Airy function.

On the other hand, if we drop the linear term, we are left with the inviscid Burgers Equation,  $u_t = -uu_x$ , which as we know exhibits steepening and breaking of the wave profile, causing a shock singularity to develop in finite time  $T_B$  for any non-trivial initial condition  $u_0$  that vanishes at infinity. Up to this breaking time,  $T_B$ , we can again solve the Cauchy Problem, either by the method of characteristics, or by solving the implicit equation  $u = u_0(x - ut)$  for  $u$  as a function of  $x$  and  $t$ .

Now, in [BS] it is proved that KdV defines a global flow on the Sobolev space  $H^4(\mathbf{R})$  of functions  $u : \mathbf{R} \rightarrow \mathbf{R}$  having derivatives of order up to four in  $L^2$ , so it is clear that dispersion from the linear  $u_{xxx}$  term must be counteracting the peaking from the nonlinear  $uu_x$  term, preventing the development of a shock singularity.

In order to understand this balancing act better, it would be useful to have a method for taking the two flows defined by  $u_t = -u_{xxx}$  and  $u_t = -uu_x$  and combining them to define the flow for the full KdV equation. (In addition, this would give us a method for solving the KdV Cauchy Problem numerically.)

In fact there is a very general technique that applies in such situations. In the pure mathematics community it is usually referred to as the Trotter Product Formula, while in the applied mathematics and numerical analysis communities it is called split-stepping. Let me state it in the context of ordinary differential equations. Suppose that  $Y$  and  $Z$  are two smooth vector fields on  $\mathbf{R}^n$ , and we know how to solve each of the differential equations  $dx/dt = Y(x)$  and  $dx/dt = Z(x)$ , meaning that we know both of the flows  $\phi_t$  and  $\psi_t$  on  $\mathbf{R}^n$  generated by  $Y$  and  $Z$  respectively. The Trotter Product Formula is a method for constructing the flow  $\theta_t$  generated by  $Y + Z$  out of  $\phi$  and  $\psi$ ; namely, letting  $\Delta t = \frac{t}{n}$ ,  $\theta_t = \lim_{n \rightarrow \infty} (\phi_{\Delta t} \psi_{\Delta t})^n$ . The intuition behind the formula is simple. Think of approximating the solution of  $dx/dt = Y(x) + Z(x)$  by Euler's Method. If we are currently at a point  $p_0$ , to propagate one more time step  $\Delta t$  we go to the point  $p_0 + \Delta t (Y(p_0) + Z(p_0))$ . Using the split-step approach on the other hand, we first take an Euler step in the  $Y(p_0)$  direction, going to  $p_1 = p_0 + \Delta t Y(p_0)$ , then take a second Euler step, but now from  $p_1$  and in the  $Z(p_1)$  direction, going to  $p_2 = p_1 + \Delta t Z(p_1)$ . If  $Y$  and  $Z$  are constant vector fields, then this gives exactly the same final result as the simple full Euler step with  $Y + Z$ , while for continuous  $Y$  and  $Z$  and small time step  $\Delta t$  it is a good enough approximation that the above limit is valid. The situation is more delicate for flows on infinite dimensional manifolds, nevertheless it was shown by F. Tappert in [Ta] that the Cauchy Problem for KdV can be solved numerically by using split-stepping to combine methods for  $u_t = -uu_x$  and  $u_t = -u_{xxx}$ .

[Tappert actually uses an interesting variant, known as Strang splitting, which was first suggested in [St] to solve multi-dimensional hyperbolic problems by split-stepping one-dimensional problems. One advantage of splitting in numerical analysis comes from the greatly reduced effort required to solve the smaller bandwidth linear systems that arise when implicit schemes are necessary to maintain stability, but in addition, Strang demonstrated that second-order accuracy of the component methods need not be compromised by the asymmetry of the splitting, as long as the pattern  $\phi_{\frac{\Delta t}{2}} \psi_{\frac{\Delta t}{2}} \psi_{\frac{\Delta t}{2}} \phi_{\frac{\Delta t}{2}}$  is used, to account for possible non-commutativity of  $Y$  and  $Z$ . (This may be seen by multiplying the respective exponential series.) Serendipitously, when output is not required, several steps of Strang splitting require only marginal additional effort:  $(\phi_{\frac{\Delta t}{2}} \psi_{\frac{\Delta t}{2}} \psi_{\frac{\Delta t}{2}} \phi_{\frac{\Delta t}{2}})^n = (\phi_{\frac{\Delta t}{2}} \psi_{\Delta t} (\phi_{\Delta t} \psi_{\Delta t})^{n-1} \phi_{\frac{\Delta t}{2}})$ .

Aside from such numerical considerations, split-stepping suggests a way to understand the mechanism by which dispersion from  $u_{xxx}$  balances shock formation from  $uu_x$  in KdV. Namely, if we consider wave profile evolution under KdV as made up of a succession of pairs of small steps (one for  $u_t = -uu_x$  and the one for  $u_t = -u_{xxx}$ ), then when  $u$ ,  $u_x$ , and  $u_{xxx}$  are not too large, the steepening mechanism will dominate. But recall that as the time  $t$  approaches the breaking time  $T_B$ ,  $u$  remains bounded, and along a breaking characteristic  $u_x$  only blows up like  $(T_B - t)^{-1}$  while  $u_{xxx}$  blows up like  $(T_B - t)^{-5}$ . Thus, near breaking in time and space, the  $u_{xxx}$  term will dwarf the non-linearity and will disperse the incipient shock. In fact, computer simulations do show just such a scenario playing out.

## Section 2

# The Korteweg-de Vries Equation

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We have seen that in the Korteweg-de Vries (or KdV) equation,  $u_t + 6uu_x + u_{xxx} = 0$ , expresses a balance between dispersion from its third-derivative term and the shock-forming tendency of its nonlinear term, and in fact many models of one-dimensional physical systems that exhibit mild dispersion and weak nonlinearity lead to KdV as the controlling equation at some level of approximation.

### 2.1 Early History, Exact Solutions, and Solitons

We will give here only a very abbreviated version of the historical origins of KdV. For more details see [P] and further references given there.

As already mentioned, KdV first arose as the modelling equation for solitary gravity waves in a shallow canal. Such waves are rare and not easy to produce, and they were apparently only first noticed in 1834 (by the naval architect, John Scott Russell). Early attempts by Stokes and Airy to model them mathematically seemed to indicate that such waves could not be stable—and their very existence was at first a matter of debate. Later work by Boussinesq and Rayleigh corrected errors in this earlier theory, and finally a paper in 1894 by Korteweg and de Vries [KdV] settled the matter by giving a convincing mathematical argument that wave motion in a shallow canal is governed by KdV, and showing by explicit computation that their equation admitted travelling-wave solutions that had exactly the properties described by Russell, including the relation of height to speed that Russell had determined experimentally in a wave tank he had constructed.

But it was only much later that the truly remarkable properties of the KdV equation became evident. In 1954, Fermi, Pasta and Ulam (FPU) used one of the very first digital computers to perform numerical experiments on a one-dimensional, anharmonic lattice model, and their results contradicted the then current expectations of how energy should distribute itself among the normal modes of such a system [FPU]. A decade later, Zabusky and Kruskal re-examined the FPU results in a famous paper [ZK]. They showed that, in a certain continuum limit, the FPU lattice was approximated by the KdV equation. They then did their own computer experiments, solving the Cauchy Problem for KdV with initial conditions corresponding to those used in the FPU experiments. In the results of these simulations they observed the first example of a “soliton”, a term that they coined to describe a remarkable particle-like behavior (elastic scattering) exhibited by certain KdV solutions. Zabusky and Kruskal showed how the coherence of solitons explained the anomalous results observed by Fermi, Pasta, and Ulam. But in solving that mystery, they had uncovered a larger one; KdV solitons were unlike anything that had been seen before, and the search for an explanation of their remarkable behavior led to a series of discoveries that changed the course of applied mathematics for the next thirty years.

We next fill in some of the mathematical details behind the above sketch, beginning with a discussion of explicit solutions to the KdV equation.

To find the travelling wave solutions of the KdV equation is straightforward; substituting

the Ansatz  $u(x, t) = f(x - ct)$  into KdV gives the ODE  $-cf' + 6ff' + f'''$ , and adding as boundary condition that  $f$  should vanish at infinity, a routine computation leads to the two-parameter family of travelling-wave solutions  $u(x, t) = 2a^2 \operatorname{sech}^2(a(x - 4a^2t + d))$ .

▷ **2.1—Exercise 1.** Carry out the details of this computation. (Hint: Get a first integral by writing  $6ff' = (3f^2)'$ .)

These are the solitary waves seen by Russell, and they are now usually referred to as the 1-soliton solutions of KdV. Note that their amplitude,  $2a^2$ , is just half their speed,  $4a^2$ , while their “width” is proportional to  $a^{-1}$ ; i.e., taller solitary waves are thinner and move faster.

These solutions were found by Korteweg and de Vries, who also carried out the more complicated calculations that arise when one assumes periodicity instead of decay as a boundary condition. The profile of the periodic travelling wave is given in terms of the Jacobi elliptic function  $\operatorname{cn}$ ,

$$u(x, t) = 2a^2k^2 \operatorname{cn}^2(a(x - 4(2k^2 - 1)a^2t)),$$

and following Korteweg and de Vries they are called cnoidal waves. Here  $0 \leq k \leq 1$  is the modulus of the elliptic function  $\operatorname{cn}$ . Note that as the modulus  $k \rightarrow 1$ ,  $\operatorname{cn}$  converges to  $\operatorname{sech}$ , and so the cnoidal waves have the solitary wave as a limiting case.

Next, following M. Toda [To], we will “derive” the  $n$ -soliton solutions of KdV. We first rewrite the 1-soliton solution as  $u(x, t) = 2\frac{\partial^2}{\partial x^2} \log \cosh(a(x - 4a^2t + \delta))$ , or  $u(x, t) = 2\frac{\partial^2}{\partial x^2} \log K(x, t)$  where  $K(x, t) = (1 + e^{2a(x - 4a^2t + \delta)})$ .

We now try to generalize, looking for solutions of the form  $u(x, t) = 2\frac{\partial^2}{\partial x^2} \log K(x, t)$ , with  $K$  of the form  $K(x, t) = 1 + A_1e^{2\eta_1} + A_2e^{2\eta_2} + A_3e^{2(\eta_1 + \eta_2)}$ , where  $\eta_i = a_i(x - 4a_i^2t + d_i)$ , and we are to choose the  $A_i$  and  $d_i$  by substituting in KdV and seeing what works.

▷ **2.1—Exercise 2.** Show that KdV is satisfied for  $u(x, t)$  of this form and for arbitrary choices of  $A_1, A_2, a_1, a_2, d_1, d_2$ , provided only that we define

$$A_3 = \left( \frac{a_2 - a_1}{a_1 + a_2} \right)^2 A_1 A_2.$$

The solutions of KdV that arise in this way are called the 2-soliton solutions of KdV.

▷ **2.1—Exercise 3.** Show that if we take  $A_i = \frac{1}{2a_i}$  then  $K(x, t) = \det B(x, t)$ , where  $B(x, t)$  is the  $2 \times 2$  matrix,  $B_{ij}(x, t) = \delta_{ij} + \frac{1}{a_i + a_j} e^{\eta_i + \eta_j}$ .

Yes, you’ve guessed it, this generalizes in the obvious way. If we define an  $n \times n$  matrix  $B(x, t)$  with the matrix elements defined in the same way, then  $u(x, t) = 2\frac{\partial^2}{\partial x^2} \log \det B(x, t)$  is a solution of KdV for all choices of  $a_i$  and  $d_i$ , and this  $2n$ -parameter family of solutions is called the  $n$ -soliton solutions of KdV.

Of course this is a complete swindle! Only knowing the answer in advance allowed us to make the correct choice of Ansatz for  $K$ . Later we shall see how to get the  $n$ -soliton family of solutions for KdV in a completely straightforward way using the Inverse Scattering Method.

But, for now, we want to look more closely at the 2-soliton solutions, and more specifically their asymptotic behavior as  $t$  approaches  $\pm\infty$ . We could do this for an arbitrary 2-soliton, but for simplicity let us take  $a_1 = a_2 = 3$ .

▷ **2.1—Exercise 4.** Show that for these choices of  $a_1$  and  $a_2$ ,

$$u(x, t) = 12 \frac{3 + 4 \cosh(2x - 8t) + \cosh(4x - 64t)}{[\cosh(3x - 36t) + 3 \cosh(x - 28t)]^2},$$

so in particular  $u(x, 0) = 6 \operatorname{sech}^2(x)$ .

▷ **2.1—Exercise 5.** Show that for  $t$  large and negative  $u(x, t)$  is asymptotically equal to  $2 \operatorname{sech}^2(x - 4t - \phi) + 8 \operatorname{sech}^2(x - 16t + \frac{\phi}{2})$ , while for  $t$  large and positive  $u(x, t)$  is asymptotically equal to  $2 \operatorname{sech}^2(x - 4t + \phi) + 8 \operatorname{sech}^2(x - 16t - \frac{\phi}{2})$ , where  $\phi = \log(3)/3$ . (This is hard. For the solution see [To], Chapter 6.)

Note what this says. If we follow the evolution from  $-T$  to  $T$  (where  $T$  is large and positive), we first see the superposition of two 1-solitons; a larger and thinner one to the left of and overtaking a shorter, fatter, and slower-moving one to the right. Around  $t = 0$  they merge into a single lump (with the shape  $6 \operatorname{sech}^2(x)$ ), and then they separate again, with their original shapes restored, but now the taller and thinner one is to the right. It is almost as if they had passed right through each other—the only effect of their interaction is the pair of phase shifts—the slower one is retarded slightly from where it would have been, and the faster one is slightly ahead of where it would have been. Except for these phase shifts, the final result is what we might expect from a linear interaction. It is only if we see the interaction as the two solitons meet that we can detect its highly nonlinear nature. (Note that at time  $t = 0$ , the maximum amplitude, 6, of the combined wave is actually less than the maximum amplitude, 8, of the taller wave when they are separated.) But of course the really striking fact is the resilience of the two individual solitons—their ability to put themselves back together after the collision. Not only is no energy radiated away, but their actual shapes are preserved.

(Remarkably, on page 384 of Russell’s 1844 paper, there is a sketch of a 2-soliton interaction experiment that Russell had carried out in his wave tank!)

We shall see later that every initial profile  $u_0$  for the KdV equation can be thought of as made up of two parts: an  $n$ -soliton solution for some  $n$ , and a dispersive “tail”. The tail is transient, i.e., it rapidly tends to zero in the sup norm (although its  $L^2$  norm is preserved), while the  $n$ -soliton part behaves in the robust way that is the obvious generalization of the 2-soliton behavior we have just analyzed.

Now back to the computer experiment of Zabusky and Kruskal. For numerical reasons, they chose to deal with the case of periodic boundary conditions—in effect studying the KdV equation  $u_t + uu_x + \delta^2 u_{xxx} = 0$  (which they label (1) ) on the circle instead of on the line. For their published report, they chose  $\delta = 0.022$  and used the initial condition  $u(x, 0) = \cos(\pi x)$ . With the above background, it is interesting to read the following extract from their 1965 report, containing the first use of the term “soliton”:

- (I) Initially the first two terms of Eq. (1) dominate and the classical overtaking phenomenon occurs; that is  $u$  steepens in regions where it has negative slope. (II) Second, after  $u$  has steepened sufficiently, the third term becomes important and serves



to prevent the formation of a discontinuity. Instead, oscillations of small wavelength (of order  $\delta$ ) develop on the left of the front. The amplitudes of the oscillations grow, and finally *each* oscillation achieves an almost steady amplitude (that increases linearly from left to right) and has the shape of an individual solitary-wave of (1). (III) Finally, each “solitary wave pulse” or *soliton* begins to move uniformly at a rate (relative to the background value of  $u$  from which the pulse rises) which is linearly proportional to its amplitude. Thus, the solitons spread apart. Because of the periodicity, two or more solitons eventually overlap spatially and interact nonlinearly. Shortly after the interaction they reappear virtually unaffected in size or shape. In other words, solitons “pass through” one another without losing their identity. *Here we have a nonlinear physical process in which interacting localized pulses do not scatter irreversibly.*

## 2.2 Constants of the Motion for the KdV Flow

After the appearance of the Zabusky-Kruskal paper, attempts were quickly made to understand what it was that was special about KdV that led to the soliton phenomenon. Perhaps because soliton behavior involved the conservation of shape, one conjecture was that the KdV flow might have unusually many constants of the motion, and a search was begun for “polynomial conservation laws”, i.e, polynomials  $P(u, u_x, u_{xx}, \dots)$  in  $u$  and its spatial partial derivatives such that  $\int_{-\infty}^{\infty} P(u(x, t), u_x(x, t), u_{xx}(x, t), \dots) dx$  would be independent of  $t$  for all solutions  $u(x, t)$  of KdV that vanish sufficiently rapidly at infinity.

We have seen that a sufficient condition for this is that any solution of KdV should satisfy a conservation law with  $P$  as the density, i.e., there should exist a corresponding flux,  $J(u, u_x, u_{xx}, \dots)$ , such that the equation  $\frac{\partial}{\partial t} P + \frac{\partial}{\partial x} J$  should follow as a formal consequence of the KdV equation. If this is the case, then we will call  $u$  a *conserved density* for KdV.

Now KdV is itself a conservation law:  $u_t + (3u^2 + u_{xx})_x = 0$ , so  $u$  is one conserved density. Also, if we multiply KdV through by  $u$ , we can rewrite the result as  $(\frac{1}{2}u^2)_t + (2u^3 + uu_{xx} - \frac{1}{2}u_x^2)_x = 0$ , so  $u^2$  is a second conserved density for KdV. Finally multiplying KdV by  $u^2$  and adding the result to  $u_x$  times the  $x$  derivative of KdV, we find that  $(-u^3 + \frac{1}{2}u_x^2)$  is a third conserved density for KdV, with associated flux  $(-\frac{9}{2}u^4 - 3u^2u_{xx} + 6uu_x^2 + u_xu_{xxx} - \frac{1}{2}u_{xx}^2)$ . For future reference we will name these conserved densities  $\tilde{F}_1(u) = u$ ,  $\tilde{F}_2(u) = u^2$ , and  $\tilde{F}_3(u, u_x) = -u^3 + \frac{1}{2}u_x^2$ .

These three were classical, in the sense that they were well-known long before the Zabusky-Kruskal paper. In fact, as we shall see below, they represent important conserved physical quantities in the case that KdV is modelling a wave in a shallow canal. A fourth conserved density was found by Whitham, and Zabusky and Kruskal discovered two more. This was prior to the existence of symbolic manipulation computer programs such as Macsyma, and by now the computations were getting horrendous. Still, with remarkable perseverance and effort the number was eventually raised to eleven, before Miura, using generating function methods, finally showed that these were in fact the first elements of an infinite sequence of conserved densities,  $\tilde{F}_k(u, u_x, u_{xx}, \dots)$  for KdV.

It is still not easy to prove the existence of the  $\tilde{F}_k$ , and we will not attempt to do so here, but rather refer the interested reader to Chapter 1 of [La3]. There was naturally speculation that KdV could somehow be regarded as an infinite dimensional Hamiltonian system, with

one of the functionals  $F_k(u) = \int_{-\infty}^{\infty} \tilde{F}_k(u) dx$  playing the rôle of the Hamiltonian, and all of them being in involution, and that turned out to be the case.

Let  $u(x, t)$  be a solution of KdV that along with all its derivatives vanishes at infinity, and let us imagine  $u$  as measuring the height of a wave in a narrow channel (above the level of undisturbed water). If we regard the water as incompressible, then  $u(x, t) dx$  is proportional to the mass of water in the wave between  $x$  and  $x + dx$  (at time  $t$ ), so we can identify the constant of the motion  $\int u(x, t) dx$  with the total mass of water in the wave, and we will denote it by  $\mu(u)$ .

▷ **2.2—Exercise 1.** Show that the 1-soliton with parameter  $a$  has mass  $4a$ .

We expect that the linear momentum carried by the wave should also be a constant of the motion. How do we compute it? It is natural to define the center of mass of the wave at time  $t$  by  $\bar{x}_u(t) = \frac{1}{\mu(u)} \int xu(x, t) dx$ .

▷ **2.2—Exercise 2.** Show that  $\bar{x}_u(t)$  moves with constant velocity. Equivalently, show that  $P_u = \int xu_t(x, t) dx$  is another constant of the motion.

In [To], Toda calls  $P_u$  the total momentum of the wave, but this does not seem physically justified to me. It suggests that the velocity of the center of mass is the same as the average translational velocity of the water particles in the  $x$  direction, as if the water were moving along with the wave. In fact, in the approximation used to derive the KdV equation, the  $x$ -component of velocity of the water particle located at  $x$  at time  $t$  is proportional to the wave height  $u(x, t)$ , so that the total  $x$ -momentum of the wave is actually  $\int u^2(x, t) dx$ .

This leaves the third classical constant of the motion:  $\int (u^3 - \frac{1}{2}u_x^2) dx$ ; we would like to give it some physical interpretation—and total energy is the obvious suspect. I don't see any convincing argument to identify it with the sum of the kinetic and potential energy of the wave, but on the other hand we will see in the next section that in our representation of KdV as a Hamiltonian system, this constant of the motion is the Hamiltonian function, and of course in classical mechanics that is the rôle normally played by the total energy.

## 2.3 KdV as a Hamiltonian System

I will assume below that the reader is familiar with the basic facts concerning symplectic manifolds and Hamiltonian systems, including the infinite dimensional case, however I have included an appendix in which these concepts are reviewed.

We shall now see how to view KdV as a Hamiltonian system in a simple and natural way. It turns out that this Hamiltonian system has a key property one would expect from any generalization to infinite dimensions of the concept of complete integrability in the Liouville sense, namely the existence of infinitely many functionally independent constants of the motion that are in involution. (Later, in discussing the inverse scattering method, we will indicate how complete integrability was proved in a more precise sense by Fadeev and Zakharov [ZF]; they demonstrated that the “scattering data” for the KdV equation obey the characteristic Poisson bracket relations for the action-angle variables of a completely integrable system.)

For simplicity, we shall take as our phase space  $P$  for KdV the Schwartz space,  $\mathcal{S}(\mathbf{R})$ , of rapidly decreasing functions  $u : \mathbf{R} \rightarrow \mathbf{R}$ , although a much larger space would be possible.

As mentioned earlier, it is proved in [BS] that KdV defines a global flow on the Sobolev space  $H^4(\mathbf{R})$  (see also [Ka1], [Ka2]), and it is not hard to see that  $P$  is an invariant subspace of this flow. For  $u, v$  in  $P$  we will denote their  $L^2$  inner product  $\int_{-\infty}^{\infty} u(x)v(x) dx$  by  $\langle u, v \rangle$  and we define

$$\Omega(u, v) = \frac{1}{2} \int_{-\infty}^{\infty} (v(x)fu(x) - u(x)fv(x)) dx,$$

where  $fu(x) = \int_{-\infty}^x u(y) dy$  denotes the indefinite integral of  $u$ . (For the periodic KdV equation we take  $P$  to be all smooth periodic functions of period  $2\pi$  and replace the  $\int_{-\infty}^{\infty}$  by  $\int_0^{2\pi}$ .)

We denote by  $\partial$  the derivative operator,  $u \mapsto u'$ , so  $\partial fu = u$ , and  $\int_{-\infty}^{\infty} \partial u = 0$  for functions  $u$  that vanish at infinity. We will also write  $u_{(k)}$  for  $\partial^k u$ , but for small  $k$  we shall also use  $u = u_{(0)}$ ,  $u_x = u_{(1)}$ ,  $u_{xx} = u_{(2)}$ , etc.

There is a simple but important relation connecting  $\Omega$ ,  $\partial$ , and the  $L^2$  inner product, namely:

$$\Omega(\partial u, v) = \langle u, v \rangle.$$

▷ **2.3—Exercise 1.** Prove this. (Hint: Show that  $\partial(u fv) = (\partial u) fv + u v$ ,  $\int_{-\infty}^{\infty} \partial(u fv) = 0$ , and  $\Omega(\partial u, v) = (1/2) \int_{-\infty}^{\infty} (v u - (\partial u) fv)$ .)

One important consequence of this is the weak non-degeneracy of  $\Omega$ . For, if  $i_v \Omega$  is zero, then in particular  $\langle u, v \rangle = \Omega(\partial u, v) = -\Omega(v, \partial u) = -(i_v \Omega)(\partial u) = 0$  for all  $u$ , so  $v = 0$ .

$\Omega$  is clearly a skew-bilinear form on  $P$ . Since  $P$  is a vector space, we can as usual identify  $P$  with its tangent space at every point, and then  $\Omega$  becomes a “constant” 2-form on  $P$ . Since it is constant, of course  $d\Omega = 0$ .

A second consequence of  $\Omega(\partial u, v) = \langle u, v \rangle$  is that if  $F : P \rightarrow \mathbf{R}$  is a smooth function (or “functional”) on  $P$  that has a gradient  $\nabla F$  with respect to the flat Riemannian structure on  $P$  defined by the  $L^2$  inner product, then the symplectic gradient of  $F$  also exists.

Recall that  $dF$ , the differential of  $F$ , is the 1-form on  $P$  defined by

$$dF_u(v) = \left. \frac{d}{d\epsilon} \right|_{\epsilon=0} F(u + \epsilon v),$$

and the gradient of  $F$  is the vector field dual to  $dF$  with respect to the  $L^2$  inner product (if such a vector field indeed exists), i.e., it is characterized by  $(dF)_u(v) = \langle (\nabla F)_u, v \rangle$ . Similarly, the symplectic gradient of  $F$  (if it exists) is the dual to  $dF$  with respect to  $\Omega$ , i.e., it satisfies  $(dF)_u(v) = \Omega((\nabla_s F)_u, v)$ . Since  $\langle (\nabla F)_u, v \rangle = \Omega((\partial(\nabla F)_u), v)$ , it follows that if  $(\nabla F)_u$  exists then  $(\nabla_s F)_u$  also exists and equals  $\partial((\nabla F)_u)$ .

**2.3.1 Remark.** Since  $P$  is not complete with respect to the  $L^2$  norm, it is **not** automatic that a continuous linear functional on  $P$  can be represented as the inner product with some element of  $P$ . Thus, the existence of a gradient vector field corresponding to a particular function  $F$  requires proof.

We shall only consider functions  $F : P \rightarrow \mathbf{R}$  of the type normally considered in the Calculus of Variations, i.e., of the form:

$$F(u) = \int_{-\infty}^{\infty} \tilde{F}(u, u_x, u_{xx}, \dots) dx,$$

where  $\tilde{F} : \mathbf{R}^{k+1} \rightarrow \mathbf{R}$  is a polynomial function without a constant term. Then the usual integration by parts argument of the Calculus of Variations shows that such an  $F$  has a gradient, given by:

$$(\nabla F)_u = \frac{\partial \tilde{F}}{\partial u} - \partial \left( \frac{\partial \tilde{F}}{\partial u_x} \right) + \partial^2 \left( \frac{\partial \tilde{F}}{\partial u_{xx}} \right) - \dots$$

**2.3.2 Remark.** The above formula is written using the standard but somewhat illogical conventions of the Calculus of Variations and needs a little interpretation.  $\tilde{F}$  is a function of variables  $y = (y_0, y_1, y_2, \dots, y_k)$ , and for example  $\partial \tilde{F} / \partial u_{xx}$  really means the function on  $\mathbf{R}$  whose value at  $x$  is  $\partial \tilde{F} / \partial y_2$  evaluated at  $y = (u_{(0)}(x), u_{(1)}(x), u_{(2)}(x), \dots, u_{(k)}(x))$ .

From what we saw above, the symplectic gradient of such an  $F$  exists and is given by:

$$(\nabla_s F)_u = \partial \left( \frac{\partial \tilde{F}}{\partial u} \right) - \partial^2 \left( \frac{\partial \tilde{F}}{\partial u_x} \right) + \partial^3 \left( \frac{\partial \tilde{F}}{\partial u_{xx}} \right) - \dots$$

Now a smooth function on a symplectic manifold is called Hamiltonian if it has a symplectic gradient, so what we have shown is that all such Calculus of Variations functionals on  $P$  are Hamiltonian and define the Hamiltonian flow  $\dot{u} = (\nabla_s F)_u$ , where  $u(t)$  denotes a smooth curve in  $P$ . If instead of  $u(t)(x)$  we write  $u(x, t)$ , this symbolic ODE in the manifold  $P$  becomes the PDE:

$$u_t = \partial \left( \frac{\partial \tilde{F}}{\partial u} \right) - \partial^2 \left( \frac{\partial \tilde{F}}{\partial u_x} \right) + \partial^3 \left( \frac{\partial \tilde{F}}{\partial u_{xx}} \right) - \dots$$

In particular if we take  $\tilde{F} = \tilde{F}_3(u, u_x) = -u^3 + u_x^2/2$ , then we get the KdV equation in standard form:  $u_t = \partial(-3u^2) - \partial^2(u_x) = -6u u_x - u_{xxx}$ .

Recall that if two smooth real-valued functions  $F$  and  $G$  on a symplectic manifold  $P$  are both Hamiltonian, then they determine a third function on  $P$ , called their *Poisson bracket*, defined by:  $\{F, G\} = \Omega(\nabla_s G, \nabla_s F)$ , and it is easy to show that this is also a Hamiltonian function and in fact  $\nabla_s \{F, G\} = [\nabla_s F, \nabla_s G]$ , (cf. the appendix.)

Specializing again to the case that  $P$  is the Schwartz space  $\mathcal{S}(\mathbf{R})$ , with the symplectic structure defined above, we get the following formula for the Poisson Bracket:

$$\{F, G\} = \Omega(\nabla_s G, \nabla_s F) = \Omega(\partial \nabla G, \partial \nabla F) = \langle \nabla G, \partial(\nabla F) \rangle$$

▷ **2.3—Exercise 2.** Note that the density  $\tilde{F}_3$  above, that gives the KdV equation, is just the third of the classical conserved densities for KdV. Show that in fact all three of the functionals  $F_i$  (corresponding to the densities  $\tilde{F}_1(u) = u$ ,  $\tilde{F}_2(u) = u^2$ , and  $\tilde{F}_3(u, u_x) = -u^3 + \frac{1}{2}u_x^2$ ) are in involution.

In fact, it turns out that the whole sequence of functionals  $F_i$  coming from the conserved densities  $\tilde{F}_i$  found by Miura are all in involution. (For the proof see [La3].)

## 2.4 KdV as a Lax Equation

In developing the Inverse Scattering Transform Gardner, Greene, Kruskal and Miura [GGKM] showed that there was an intimate relation between the KdV equation and the

time-independent Schrödinger operators  $-\frac{d^2}{dx^2} + u$ —namely if a one-parameter family of potentials  $u(x, t)$  evolved according to the KdV equation, then the corresponding one-parameter  $L(t)$  of self-adjoint operators on  $L^2(\mathbf{R})$  that are given by the Schrödinger operators with potentials  $u(t)(x) = u(x, t)$  (i.e.,  $L(t)\psi(x) = -\frac{d^2}{dx^2}\psi(x) + u(x, t)\psi(x)$ ) are isospectral. Peter Lax [La1] took this observation one step further. He showed that one could recast the KdV equation in a form now known as a *Lax Equation*, and as such it is equivalent to the statement that the  $L(t)$  are evolving by unitary equivalence, i.e., there is a smooth one-parameter family,  $U(t)$ , of unitary operators on  $L^2(\mathbf{R})$  such that  $U(0) = I$  and  $L(t) = U(t)L(0)U(t)^{-1}$ . We will first develop the concept of a Lax Equation in an abstract setting, and then apply these considerations to the KdV situation. By the way, in the following it will be convenient to take KdV in the form  $u_t - 6uu_x + u_{xxx} = 0$ .

Suppose we have a smooth one-parameter family  $U(t)$  of unitary transformations of a Hilbert space  $H$  with  $U(0) = I$ .  $U_t(t)$ , the derivative of  $U(t)$ , is a tangent vector at  $U(t)$  of the group  $\mathcal{U}(H)$  of unitary transformations of  $H$ , so  $B(t) = U_t(t)U(t)^{-1} = U_t(t)U(t)^*$  is a tangent vector to  $\mathcal{U}(H)$  at the identity,  $I$ . Differentiating  $UU^* = I$  gives  $U_tU^* + UU_t^* = 0$ , and since  $U_t = BU$  and  $U_t^* = U^*B^*$ ,  $0 = BUU^* + UU^*B^*$ , so  $B^* = -B$ ; i.e.,  $B(t)$  is a family of skew-adjoint operators on  $H$ . Conversely, a smooth map  $t \mapsto B(t)$  of  $\mathbf{R}$  into the skew-adjoint operators defines a time-dependent right invariant vector field  $X_U(t) = B(t)U$  on  $\mathcal{U}(H)$  and so (at least in finite dimensions) a smooth curve  $U(t)$  of unitary operators starting from  $I$  such that  $U_t(t) = B(t)U(t)$ .

Now suppose that  $L(0)$  is a self-adjoint operator on  $H$ , and define a family of conjugate operators  $L(t)$  by  $L(t) = U(t)L(0)U(t)^{-1}$ , so  $L(0) = U(t)^*L(t)U(t)$ . Differentiating the latter with respect to  $t$ ,  $0 = U_t^*LU + U^*L_tU + U^*LU_t = U^*(-BL + L_t + LB)U$ . Hence, writing  $[B, L] = BL - LB$  as usual for the commutator of  $B$  and  $L$ , we see that  $L(t)$  satisfies the so-called *Lax Equation*,  $L_t = [B, L]$ .

Given a smooth family of skew-adjoint operators  $B(t)$ , the Lax Equation is a time-dependent linear ODE in the vector space  $\mathcal{S}$  of self-adjoint operators on  $H$ , whose special form expresses the fact that the evolution is by unitary conjugation. Indeed, since the commutator of a skew-adjoint operator and a self-adjoint operator is again self-adjoint,  $B(t)$  defines a time-dependent vector field,  $Y$ , on  $\mathcal{S}$  by  $Y(t)(L) = [B(t), L]$ . Clearly a smooth curve  $L(t)$  in  $\mathcal{S}$  satisfies the Lax Equation if and only if it is a solution curve of  $Y$ . By uniqueness of solutions of linear ODE, the solution  $L(t)$  of this ODE with initial condition  $L(0)$  must be the one-parameter family  $U(t)L(0)U(t)^{-1}$  constructed above.

Given any  $\psi(0)$  in  $H$ , define  $\psi(t) = U(t)\psi(0)$ . Since  $U(t)L(0) = L(t)U(t)$ , it follows that if  $\psi(0)$  is an eigenvector of  $L(0)$  belonging to the eigenvalue  $\lambda$ , then  $\psi(t)$  is an eigenvector of  $L(t)$  belonging to the *same* eigenvalue  $\lambda$ . Differentiating the relation defining  $\psi(t)$  gives  $\psi_t = B\psi(t)$ , so we may consider  $\psi(t)$  to be defined as the solution of this linear ODE with initial value  $\psi(0)$ . Since this is one of the main ways in which we will use Lax Equations, we will restate it as what we shall call the:

**Isospectral Principle.** *Let  $L(t)$  and  $B(t)$  be smooth one-parameter families of self-adjoint and skew-adjoint operators respectively on a Hilbert space  $H$ , satisfying the Lax Equation  $L_t = [B, L]$ , and let  $\psi(t)$  be a curve in  $H$  that is a solution of the time-dependent linear ODE  $\psi_t = B\psi$ . If the initial value,  $\psi(0)$ , is an eigenvector of  $L(0)$  belonging to an eigenvalue  $\lambda$ , then  $\psi(t)$  is an eigenvector of  $L(t)$  belonging to the same eigenvalue  $\lambda$ .*

We now apply the above with  $H = L^2(\mathbf{R})$ . We will see that if  $u$  satisfies KdV, then

the family of Schrödinger operators  $L(t)$  on  $H$  defined above satisfies the Lax Equation  $L_t = [B, L]$ , where

$$B(t)\psi(x) = -4\psi_{xxx}(x) + 3(u(x, t)\psi_x(x) + (u(x, t)\psi(x))_x),$$

or more succinctly,  $B = -4\partial^3 + 3(u\partial + \partial u)$ . Here and in the sequel it is convenient to use the same symbol both for an element  $w$  of the Schwartz space,  $\mathcal{S}(\mathbf{R})$ , and for the bounded self-adjoint multiplication operator  $v \mapsto wv$  on  $H$ . Since  $H$  is infinite dimensional and our operators  $B$  and  $L$  are unbounded on  $H$ , some care is needed for a rigorous treatment. But this is relatively easy. Note that all the operators involved have the Schwartz space as a common dense domain.)

Note that since  $\partial$  is skew-adjoint, so is any odd power, and in particular  $4\partial^3$  is skew-adjoint. Also, the multiplication operator  $u$  is self-adjoint, while the anti-commutator of a self-adjoint and a skew-adjoint operator is skew-adjoint, so  $u\partial + \partial u$  and hence  $B$  is indeed skew-adjoint.

Since clearly  $L_t = u_t$ , while  $u_t - 6uu_x + u_{xxx} = 0$  by assumption, to prove that  $L_t = [B, L]$  we need only check that  $[B, L] = 6uu_x - u_{xxx}$ .

▷ **2.4—Exercise 1.** Prove this. (Hint:  $[B, L] = 4[\partial^3, \partial^2] - 4[\partial^3, u] - 3[u\partial, \partial^2] + 3[u\partial, u] - 3[\partial u, \partial^2] + 3[\partial u, u]$ , so it will suffice to verify the following six commutator relations:  $[\partial^3, \partial^2] = 0$ ,  $[\partial^3, u] = u_{xxx} + 3u_{xx}\partial + 3u_x\partial^2$ ,  $[u\partial, \partial^2] = -u_{xx}\partial - 2u_x\partial^2$ ,  $[u\partial, u] = uu_x$ ,  $[\partial u, \partial^2] = -3u_{xx}\partial - 2u_x\partial^2 - u_{xxx}$ , and  $[\partial u, u] = uu_x$ .)

Let us now apply the Isospectral Principle to this example.

**KdV Isospectrality Theorem.** Suppose  $u(x, t)$  is a solution of the KdV equation,

$$u_t - 6uu_x + u_{xxx} = 0,$$

whose initial value  $u(x, 0)$  is in the Schwartz space  $\mathcal{S}(\mathbf{R})$ , and that  $\psi(x)$  is an eigenfunction of the Schrödinger Equation with potential  $u(x, 0)$  and eigenvalue  $\lambda$ :

$$-\frac{d^2}{dx^2}\psi(x) + u(x, 0)\psi(x) = \lambda\psi(x).$$

Let  $\psi(x, t)$  be the solution of the evolution equation  $\psi_t = B\psi$ , i.e.,

$$\frac{\partial\psi}{\partial t} = -4\frac{\partial^3\psi}{\partial x^3} + 3\left(u(x, t)\frac{\partial\psi}{\partial x}(x, t) + \frac{\partial}{\partial x}(u(x, t)\psi(x, t))\right)$$

with the initial value  $\psi(x, 0) = \psi(x)$ . Then  $\psi(x, t)$  is an eigenfunction for the Schrödinger Equation with potential  $u(x, t)$  and the same eigenvalue  $\lambda$ :

$$-\psi_{xx}(x, t) + u(x, t)\psi(x, t) = \lambda\psi(x, t),$$

and moreover, if  $\psi(x)$  is in  $L^2$ , then the  $L^2$  norm of  $\psi(\cdot, t)$  is independent of  $t$ . Finally,  $\psi(x, t)$  also satisfies the first-order evolution equation

$$\psi_t - (4\lambda + 2u)\psi_x + u_x\psi = 0.$$

PROOF. Except for the final statement this is an immediate application of the Isospectrality Principle. Differentiating the eigenvalue equation for  $\psi(x, t)$  with respect to  $x$  gives  $\psi_{xxx} = u_x\psi + (u - \lambda)\psi_x$ , and substituting this into the assumed evolution equation for  $\psi$  gives the asserted first-order equation for  $\psi$ . ■

By the way, I should re-emphasize that the essential point is that when a potential evolves via KdV, the corresponding Schrödinger operators are isospectral, and this is already clearly stated in [GGKM]. Lax’s contribution was to explain the mechanism behind this remarkable fact and to formulate it in a way that was easy to generalize. In fact, almost all generalizations of the phenomena first recognized in KdV have used the Lax Equation as a jumping-off place.

## 2.5 The KdV Heierarchy

Let me explain why you should find the Lax form of the KdV equation striking and more that a little surprising. Let’s examine both sides of the equation  $L_t = [B, L]$  carefully. On the left, since the self-adjoint operator  $L(t)$  is the constant (in time) second order differential operator  $-\partial^2$  plus the zero-order operator multiplication by  $u(t)$ , its time derivative,  $L_t$ , is the zero-order operator multiplication by  $u_t$ . On the right we have the difference of the two fifth order differential operators  $B(t)L(t)$  and  $L(t)B(t)$ . Now of course the operators  $L(t)$  and  $B(t)$  do **not** commute, but since they are acting on scalar-valued functions, the top-order (i.e., fifth order) terms (or “symbols”) of their products is independent of the order of composition by a well-known trivial calculation. Thus,  $[B, L]$  should be a fourth order operator! What happened to the terms of order one, two, three, and four? Of course they have miraculously cancelled (as you will have noticed if you did the above exercise) due to the special form of  $B(t)$ . The fact that the zero order “right hand side”,  $6uu_x - u_{xxx}$  of the KdV equation  $u_t = 6uu_x - u_{xxx}$  can be written as the commutator of  $L(t)$  and a third order operator  $B(t)$  is what should have surprised you, it is what accounts for the remarkable “integrability” properties of KdV. If you replace  $B(t)$  by another skew-adjoint third order operator that is not just a multiple of  $B(t)$  you will see that it is never of order zero. But what if we replace  $B(t)$  with some higher order differential operator?

Peter Lax asked and answered this question in [La1], the paper in which he first derived the above Lax form of the KdV equation. The natural generalization for  $B$ , Lax points out, is an operator  $B_j$  of order  $2j + 1$  of the form  $a\partial^{2j+1} + \sum_{i=1}^j (b_i\partial^{2i-1} + \partial^{2i-1}b_i)$ , where the  $b_i$  are polynomials in  $u$  and its partial derivatives. If we demand that  $[L, B_j]$  be a zero order operator, multiplication by some polynomial  $K_j(u)$  in  $u$  and its derivatives, this gives  $j$  conditions that uniquely determine the  $b_1, \dots, b_j$ . For  $j = 0$  we get  $B_0 = \partial$  and  $K_0(u) = u_x$ , so the analogue of the KdV equation is just the linear advection equation  $u_t = u_x$  which is therefore also called the “zero-th flow of the KdV Heierarchy. Of course  $B_1 = B$ , and KdV itself is the “first flow of the KdV Heierarchy”, and in general the evolution equation  $u_t = K_j(u)$  is referred to as *the  $j$ -th flow of the KdV Heierarchy*. What is more, it turns out that each of these higher order *KdV* flows is a Hamiltonian flow on our phase space  $\mathcal{S}(\mathbf{R})$  with respect to the symplectic structure we have described above. The corresponding Hamiltonian functions  $F_j : \mathcal{S}(\mathbf{R}) \rightarrow \mathbf{R}$  are all Calculus of Variations functionals, i.e., they are of the form  $F_j(u) = \int_{-\infty}^{\infty} \tilde{F}_j(u) dx$ , where  $\tilde{F}_j(u)$  is a polynomial differential operator of order  $j$ . By now you probably won’t be surprised to learn that these  $F_j$  are all in involution

(so all the flows of the KdV hierarchy commute), and hence each  $F_j$  is a conserved quantity for the KdV flow. In fact,  $F_1, F_2, F_3$  are the classical conserved quantities of KdV, and the higher  $F_j$  are just the sequence of conserved quantities discovered in [GGKM].



## Section 3

# Introduction to the Inverse Scattering Transform

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### 3.1 The Scattering Data and its Evolution

We now fix a “potential function”  $u$  in the Schwartz space  $\mathcal{S}(\mathbf{R})$  and look more closely at the space  $E_\lambda(u)$  of  $\lambda$  eigenfunctions of the Schrödinger operator with this potential. By definition,  $E_\lambda(u)$  is just the kernel of the linear operator  $L^u(\psi) = -\frac{d^2\psi}{dx^2} + u\psi - \lambda\psi$  acting on the space  $C^\infty(\mathbf{R})$ , and by the elementary theory of second-order linear ODE it is, for each choice of  $\lambda$ , a two-dimensional linear subspace of  $C^\infty(\mathbf{R})$ . Using the special form of  $L^u$  we can describe  $E_\lambda(u)$  more precisely. We will ignore the case  $\lambda = 0$ , and consider the case of positive and negative  $\lambda$  separately.

Suppose  $\lambda = -\kappa^2$ ,  $\kappa > 0$ . Note that any  $\psi$  in  $E_\lambda(u)$  will clearly be of the form  $\psi(x) = ae^{\kappa x} + be^{-\kappa x}$  in any interval on which  $u$  vanishes identically. Thus if  $u$  has compact support, say  $u(x) = 0$  for  $|x| > M$ , then we can find a basis  $\{\psi_{\lambda,-\infty}^+, \psi_{\lambda,-\infty}^-\}$  for  $E_\lambda(u)$  such that  $\psi_{\lambda,-\infty}^\pm(x) = e^{\pm\kappa x}$ , (or equivalently,  $\psi_{\lambda,-\infty}^\pm(x)e^{\mp\kappa x} = 1$ ) for  $x < -M$ . Similarly there is a second basis  $\{\psi_{\lambda,\infty}^+, \psi_{\lambda,\infty}^-\}$  for  $E_\lambda(u)$  such that  $\psi_{\lambda,\infty}^\pm(x) = e^{\pm\kappa x}$  (or  $\psi_{\lambda,\infty}^\pm(x)e^{\mp\kappa x} = 1$ ) for  $x > M$ .

When  $u$  does not have compact support, but is only rapidly decreasing then, by an argument that we will sketch below, it follows that there still exist two bases for  $E_\lambda(u)$   $\{\psi_{\lambda,-\infty}^+, \psi_{\lambda,-\infty}^-\}$ ,  $\{\psi_{\lambda,\infty}^+, \psi_{\lambda,\infty}^-\}$  such that  $\psi_{\lambda,-\infty}^\pm(x) \sim e^{\pm\kappa x}$  at  $-\infty$  and  $\psi_{\lambda,\infty}^\pm(x) \sim e^{\pm\kappa x}$  at  $+\infty$  (i.e.,  $\lim_{x \rightarrow -\infty} \psi_{\lambda,-\infty}^\pm(x)e^{\mp\kappa x} = 1$  and  $\lim_{x \rightarrow \infty} \psi_{\lambda,\infty}^\pm(x)e^{\mp\kappa x} = 1$ ).

Using these bases it is easy to detect when  $\lambda$  is a so-called “discrete eigenvalue” of  $L^u$ , i.e., when  $E_\lambda(u)$  contains a non-zero element  $\psi$  of  $L^2(\mathbf{R})$ . Let us define functions  $f(\lambda)$  and  $c(\lambda)$  by  $\psi_{\lambda,-\infty}^+ = f(\lambda)\psi_{\lambda,\infty}^+ + c(\lambda)\psi_{\lambda,\infty}^-$ . We can assume  $\psi$  has  $L^2$  norm one, and since  $\psi_{\lambda,-\infty}^-$  blows up at  $-\infty$  while  $\psi_{\lambda,\infty}^+$  blows up at  $\infty$ ,  $\psi$  must be both a multiple of  $\psi_{\lambda,-\infty}^+$  and of  $\psi_{\lambda,\infty}^-$ , and since  $\psi \neq 0$  it follows that  $f(\lambda) = 0$ . Conversely, if  $f(\lambda) = 0$  then  $\psi_{\lambda,-\infty}^+ = c(\lambda)\psi_{\lambda,\infty}^-$  decays exponentially both at  $\infty$  and  $-\infty$  and so we can normalize it to get an element of  $E_\lambda(u)$  with  $L^2$  norm one. Thus the discrete eigenvalues of  $L^u$  are precisely the roots of the function  $f$ .

It follows from standard arguments of Sturm-Liouville theory that in fact  $L^u$  has only finitely many discrete eigenvalues,  $\lambda_1, \dots, \lambda_N$ , with corresponding  $L^2$  normalized eigenfunctions  $\psi_1, \dots, \psi_N$ , and these determine so-called “normalization constants”  $c_1, \dots, c_N$  by  $\psi_n = c_n\psi_{\lambda_n,\infty}^-$ , i.e., if we write  $\lambda_n = -\kappa_n^2$ , then  $c_n$  is characterized by  $\psi_n(x) \sim c_n e^{-\kappa_n x}$  as  $x \rightarrow \infty$ . We note that the  $\psi_n$  and hence the normalization constants  $c_n$  are only determined up to sign, but we will only use  $c_n^2$  in the Inverse Scattering Transform.

For  $\lambda = k^2$ ,  $k > 0$  there are similar considerations. In this case if  $u(x)$  vanishes for  $|x| > M$  then any element of  $E_\lambda(u)$  will be of the form  $ae^{ikx} + be^{-ikx}$  for  $x < -M$  and also of the form  $ce^{ikx} + de^{-ikx}$  for  $x > M$ . If  $u$  is only rapidly decaying then this time we can find two bases  $\{\psi_{\lambda,-\infty}^+, \psi_{\lambda,-\infty}^-\}$  and  $\{\psi_{\lambda,\infty}^+, \psi_{\lambda,\infty}^-\}$  for  $E_\lambda(u)$  such that  $\psi_{\lambda,-\infty}^\pm(x) \sim e^{\pm ikx}$  at  $-\infty$

while  $\psi_{\lambda,\infty}^{\pm}(x) \sim e^{\pm ikx}$  at  $+\infty$ . Then  $\psi_{\lambda,-\infty}^{-} = \alpha\psi_{\lambda,\infty}^{-} + \beta\psi_{\lambda,\infty}^{+}$ , where  $\alpha$  can be shown to be non-zero. Dividing by  $\alpha$  we get a particular eigenfunction  $\psi_k$ , called the Jost solution, with the special asymptotic behavior  $\psi_k(x) \sim a(k)e^{-ikx}$  as  $x \rightarrow -\infty$  and  $\psi_k(x) \sim e^{-ikx} + b(k)e^{ikx}$  as  $x \rightarrow \infty$ .

The functions  $a(k)$  and  $b(k)$  are called the transmission coefficient and reflection coefficient respectively, and  $b(k)$  together with the above normalizing constants  $c_1, \dots, c_n$  make up the ‘‘Scattering Data’’,  $\mathcal{S}(u)$  for  $u$ .

While it may seem intuitively clear that the bases  $\psi_{\lambda,\pm\infty}^{\pm}$  must exist, to give rigorous asymptotic arguments required for the proof of the crucial theorem on the time evolution of the Scattering Data it is essential to supply precise definitions of these bases, and we do this next.

For a warm-up, consider the simpler problem of the first order ODE  $L^u\psi = \frac{d\psi}{dx} - u\psi$ . If we make the substitution  $\psi = e^{\lambda x}\phi$ , then the eigenvalue equation  $L^u(\psi) = \lambda\psi$  becomes  $\frac{d\phi}{dx} = u\phi$ , so (assuming  $u$  depends on a parameter  $t$ ) we have  $\phi(x, t) = \exp(\int_{-\infty}^x u(\xi, t) d\xi)$ . Note that  $\lim_{x \rightarrow -\infty} \phi(x, t) = 1$  while  $\lim_{x \rightarrow \infty} \phi(x, t) = \exp(\int_0^{\infty} u(\xi, t) d\xi) = c(t)$ . If  $\psi(x, t)$  is an eigenfunction of  $L^u$  it follows that  $\psi(x, t) \sim c(t)e^{\lambda x}$  (i.e.,  $\lim_{x \rightarrow \infty} \psi(x, t)e^{-\lambda x} = c(t)$ ). But moreover, *since  $u(x, t)$  is rapidly decaying we can even differentiate under the integral sign to obtain  $\psi_t(x, t) \sim c'(t)e^{\lambda x}$ .*

If an asymptotic relation depends on a parameter, one cannot in general differentiate with respect to that parameter unless one knows that the asymptotic relation holds uniformly in the parameter, and since we will need to derive a relation similar to the above for eigenfunctions of Schrödinger operators, we must now make an argument similar to the above (but a somewhat more complicated) to justify differentiation in that case.

If we make the substitution  $\psi = \phi e^{-\kappa x}$  in our eigenvalue equation  $\psi_{xx} = \kappa^2\psi + u\psi$ , then we get after simplifications  $\phi_{xx} - 2\kappa\phi_x = u\phi$ , or  $\partial(\partial - 2\kappa)\phi = u\phi$ . Recall the method of solving the inhomogeneous equation  $\partial(\partial - 2\kappa)\phi = f$  by ‘‘variation of parameters’’. Since 1 and  $e^{2\kappa x}$  form a basis for the solutions of the homogeneous equation, we look for a solution of the form  $\phi = \Theta_1 + \Theta_2 e^{2\kappa x}$ , and to make the system determined we add the relation  $\Theta_1' + \Theta_2' e^{2\kappa x} = 0$ . This leads to the equations  $\Theta_1' = -\frac{f}{2\kappa}$  and  $\Theta_2' = \frac{f}{2\kappa} e^{2\kappa x}$  so the solution to the inhomogeneous equation is just  $\phi = -\frac{1}{2\kappa} \int_0^x f(\xi) d\xi + \frac{e^{2\kappa x}}{2\kappa} \int_0^x f(\xi) e^{-2\kappa x} d\xi$ .

If we now take  $f = u\phi$  (and use  $\phi e^{-\kappa x} = \psi$ ) then we get the relation

$$\phi(x, t) = \frac{1}{2\kappa} \int_x^0 u(\xi, t)\phi(\xi, t) d\xi - \frac{e^{2\kappa x}}{2\kappa} \int_x^0 u(\xi, t)\psi(\xi, t)e^{-\kappa x} d\xi.$$

Assuming that  $-\kappa^2$  is a discrete eigenvalue, and that  $\psi$  has  $L^2$  norm 1,  $u\psi$  will also be in  $L^2$  and we can estimate the second integral using the Schwartz Inequality. We see that in fact  $|\int_x^0 u(\xi)\psi(\xi)e^{-\kappa x} d\xi| < O(e^{-\kappa x})$ , so the second term is  $O(e^{\kappa x})$ , and it follows that  $\psi(x, t) \sim c(t)e^{\kappa x}$  at  $-\infty$  where  $c(t) = \phi(-\infty, t) = \frac{1}{2\kappa} \int_{-\infty}^0 u(\xi, t)\phi(\xi, t) d\xi$ . In other words, the normalizing constant is well defined. But what is more important, it also follows that if  $u(x, t)$  satisfies KdV, then the normalizing constant  $c(t)$  for a fixed eigenvalue  $-\kappa^2$  is a differentiable function of  $t$  and satisfies  $\psi_t(x, t) \sim c'(t)e^{\kappa x}$ . This follows from the fact that we can differentiate the formula for  $c(t)$  under the integral sign because  $u$  is rapidly decreasing.

Note that differentiating the relation  $\psi e^{\kappa x} = \phi$  gives  $\psi_x e^{\kappa x} = \phi_x - \kappa\psi$ . But the formula for  $\phi$  shows that  $\phi_x$  converges to zero at  $-\infty$ , so  $\psi_x(x, t) \sim -\kappa c(t)e^{\kappa x}$ . From the KdV

Isospectrality Theorem, we know that if  $u(x, t)$  satisfies KdV, then  $\psi(x, t)$  satisfies  $\psi_t - (-4\kappa^2 + 2u)\psi_x + u_x\psi = 0$ . It follows that the left hand side times  $e^{\kappa x}$  converges to  $c'(t) + 4\kappa^2(-\kappa c(t))$  as  $x \rightarrow \infty$  and hence  $c'(t) - 4\kappa^3 c(t) = 0$ , so  $c(t) = c(0)e^{4\kappa^3 t}$ .

By a parallel argument (which we omit) it follows that the transmission and reflection coefficients are also well defined and that the Jost solution  $\psi_k(x, t)$  satisfies  $(\psi_k)_t \sim a_t(k, t)e^{-ikx}$  at  $-\infty$  and  $(\psi_k)_t \sim b_t(k, t)e^{ikx}$  at  $\infty$ , and then one can show from the KdV Isospectrality Theorem that the transmission coefficients are constant, while the reflection coefficients satisfy  $b(k, t) = b(k, 0)e^{8ik^3 t}$ .

▷ **3.1—Exercise 1.** Supply the omitted proof.

**Theorem on Evolution of the Scattering Data.** *Let  $u(t) = u(x, t)$  be a smooth curve in  $\mathcal{S}(\mathbf{R})$  satisfying the KdV equation  $u_t - 6uu_x + u_{xxx} = 0$  and assume that the Schrödinger operator with potential  $u(t)$  has discrete eigenvalues  $-\kappa_1^2, \dots, -\kappa_N^2$  whose corresponding normalized eigenfunctions have normalization constants  $c_1(t), \dots, c_n(t)$ . Let the transmission and reflection coefficients of  $u(t)$  be respectively  $a(k, t)$  and  $b(k, t)$ . Then the transmission coefficients are all constants of the motion, i.e.,  $a(k, t) = a(k, 0)$ , while the Scattering Data,  $c_n(t)$  and  $b(k, t)$ , satisfy:*

- 1)  $c_n(t) = c_n(0)e^{4\kappa_n^3 t}$ ,
- 2)  $b(k, t) = b(k, 0)e^{8ik^3 t}$ .

We note a striking (and important) fact: not only do we now have an explicit and simple formula for the evolution of the scattering data  $\mathcal{S}(u(t))$  when  $u(t)$  evolves by the KdV equation, but further **this formula does not require any knowledge of  $u(t)$** .

The fact that the transmission coefficients  $a(k)$  are constants of the motion while the logarithms of the reflection coefficients,  $b(k)$  vary linearly with time suggest that perhaps they can somehow be regarded as action-angle variables for the KdV equation, thereby identifying KdV as a completely integrable system in a precise sense. While  $a(k)$  and  $b(k)$  are not themselves canonical variables, Zakharov and Fadeev in [ZF] showed that certain functions of  $a$  and  $b$  did satisfy the Poisson commutation relations for action-angle variables. Namely, the functions  $p(k) = (k/\pi) \log |a(k)|^2 = (k/\pi) \log [1 + |b(k)|^2]$  and  $q(k) = \arg(b(k))$  satisfy  $\{p(k), q(k')\} = \delta(k - k')$  and  $\{p(k), p(k')\} = \{q(k), q(k')\} = 0$ .

The above formula for the evolution of the Scattering Data is one of the key ingredients for The Inverse Scattering Method, and we are finally in a position to describe this elegant algorithm for solving the Cauchy problem for KdV.

### The Inverse Scattering Method.

To solve the KdV initial value problem  $u_t - 6uu_x + u_{xxx} = 0$  with given initial potential  $u(x, 0)$  in  $\mathcal{S}(\mathbf{R})$ :

- 1) Apply the “Direct Scattering Transform”. That is, find all the discrete eigenvalues  $-\kappa_1^2, \dots, -\kappa_N^2$  for the Schrödinger operator with potential  $u(x, 0)$ , and the the Scattering Data  $\mathcal{S}(u(x, 0))$  for  $u(x, 0)$ , consisting of the normalizing constants  $c_n(0)$  and the reflection coefficients  $b(k, 0)$ .
- 2) Use the explicit evolution formulae:  $c_n(t) = c_n(0)e^{4\kappa_n^3 t}$  and  $b(k, t) = b(k, 0)e^{8ik^3 t}$ , to find the scattering data  $\mathcal{S}(u(x, t))$ .

- 3) Use the Inverse Scattering Transform (described in the next section) to compute  $u(t)$  from  $\mathcal{S}(u(x, t))$ .

### 3.2 The Gelfand-Levitan-Marchenko Equation

Recovering the potential  $u$  of a Schrödinger operator  $L^u$  from the Scattering Data  $\mathcal{S}(u)$  was not something invented for the purpose of solving the KdV initial value problem. Rather, it was a question of basic importance to physicists doing Cyclotron experiments, and the theory was worked out in the mid-1950's by Kay and Moses [KM], by Gelfand and Levitan [GL], and Marchenko [M].

Denote the discrete eigenvalues of  $u$  by  $-\kappa_1^2, \dots, -\kappa_N^2$ , the normalizing constants by  $c_1, \dots, c_N$ , and the reflection coefficients by  $b(k)$ , and define a function

$$B(\xi) = \sum_{n=1}^N c_n^2 e^{-\kappa_n \xi} + \frac{1}{2\pi} \int_{-\infty}^{\infty} b(k) e^{ik\xi} dk.$$

**Inverse Scattering Theorem.** *The potential  $u$  can be recovered using the formula  $u(x) = -2 \frac{d}{dx} K(x, x)$ , where  $K(x, z)$  is the unique function on  $\mathbf{R} \times \mathbf{R}$  that is zero for  $z < x$  and satisfies the Gelfand-Levitan-Marchenko Integral Equation:*

$$(GLM) \quad K(x, z) + B(x+z) + \int_{-\infty}^{\infty} K(x, y) B(y+z) dy = 0.$$

Below we will demonstrate how the Inverse Scattering Method can be used to get formulas for the KdV multi-solitons by solving the GLM equation explicitly for the case of reflectionless potentials. But first a couple of general remarks about solving the GLM equation. We assume in the following that  $B$  is rapidly decreasing.

Let  $C(\mathbf{R} \times \mathbf{R})$  denote the Banach space of bounded, continuous real-valued functions on  $\mathbf{R} \times \mathbf{R}$  with the sup norm. Define  $\mathcal{F}^B : C(\mathbf{R} \times \mathbf{R}) \rightarrow C(\mathbf{R} \times \mathbf{R})$  by the formula

$$\mathcal{F}^B(K)(x, z) = -B(x+z) - \int_{-\infty}^{\infty} K(x, y) B(y+z) dy.$$

Then  $K$  satisfies the Gelfand-Levitan-Marchenko equation if and only if it is a fixed-point of  $\mathcal{F}^B$ . It is clear that  $\mathcal{F}^B$  is Lipschitz with constant  $\|B\|_{L^1}$ , so if  $\|B\|_{L^1} < 1$  then by the Banach Contraction Principle the Gelfand-Levitan-Marchenko equation has a unique solution, and it is the limit of the sequence  $K_n$  defined by  $K_1(x, z) = -B(x+z)$ ,  $K_{n+1} = \mathcal{F}^B(K_n)$ .

Secondly, we note that if the function  $B$  is “separable” in the sense that it satisfies an identity of the form  $B(x+z) = \sum_{n=1}^N X_n(x) Z_n(z)$ , then the Gelfand-Levitan-Marchenko equation takes the form:

$$K(x, z) + \sum_{n=1}^N X_n(x) Z_n(z) + \sum_{n=1}^N Z_n(z) \int_x^{\infty} K(x, y) X_n(y) dy = 0.$$

and it follows that  $K(x, z)$  must have the form  $K(x, z) = \sum_{n=1}^N L_n(x)Z_n(z)$ . If we substitute this for  $K$  in the previous equation and define  $a_{nm}(x) = \int_x^\infty Z_m(y)X_n(y) dy$  then we have reduced the problem to solving  $N$  linear equations for the unknown functions  $L_n$ , namely:  $L_n(x) + X_n(x) + \sum_{m=1}^N a_{nm}(x)L_m(x) = 0$ , or  $X_n(x) + \sum_{m=1}^N A_{nm}(x)L_m(x) = 0$ , where  $A_{nm}(x) = \delta_{nm} + a_{nm}(x)$ . Thus finally we have:

$$K(x, x) = - \sum_{n=1}^N Z_n(x) \sum_{m=1}^N A_{nm}^{-1}(x)X_m(x).$$

### 3.3 An Explicit Formula for KdV Multi-Solitons.

A potential  $u$  is called ‘‘reflectionless’’ if all the reflection coefficients are zero. Because of the relation  $b(k, t) = b(k, 0)e^{8ik^3t}$ , it follows that if  $u(x, t)$  evolves by KdV and if it is reflectionless at  $t = 0$  then it is reflectionless for all  $t$ . If the discrete eigenvalues of such a potential are  $-\kappa_1^2, \dots, -\kappa_N^2$  and the normalizing constants are  $c_1, \dots, c_N$ , then  $B(\xi) = \sum_{n=1}^N c_n^2 e^{-\kappa_n \xi}$ , so  $B(x+z) = \sum_{n=1}^N X_n(x)Z_n(z)$ , where  $X_n(x) = c_n^2 e^{-\kappa_n x}$ , and  $Z_n(z) = e^{-\kappa_n z}$  and we are in the separable case just considered. Recall that:

$$\begin{aligned} a_{nm}(x) &= \int_x^\infty Z_m(y)X_n(y) dy \\ &= c_n^2 \int_x^\infty e^{-(\kappa_n + \kappa_m)y} dy \\ &= c_n^2 \frac{e^{-(\kappa_n + \kappa_m)x}}{(\kappa_n + \kappa_m)}, \end{aligned}$$

and that

$$\begin{aligned} A_{nm}(x) &= \delta_{nm} + a_{nm}(x) \\ &= \delta_{nm} + c_n^2 \frac{e^{-(\kappa_n + \kappa_m)x}}{(\kappa_n + \kappa_m)}. \end{aligned}$$

Differentiation gives  $\frac{d}{dx} A_{nm}(x) = -c_n^2 e^{-(\kappa_n + \kappa_m)x}$ , so by the formula above:

$$\begin{aligned} K(x, x) &= - \sum_{n=1}^N Z_n(x) \sum_{m=1}^N A_{nm}^{-1}(x)X_m(x) \\ &= \sum_{n=1}^N e^{-\kappa_n x} \sum_{m=1}^N A_{nm}^{-1}(x)(-c_m^2 e^{-\kappa_m x}) \\ &= \sum_{n=1}^N \sum_{m=1}^N A_{nm}^{-1} \frac{d}{dx} A_{mn}(x) \\ &= \text{tr} \left( A^{-1}(x) \frac{d}{dx} A(x) \right) \\ &= \frac{1}{\det(A(x))} \frac{d}{dx} \det A(x) \\ &= \frac{d}{dx} \log \det A(x). \end{aligned}$$

and so  $u(x) = -2 \frac{d}{dx} K(x, x) = -2 \frac{d^2}{dx^2} \log \det A(x)$ .

If  $N = 1$  and we put  $\kappa = \kappa_1$  it is easy to see that this formula reduces to our earlier formula for travelling wave solutions of the KdV equation:  $u(x, t) = -\frac{\kappa^2}{2} \operatorname{sech}^2(\kappa(x - \kappa^2 t))$ . We can also use it to find explicit solutions  $u(x, t)$  for  $N = 2$ . Let  $g_i(x, t) = \exp(\kappa_i^3 t - \kappa_i x)$ , and set  $A = \frac{(\kappa_1 - \kappa_2)^2}{(\kappa_1 + \kappa_2)^2}$ , then

$$u(x, t) = -2 \frac{\kappa_1^2 g_1 + \kappa_2^2 g_2 + 2(\kappa_1 - \kappa_2)^2 g_1 g_2 + A g_1 g_2 (\kappa_1^2 g_2 + \kappa_2^2 g_1)}{(1 + g_1 + g_2 + A g_1 g_2)^2}.$$

For general  $N$  the solutions  $u(x, t)$  that we get this way are referred to as the pure  $N$ -soliton solutions of the KdV equation. It is not hard to show by an asymptotic analysis that for large large negative times and large positive times they behave as a superposition of the above travelling wave solutions, and that after the larger, faster moving waves have all passed through the slower moving shorter ones and they have become well-separated, the only trace of their interactions are certain predictable “phase-shifts”, i.e., certain constant translations of the locations of their maxima from where they would have been if they had not interacted.

# Section 4

## The ZS-AKNS Scheme

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### 4.1 Zero Curvature Lax Equations

In this section, we will explain a general technique developed Zakharov and Shabat and by Ablowitz, Kaup, Newell, and Segur for generating Lax Equations of a special type (called ZCC, or Zero Curvature Condition equations). The Cauchy Problem for ZCC equations can be solved using a generalization of the Inverse Scattering Transform. Zakharov and Shabat introduced this method to study an important special equation (the so-called Non-linear Schrödinger Equation, or NLS) [ZS], and soon thereafter Ablowitz, Kaup, Newell, and Segur [AKNS1] showed that one relatively minor modification of the Zakharov and Shabat approach recovers the theory of the KdV equation, while another leads to an Inverse Scattering Theory analysis for a third very important evolution equation, the Sine-Gordon Equation (SGE). They went on [AKNS2] to develop the Zakharov and Shabat technique into a general method for PDE with values in  $2 \times 2$ -matrix groups [AKNS2], and Zakharov and Shabat further generalized it to the case of  $n \times n$ -matrix groups. Following current custom, we will refer to this method as the ZS-AKNS Scheme.

To prepare for the introduction of the ZS-AKNS Scheme, we next develop the infrastructure on which Zero Curvature Equations are based. We fix a matrix Lie Group  $\mathbf{G}$  and denote its Lie algebra by  $\mathcal{G}$ . That is,  $\mathbf{G}$  is some closed subgroup of the group  $\mathbf{GL}(n, \mathbf{C})$  of all  $n \times n$  complex matrices, and  $\mathcal{G}$  is the set of all  $n \times n$  complex matrices,  $X$ , such that  $\exp(X)$  is in  $\mathbf{G}$ . If you feel more comfortable working with a concrete example, think of  $\mathbf{G}$  as the group  $\mathbf{SL}(n, \mathbf{C})$  of all  $n \times n$  complex matrices of determinant 1, and  $\mathcal{G}$  as its Lie algebra  $\mathfrak{sl}(n, \mathbf{C})$  of all  $n \times n$  complex matrices of trace zero. In fact, for the original ZS-AKNS Scheme,  $\mathbf{G} = \mathbf{SL}(2, \mathbf{C})$  and  $\mathcal{G} = \mathfrak{sl}(2, \mathbf{C})$ , and we will carry out most of the later discussion with these choices, but for what we will do next the precise nature of  $\mathbf{G}$  is irrelevant.

Let  $\nabla$  be a flat connection for the trivial principal bundle  $\mathbf{R}^2 \times \mathbf{G}$ . Then we can write  $\nabla = d - \omega$ , where  $\omega$  is a 1-form on  $\mathbf{R}^2$  with values in the Lie algebra  $\mathcal{G}$ . Using coordinates  $(x, t)$  for  $\mathbf{R}^2$  we can then write  $\omega = A dx + B dt$  where  $A$  and  $B$  are smooth maps of  $\mathbf{R}^2$  into  $\mathcal{G}$ .

If  $X$  is a vector field on  $\mathbf{R}^2$ , then the covariant derivative operator in the direction  $X$  is  $\nabla_X = \partial_X - \omega(X)$ , and in particular, the covariant derivatives in the coordinate directions  $\frac{\partial}{\partial x}$  and  $\frac{\partial}{\partial t}$  are  $\nabla_{\frac{\partial}{\partial x}} = \frac{\partial}{\partial x} - A$  and  $\nabla_{\frac{\partial}{\partial t}} = \frac{\partial}{\partial t} - B$ .

Since we are assuming that  $\nabla$  is flat, it determines a global parallelism. If  $(x_0, t_0)$  is any point of  $\mathbf{R}^2$ , then we have a map  $\psi : \mathbf{R}^2 \rightarrow \mathbf{G}$ , where  $\psi(x, t)$  is the parallel translation operator from  $(x_0, t_0)$  to  $(x, t)$ . Considered as a section of our trivial principal bundle,  $\psi$  is covariant constant, i.e.,  $\nabla_X \psi = 0$  for any tangent vector field  $X$ . In particular, taking  $X$  to be  $\frac{\partial}{\partial x}$  and  $\frac{\partial}{\partial t}$  gives the relations  $\psi_x = A\psi$  and  $\psi_t = B\psi$ .

There are many equivalent ways to express the flatness of the connection  $\nabla$ . On the one hand the curvature 2-form  $d\omega - \omega \wedge \omega$  is zero. Equivalently, the covariant derivative operators in the  $\frac{\partial}{\partial x}$  and  $\frac{\partial}{\partial t}$  directions commute, i.e.,  $[\frac{\partial}{\partial x} - A, \frac{\partial}{\partial t} - B] = 0$ , or finally,

equating the cross-derivatives of  $\psi$ ,  $(A\psi)_t = \psi_{xt} = \psi_{tx} = (B\psi)_x$ . Expanding the latter gives  $A_t\psi + A\psi_t = B_x\psi + B\psi_x$  or  $A_t\psi + AB\psi = B_x\psi + BA\psi$ , and right multiplying by  $\psi^{-1}$  we arrive at the so-called “Zero-Curvature Condition”:  $A_t - B_x + [A, B] = 0$ . Rewriting this as  $-A_t = -B_x + [B, -A]$ , and noting that  $[B, \frac{\partial}{\partial x}] = -B_x$ , we see that the Zero-Curvature Condition has an equivalent formulation as a Lax Equation:

$$(ZCC) \quad \left( \frac{\partial}{\partial x} - A \right)_t = \left[ B, \frac{\partial}{\partial x} - A \right],$$

and it is ZCC that plays the central rôle in the ZS-AKNS Scheme.

Recall what ZCC is telling us. If we look at  $t$  as a parameter, then the operator  $\frac{\partial}{\partial x} - A(x, t_0)$  is the covariant derivative in the  $x$ -direction along the line  $t = t_0$ , and the Lax Equation ZCC says that as a function of  $t_0$  these operators are all conjugate. Moreover the operator  $\psi(t_0, t_1)$  implementing the conjugation between the time  $t_0$  and the time  $t_1$  satisfies  $\psi_t = B\psi$ , which means it is parallel translation from  $(x, t_0)$  to  $(x, t_1)$  computed by going “vertically” along the curve  $t \mapsto (x, t)$ . But since  $\frac{\partial}{\partial x} - A(x, t_0)$  generates parallel translation along the horizontal curve  $x \mapsto (x, t_0)$ , what this amounts to is the statement that parallel translating horizontally from  $(x_0, t_0)$  to  $(x_1, t_0)$  is the same as parallel translation vertically from  $(x_0, t_0)$  to  $(x_0, t_1)$  followed by parallel translation horizontally from  $(x_0, t_1)$  to  $(x_1, t_1)$  followed by parallel translation vertically from  $(x_1, t_1)$  to  $(x_1, t_0)$ . Thus, in the case of ZCC, the standard interpretation of the meaning of a Lax Equation reduces to a special case of the theorem that if a connection has zero curvature, then the holonomy around a contractible path is trivial.

## 4.2 Some ZS-AKNS Examples

The ZS-AKNS Scheme is a method for solving the initial value problem for certain (hierarchies of) evolution equations on a space of “potentials”  $P$ . In general  $P$  will be of the form  $\mathcal{S}(\mathbf{R}, V)$ , where  $V$  is some finite dimensional real or complex vector space, i.e., each potential  $u$  will be a map  $x \mapsto u(x)$  of Schwartz class from  $\mathbf{R}$  into  $V$ . (A function  $u$  with values in  $V$  is of Schwartz class if, for each linear functional  $\ell$  on  $V$ , the scalar valued function  $\ell \circ u$  is of Schwartz class, or equivalently if, when we write  $u$  in terms of a fixed basis for  $V$ , its components are of Schwartz class.) The evolution equations in question are of the form  $u_t = F(u)$  where the map  $F : P \rightarrow P$  is a “polynomial differential operator”—i.e., it has the form  $F(u) = p(u, u_x, u_{xx}, \dots)$ , where  $p$  is a polynomial mapping of  $V$  to itself.

When we say we want to solve the initial value (or “Cauchy”) problem for such an equation, we of course mean that given  $u^0 = u(x, 0)$  in  $P$  we want to find a smooth map  $t \mapsto u(t) = u(x, t)$  of  $\mathbf{R}$  to  $P$  with  $u(0) = u^0$  and  $u_t(x, t) = p(u(x, t), u_x(x, t), u_{xx}(x, t), \dots)$ . In essence, we want to think of  $F$  as a vector field on  $P$  and construct the flow  $\phi_t$  that it generates. (Of course, if  $P$  were a finite dimensional manifold, then we could construct the flow  $\phi_t$  by solving a system of ODE’s, and as we shall see, the ZS-AKNS Scheme allows us in certain cases to solve the PDE  $u_t = p(u, u_x, u_{xx}, \dots)$  by reducing it to ODE’s.)

The first and crucial step in using the ZS-AKNS Scheme to study a particular such evolution equation consists in setting up an interpretation of  $A$  and  $B$  so that the equation  $u_t = p(u, u_x, u_{xx}, \dots)$  becomes a special case of ZCC.

To accomplish this, we first identify  $V$  with a subspace of  $\mathcal{G}$  (so that  $P = \mathcal{S}(\mathbf{R}, V)$ )



becomes a subspace of  $\mathcal{S}(\mathbf{R}, \mathcal{G})$ , and define a map  $u \mapsto A(u)$  of  $P$  into  $C^\infty(\mathbf{R}, \mathcal{G})$  of the form  $A(u) = \text{const} + u$ , so that if  $u$  depends parametrically on  $t$ , then  $(\frac{\partial}{\partial x} - A(u))_t = -u_t$ .

Finally (and this is the difficult part) we must define a map  $u \mapsto B(u)$  of  $P$  into  $C^\infty(\mathbf{R}, \mathcal{G})$  so that  $[B(u), \frac{\partial}{\partial x} - A(u)] = -p(u, u_x, u_{xx}, \dots)$ .

To interpret the latter equation correctly, and in particular to make sense out of the commutator bracket in a manner consistent with our earlier interpretation of  $A$  and  $B$ , it is important to be clear about the interpretation  $A(u)$  and  $B(u)$  as operators, and in particular to be precise about the space on which they are operating. This is just the space  $C^\infty(\mathbf{R}, \mathbf{gl}(2, \mathbf{C}))$  of smooth maps  $\psi$  of  $\mathbf{R}$  into the space of all complex  $2 \times 2$  matrices. Namely, we identify  $A(u)$  with the zero-order differential operator mapping  $\psi$  to  $A(u)\psi$ , the pointwise matrix product of  $A(u)(x)$  and  $\psi(x)$ , and similarly with  $B(u)$ . (This is a complete analogy with the KdV situation, where in interpreting the Schrödinger operator, we identified our potential  $u$  with the operator of multiplication by  $u$ .) Of course  $(\frac{\partial}{\partial x}\psi)(x) = \psi_x$ .

We will now illustrate this with three examples: the KdV equation, the Nonlinear Schrödinger Equation (NLS), and the Sine-Gordon Equation (SGE). In each case  $V$  will be a one-dimensional space that is embedded in the space of off-diagonal complex matrices  $\begin{pmatrix} 0 & b \\ c & 0 \end{pmatrix}$ , and in each case  $A(u) = \mathbf{a}\lambda + u$ , where  $\lambda$  is a complex parameter, and  $\mathbf{a}$  is the constant, diagonal, trace zero matrix  $\mathbf{a} = \begin{pmatrix} -i & 0 \\ 0 & i \end{pmatrix}$ .

**Example 1.** [AKNS1] Take  $u(x) = \begin{pmatrix} 0 & q(x) \\ -1 & 0 \end{pmatrix}$ , and let

$$B(u) = \mathbf{a}\lambda^3 + u\lambda^2 + \begin{pmatrix} \frac{i}{2}q & \frac{i}{2}q_x \\ 0 & -\frac{i}{2}q \end{pmatrix} \lambda + \begin{pmatrix} \frac{q_x}{4} & \frac{-q^2}{2} - \frac{q_{xx}}{4} \\ \frac{q}{4} & \frac{q_x}{4} \end{pmatrix}.$$

Then an easy computation shows that ZCC is satisfied if and only if  $q$  satisfies KdV in the form  $q_t = -\frac{1}{4}(6qq_x + q_{xxx})$ .

**Example 2.** [ZS] Take  $u(x) = \begin{pmatrix} 0 & q(x) \\ -\bar{q}(x) & 0 \end{pmatrix}$ , and let

$$B(u) = \mathbf{a}\lambda^2 + u\lambda + \begin{pmatrix} \frac{i}{2}|q|^2 & \frac{i}{2}q_x \\ \frac{i}{2}\bar{q}_x & -\frac{i}{2}|q|^2 \end{pmatrix}.$$

In this case ZCC is satisfied if and only if  $q(x, t)$  satisfies the so-called Nonlinear Schrödinger Equation (NLS)  $q_t = \frac{i}{2}(q_{xx} + 2|q|^2q)$ .

**Example 3.** [AKNS1] Take  $u = \begin{pmatrix} 0 & -\frac{q_x(x)}{2} \\ \frac{q_x(x)}{2} & 0 \end{pmatrix}$ , and let  $B(u) = \frac{1}{\lambda}v$  where  $v(x) = \frac{i}{4} \begin{pmatrix} \cos q(x) & \sin q(x) \\ \sin q(x) & -\cos q(x) \end{pmatrix}$ . In this case, ZCC is satisfied if and only if  $q$  satisfies the Sine-Gordon Equation (SGE) in the form  $q_{xt} = \sin q$ .

# Appendix A

## Symplectic Manifolds and Hamiltonian Systems

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If  $P$  is a finite dimensional smooth manifold, then a symplectic structure for  $P$  is a closed non-degenerate 2-form  $\Omega$  on  $P$ . Non-degenerate means that at each point  $p$  of  $P$ , the map  $v \mapsto i_v \Omega = \Omega(v, \cdot)$  of  $TP_p$  to its dual  $T^*P_p$  is a linear isomorphism. It then follows that if  $F : P \rightarrow \mathbf{R}$  is a smooth real-valued function on  $P$ , then there is a uniquely determined vector field  $X$  on  $P$  such that  $i_X \Omega = dF$ , and we call  $X$  the symplectic gradient of  $F$  and denote it by  $\nabla_{\mathfrak{s}} F$ .

By an important theorem of Darboux, ([Ar], Chapter 8) in the neighborhood of any point of  $P$  there exist ‘‘canonical coordinates’’  $q_1, \dots, q_n, p_1, \dots, p_n$  in which  $\Omega$  has the form  $\sum_i dp_i \wedge dq_i$ , and in these coordinates  $\nabla_{\mathfrak{s}} H = \sum_i (\frac{\partial H}{\partial p_i} \frac{\partial}{\partial q_i} - \frac{\partial H}{\partial q_i} \frac{\partial}{\partial p_i})$ , or equivalently the solution curves of  $\nabla_{\mathfrak{s}} H$  satisfy Hamilton’s equations  $\frac{dp_i}{dt} = -\frac{\partial H}{\partial q_i}$ ,  $\frac{dq_i}{dt} = \frac{\partial H}{\partial p_i}$ .

We next recall some facts about Lie derivatives. If  $X$  is a smooth vector field on a smooth manifold  $M$ , generating a flow  $\phi_t$ , and if  $T$  is any smooth tensor field on  $M$ , then the Lie derivative of  $T$  with respect to  $X$  is the tensor field  $\mathcal{L}_X T = \frac{d}{dt}|_{t=0} \phi_t^*(T)$ . If  $\mathcal{L}_X T = 0$ , then we shall say that ‘‘ $X$  preserves  $T$ ’’, for this is the necessary and sufficient condition that the flow  $\phi_t$  preserve  $T$ , i.e., that  $\phi_t^*(T) = T$  for all  $t$ . There is a famous formula of Cartan for the Lie derivative operator  $\mathcal{L}_X$  restricted to differential forms, identifying it with the anti-commutator of the exterior derivative operator  $d$  and the interior product operator  $i_X$ :

$$\mathcal{L}_X = di_X + i_X d.$$

If  $\theta$  is a closed  $p$ -form, this gives  $\mathcal{L}_X \theta = d(i_X \theta)$ , so  $X$  preserves  $\theta$  if and only if the  $(p-1)$ -form  $i_X \theta$  is closed. In particular this demonstrates the important fact that a vector field  $X$  on a symplectic manifold  $P$  is symplectic (i.e., preserves the symplectic form,  $\Omega$ ) if and only if  $i_X \Omega$  is a closed 1-form (and hence, at least locally, the differential of a smooth function). The well known identity  $\mathcal{L}_{[X,Y]} = [\mathcal{L}_X, \mathcal{L}_Y]$  implies that the space of symplectic vector fields on  $P$  is a Lie algebra, which we can think of as the Lie algebra of the group of symplectic diffeomorphisms of  $P$ . It is an interesting and useful fact that the space of Hamiltonian vector fields on  $P$ , i.e., those for which  $i_X \Omega$  is an exact form,  $dF$ , is not only a linear subspace, but is even a Lie subalgebra of the symplectic vector fields, and moreover the commutator subalgebra of the symplectic vector fields is included in the Hamiltonian vector fields. To demonstrate this we shall show that if  $i_X \Omega$  and  $i_Y \Omega$  are closed forms, then  $i_{[X,Y]} \Omega$  is not only closed but even exact, and in fact it is the differential of the function  $\Omega(Y, X)$ . First, using the fact that Lie derivation satisfies a Leibnitz formula with respect to any natural bilinear operation on tensors (so in particular with respect to the interior product),  $\mathcal{L}_X (i_Y \Omega) = i_{(\mathcal{L}_X Y)} \Omega + i_Y (\mathcal{L}_X \Omega)$ . Thus, since  $\mathcal{L}_X Y = [X, Y]$  and  $\mathcal{L}_X \Omega = 0$ ,  $\mathcal{L}_X (i_Y \Omega) = i_{[X,Y]} \Omega$ . Finally, since  $d(i_Y \Omega) = 0$ , Cartan’s formula for  $\mathcal{L}_X (i_Y \Omega)$  gives  $i_{[X,Y]} \Omega = di_X (i_Y \Omega) = d(\Omega(Y, X))$ .

**5.0.1 Remark.** Cartan’s Formula can be proved easily as follows. There is an important involutory automorphism  $\omega \mapsto \bar{\omega}$  of the algebra  $A$  of differential forms on a manifold. Namely, it is the identity on forms of even degree and is minus the identity on forms of odd degree. A linear map  $\partial : A \rightarrow A$  is called an *anti-derivation* if  $\partial(\lambda\omega) = \partial\lambda \wedge \omega + \bar{\lambda} \wedge \partial\omega$ . It

is of course well-known that the exterior derivative,  $d$ , is an anti-derivation (of degree  $+1$ ), and an easy check shows that the interior product  $i_X$  is an anti-derivation (of degree  $-1$ ). Moreover, the anti-commutator of two anti-derivations is clearly a derivation, so that  $\mathcal{L}_X$  and  $di_X + i_Xd$  are both derivations of  $A$ , and hence to prove they are equal it suffices to check that they agree on a set of generators of  $A$ . But  $A$  is generated by forms of degree zero (i.e., functions) and the differentials of functions, and it is obvious that  $\mathcal{L}_X$  and  $di_X + i_Xd$  agree on these.

We shall also have to deal with symplectic structures on infinite dimensional manifolds. In this case we still require that  $\Omega$  is a closed form and we also still require that  $\Omega$  is *weakly* non-degenerate, meaning that for each point  $p$  of  $P$ , the map  $v \mapsto i_v\Omega$  of  $TP_p$  to  $TP_p^*$  is injective. In finite dimensions this of course implies that  $\Omega$  is strongly non-degenerate—meaning that the latter map is in fact an isomorphism—but that is rarely the case in infinite dimensions, so we will *not* assume it. Thus, if  $F$  is a smooth function on  $P$ , it does not automatically follow that there is a symplectic gradient vector field  $\nabla_s F$  on  $P$  satisfying  $\Omega((\nabla_s F)_p, v) = dF_p(v)$  for all  $v$  in  $TP_p$ —this must be proved separately. However, if a symplectic gradient does exist, then weak non-degeneracy shows that it is unique. In the infinite dimensional setting we call a function  $F : P \rightarrow \mathbf{R}$  a *Hamiltonian* function if it has a symplectic gradient, and vector fields of the form  $\nabla_s F$  will be called Hamiltonian vector fields. Obviously the space of Hamiltonian functions is linear, and in fact the formula  $d(FG) = FdG + GdF$  shows that it is even an algebra, and that  $\nabla_s(FG) = F\nabla_s G + G\nabla_s F$ . We shall call a vector field  $X$  on  $P$  symplectic if the 1-form  $i_X\Omega$  is closed but not necessarily exact, for as we have seen, this is the condition for the flow generated by  $X$  to preserve  $\Omega$ .

Of course if  $P$  is a vector space, the distinction between Hamiltonian and symplectic disappears: if  $i_X\Omega$  is closed, then  $H(p) = \int_0^1 \Omega_{tp}(X_{tp}, p) dt$  defines a Hamiltonian function with  $\nabla_s H = X$ . Moreover, in this case it is usually straightforward to check if  $i_X\Omega$  is closed. Given  $u, v$  in  $P$ , consider them as constant vector fields on  $P$ , so that  $[u, v] = 0$ . Then the formula  $d\theta(u, v) = u(\theta(v)) - v(\theta(u)) - \theta([u, v])$  for the exterior derivative of a 1-form shows that symmetry of  $\frac{d}{dt}\big|_{t=0} \Omega(X_{p+tu}, v)$  in  $u$  and  $v$  is necessary and sufficient for  $i_X\Omega$  to be closed (and hence exact). In case  $\Omega$  is a constant form (i.e.,  $\Omega_p(u, v)$  is independent of  $p$ ), then  $\frac{d}{dt}\big|_{t=0} \Omega(X_{p+tu}, v) = \Omega((DX_p)(u), v)$ , where  $(DX)_p(u) = \frac{d}{dt}\big|_{t=0} X_{p+tu}$  is the differential of  $X$  at  $p$ . Since  $\Omega$  is skew-symmetric in  $u$  and  $v$ , this shows that if  $\Omega$  is constant, then  $X$  is Hamiltonian if and only if  $(DX)_p$  is “skew-adjoint” with respect to  $\Omega$ .

If two smooth real-valued functions  $F_1$  and  $F_2$  on a symplectic manifold  $P$  are Hamiltonian, i.e., if they have symplectic gradients  $\nabla_s F_1$  and  $\nabla_s F_2$ , then they determine a third function on  $P$ , called their *Poisson bracket*, defined by:

$$\{F_1, F_2\} = \Omega(\nabla_s F_2, \nabla_s F_1).$$

The formula  $i_{[X, Y]}\Omega = d(\Omega(Y, X))$  shows that the Poisson bracket is also a Hamiltonian function, and in fact

$$\nabla_s \{F_1, F_2\} = [\nabla_s F_1, \nabla_s F_2].$$

What this formula says is that Hamiltonian functions  $F : P \rightarrow \mathbf{R}$  are not only a commutative and associative algebra under pointwise product, but also a Lie algebra under Poisson bracket, and  $F \mapsto \nabla_s F$  is a Lie algebra homomorphism of this Lie algebra onto the Lie algebra of Hamiltonian vector fields on  $P$ . In particular, we see that the Poisson bracket satisfies the Jacobi identity,

$$\{\{F_1, F_2\}, F_3\} + \{\{F_2, F_3\}, F_1\} + \{\{F_3, F_1\}, F_2\} = 0,$$

and the Leibnitz Rule  $\nabla_{\mathbf{s}}(FG) = F \nabla_{\mathbf{s}} G + G \nabla_{\mathbf{s}} F$  gives:

$$\{F_1, F_2 F_3\} = \{F_1, F_2\} F_3 + F_2 \{F_1, F_3\},$$

which we will also call the Leibnitz Rule.

Since  $\{F_1, F_2\} = \Omega(\nabla_{\mathbf{s}} F_2, \nabla_{\mathbf{s}} F_1) = dF_2(\nabla_{\mathbf{s}} F_1) = \nabla_{\mathbf{s}} F_1(F_2)$ , we can interpret the Poisson bracket of  $F_1$  and  $F_2$  as the rate of change of  $F_2$  along the solution curves of the vector field  $\nabla_{\mathbf{s}} F_1$ . If we are considering some fixed Hamiltonian system  $\frac{dx}{dt} = \nabla_{\mathbf{s}} H_x$  on  $P$ , then we can write this as  $\frac{dF}{dt} = \{H, F\}$ , and we see that *the vanishing of the Poisson bracket  $\{H, F\}$  is the necessary and sufficient condition for  $F$  to be a constant of the motion*. By the Jacobi Identity, a corollary to this observation is that the Poisson Bracket of two constants of the motion is also a constant of the motion. And since  $\{H, H\} = 0$ ,  $H$  itself is always a constant of the motion.

Since the Poisson bracket is skew-symmetric,  $\{F_1, F_2\}$  is zero if and only if  $\{F_2, F_1\}$  is zero, and in this case we say that  $F_1$  and  $F_2$  are *in involution*. More generally  $k$  Hamiltonian functions  $F_1, \dots, F_k$  are said to be in involution if all of the Poisson brackets  $\{F_i, F_j\}$  vanish. Note that since  $\nabla_{\mathbf{s}} \{F_i, F_j\} = [\nabla_{\mathbf{s}} F_i, \nabla_{\mathbf{s}} F_j]$ , if the  $F_i$  are in involution then the vector fields  $\nabla_{\mathbf{s}} F_i$  commute, i.e.,  $[\nabla_{\mathbf{s}} F_i, \nabla_{\mathbf{s}} F_j] = 0$ , or equivalently the flows they generate commute. In particular we see that *if  $F_1, \dots, F_n$  are in involution and if each  $\nabla_{\mathbf{s}} F_i$  generates a one-parameter group of diffeomorphisms  $\phi_t^i$  of  $P$ , then  $(t_1, \dots, t_n) \mapsto \phi_{t_1}^1 \circ \phi_{t_2}^2 \circ \dots \circ \phi_{t_n}^n$  defines a symplectic action of the abelian group  $\mathbf{R}^n$  on  $P$ .*

Suppose  $P$  is a symplectic manifold of dimension  $2n$  and that there exist  $n$  functions  $F_i$  such that the  $dF_i$  are everywhere linearly independent. If the functions  $F_i$  are in involution with each other and with a function  $H$ , then the so-called Arnold-Liouville Theorem ([Ar], Chapter 10) states that the Hamiltonian system  $\nabla_{\mathbf{s}} H$  is completely integrable in the sense mentioned earlier, i.e., there exist action-angle variables  $q_1, \dots, q_n, p_1, \dots, p_n$ . In fact, complete integrability of a  $2n$  dimensional Hamiltonian system is often *defined* as the existence of  $n$  functionally independent constants of the motion in involution.

# Appendix B

## Wave Equations as Continuum Limits of Lattice Models

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### Introduction.

In this appendix we will indicate one way that physically natural wave equations can be deduced more or less directly from first principles. While, much of what we do below can be generalized to  $n$  space dimensions, we shall as usual, concentrate on the 1-dimensional case.

We imagine a 1-dimensional physical medium that it may help to think of as a stretched piano wire or a steel bar of small cross-section, but as we shall see later there are other useful interpretations. We think of this initially as a continuum that is placed along the  $x$ -axis from 0 to its length  $\ell$ . We assume that the property of this system that interests us can be described by a “scalar field”  $u$ , that we will usually take to be real-valued (although the case that  $u$  is complex-valued is also of interest). The value of  $u$  at the point  $x \in [0, \ell]$  and time  $t$  is  $u(x, t)$ . The time evolution of the system will then be described by some sort of evolution PDE for  $u$  of the general form  $u_{tt} = F(u)$  or  $u_t = G(u)$ , and we want to deduce the general form of the right hand side from basic physical laws.

Our strategy will be to take an atomistic viewpoint—real physical media after all are discrete, not continuous, made up of particles (“molecules”) arranged in space with a very small average distance  $h$  separating nearest neighbors. In our simplified model, we will suppose that there are  $N$  identical particles, located at the lattice points  $p_i = ih$  where  $0 \leq i \leq N - 1$ , and  $h = \ell/(N - 1)$ . We shall refer to the particle at  $p_i$  as  $P_i$ .

We assume each  $P_i$  is a Newtonian particle with a mass  $m$  and that the property we are concerned with is associated to a degree of freedom of the particle that is uncoupled from its other degrees of freedom, and that we will denote by  $x_i$ . We do not at this point fix a precise interpretation of  $x_i$  in terms of say the spatial location of the particle  $P_i$ . In a particular model, it will often represent the deviation of  $P_i$  from an equilibrium configuration. The relation between the field  $u$  and the particles  $P_i$  is that  $u$  should interpolate the values  $x_i$  at the points  $p_i$ , i.e.,  $u(p_i, t) = x_i(t)$ .

Note that if the density of our medium is  $\rho$  then the mass of a length  $h$  between  $p_i$  and  $p_{i+1}$  is  $m = \rho h$ , which we think of as being concentrated in the particle  $P_i$ . Eventually we will pass to a continuum limit by letting  $N$  tend to infinity (and hence  $h \rightarrow 0$ ), keeping the density,  $\rho$ , fixed.

Since the evolution of the  $x_i$  in time is governed by Newton’s Third Law of Motion, “force = mass  $\times$  acceleration”, i.e.,  $m\ddot{x}_i = F_i$ , to specify a model, we must specify the force,  $F_i$ , on each particle  $P_i$ . Assuming the system is isolated,  $F_i$  will be a sum of terms,  $F_i = \sum_j F_{i,j}$ , where  $F_{i,j}$  is the force on the particle  $P_i$  due to the particle  $P_j$ , and by Newton’s Second Law, equating action and reaction,  $F_{i,j} = -F_{j,i}$ . We will restrict attention to the case of so-called *nearest-neighbor interactions*. This means that we assume  $F_{ij} = 0$  unless  $P_j$  is one of the two nearest neighbors of  $P_i$ , i.e.,  $j = i + 1$  or  $j = i - 1$ , so  $F_i = F_{i,i+1} + F_{i,i-1} = F_{i,i+1} - F_{i-1,i}$ . Since the particles are identical, there is a “universal” force law expressing  $F_{i,i+1}$  as a fixed function of  $x_i$  and  $x_{i+1}$ . We will make the natural assumption that our force law is translation invariant, so it only depends on the difference  $x_i - x_{i+1}$ :  $F_{i,i+1} = F(x_i - x_{i+1})$ ,

where  $F(0) = 0$ . Thus  $F_i = F(x_i - x_{i+1}) - F(x_{i-1} - x_i)$ , and to complete the specification of a model, we may specify either the force function  $F$ , or equivalently the potential function  $V(r) = -\int_0^r F(y) dy$  (in terms of which  $F(y) = -V'(y)$ ).

Now, as we remarked above, in the models we shall consider,  $x_i$  will be a measure of the deviation from equilibrium of  $P_i$ . In particular, if all the  $x_i$  are zero, then all the forces  $F_i$  will also be zero, and it follows that  $V'(0) = 0$ , or in other words 0 is a critical point of  $V$ , so  $V$  has the Taylor expansion  $V(y) = \frac{k}{2}y^2 + R(y)y^3$  near 0. We shall assume that in fact 0 is a non-degenerate minimum of  $V$ , i.e.,  $k > 0$ . Physically this means that taking all  $x_i$  equal 0 gives a stable equilibrium of the system, in the sense that any small deviation from this state will create forces that drive the system back towards equilibrium. Since  $V'(y) = ky + S(y)y^2$  (where  $S(y) = yR'(y) + 3R(y)$ ), and  $F = -V'$ ,

$$\begin{aligned} F_i &= V'(x_{i-1} - x_i) - V'(x_i - x_{i+1}) \\ &= k(x_{i+1} + x_{i-1} - 2x_i) + T(x_{i-1}, x_i, x_{i+1}), \end{aligned}$$

where  $T(x_{i-1}, x_i, x_{i+1}) = S(x_{i-1} - x_i)(x_{i-1} - x_i)^2 - S(x_i - x_{i+1})(x_i - x_{i+1})^2$ .

The constant  $k$  has the interpretation of the spring constant for a piece of the medium of length  $h$ , so if  $\kappa$  is the Young's modulus for the medium (the spring constant for a piece of unit length) then  $k = \kappa/h$ . (If you halve the length of a spring, it becomes twice as hard to stretch it.) So, if we write  $c = \sqrt{\frac{\kappa}{\rho}}$  and recall that  $m = \rho h$ , we have  $\frac{k}{m} = c^2 \frac{1}{h^2}$ , and we can rewrite the above formula for  $F_i$  as

$$\frac{1}{m}F_i = c^2 \left( \frac{x_{i+1} + x_{i-1} - 2x_i}{h^2} \right) + \frac{1}{m}T(x_{i-1}, x_i, x_{i+1}).$$

Let us first consider the case where our medium rigorously satisfies Hooke's Law, i.e., the remainder term  $R(y)$  (and hence also  $S$  and  $T$ ) are identically zero. (Or else assume that the deviations from equilibrium are so small that the quadratic terms in the  $x_i$  can be ignored.) Thus the forces  $F_i$  are linear, and Newton's Equations of Motion become simply

$$\ddot{x}_i = c^2 \left( \frac{x_{i+1} + x_{i-1} - 2x_i}{h^2} \right).$$

We can now easily "pass to the continuum limit". That is, by letting  $N$  tend to infinity (so  $h$  tends to zero) we can derive a PDE for the function  $u(x, t)$ . If we take  $x = p_i$ , then by definition  $u(x, t) = x_i(t)$  and since  $p_i + h = p_{i+1}$  while  $p_i - h = p_{i-1}$ , the latter form of Newton's equations gives:

$$u_{tt}(x, t) = c^2 \frac{u(x+h, t) + u(x-h, t) - 2u(x, t)}{h^2}.$$

Next recall Taylor's formula:

$$f(x \pm h) = f(x) \pm hf'(x) + \frac{h^2}{2!}f''(x) \pm \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f''''(x) + O(h^5).$$

If we now take  $f(x) = u(x, t)$ , this gives:

$$\frac{u(x+h, t) + u(x-h, t) - 2u(x, t)}{h^2} = u_{xx}(x, t) + \left(\frac{h^2}{12}\right)u_{xxxx}(x, t) + O(h^4),$$

so letting  $h \rightarrow 0$ , we find  $u_{tt} = c^2 u_{xx}$ , i.e.,  $u$  satisfies the linear wave equation, with propagation speed  $c$ .

**Example.** Longitudinal vibrations (sound waves) in a metal bar.

In this interpretation of the above, we assume that the atoms are in equilibrium when the all the particles  $P_i$  are in the locations  $p_i$ , and that the actual positions of the particles at time  $t$  are  $X_i(t) = p_i + x_i(t)$ . Note that the particles are moving longitudinally (i.e., along the length of the medium). This models the sound vibrations in a clamped metal bar when it is struck at one end.

**Example.** Transverse vibrations of a stretched wire (piano string).

In this interpretation we assume that the articles are constrained to move orthogonally to the medium. That is, the particles are in equilibrium when located at the points  $(p_i, 0)$  of the  $xy$ -plane, and the actual position of the particle at time  $t$  is  $(p_i, x_i(t))$ . If we think of this as a stretched piano wire and if the tension along the string is  $T$ , then  $F_i$  is the vertical or  $y$ -component of the tension, which is

$$T \frac{(x_i - x_{i+1})}{\sqrt{h^2 + (x_i - x_{i+1})^2}} = \frac{T}{h} \frac{(x_i - x_{i+1})}{\sqrt{1 + \left(\frac{x_i - x_{i+1}}{h}\right)^2}}.$$

If we assume that the slope of the wire,  $x_i - x_{i+1}/h$ , is small compared with 1, we can approximate this by  $\frac{T}{h}(x_i - x_{i+1})$ , which reduces to the general case above if we take  $k = \frac{T}{h}$ , i.e., if we identify  $T$  with the Young's modulus  $\kappa$ . It follows that with the above assumption that the slope of the wire is small, we again get a wave equation with the propagation speed  $c$  equal to  $\sqrt{\frac{T}{\rho}}$ .

**Exercise.** The Sine-Gordon Equation as a continuum limit.

If we put a piano wire under tension and clamp the ends, then it resists twisting as well as stretching. If attach a pendulum  $P_i$  at each of the points  $p_i$ , we get a lattice of torsion pendulums, and we let  $x_i$  denote the angle that the  $P_i$  makes with a fixed direction, say the vertical. In this case  $m_i$  should measure moment of inertia of  $P_i$  around the wire, and  $F_i$  the torque on  $P_i$  due to the twisting of the wire between  $P_i$  and  $P_{i+1}$ . (We neglect the external force of gravity.) Show that the Sine-Gordon equation can be obtained as a continuum limit this lattice. (See Remoissenet, M., *Waves Called Solitons: Concepts and Experiments*, Springer, 1994.)

**Exercise.** The Lagrangian approach to finding continuum limits.

The kinetic energy of our nearest neighbor lattice is  $K = \frac{m}{2} \sum_i \dot{x}_i^2$ , and the potential energy is  $U = \frac{k}{2} \sum_i ((x_i - x_{i+1})^2 + (x_{i-1} - x_i)^2)$ . Show that as  $N \rightarrow \infty$ , these approach respectively to  $K = \frac{\rho}{2} \int_0^\ell u_t(x, t)^2 dx$  and  $U = \frac{\kappa}{2} \int_0^\ell u_x(x, t)^2 dx$ , and hence the action of the system (in a time interval  $[a, b]$ ) converges to  $A = \int_a^b dt \int_0^\ell (\frac{\rho}{2} u_t(x, t)^2 - \frac{\kappa}{2} u_x(x, t)^2) dx$ . Show that the Euler-Lagrange equations for extremalizing this action is just the linear wave equation for  $u$  derived above.

So far we have only dealt with the case of a harmonic lattice, that is one with quadratic potential. We are now going to generalize this by looking at the effect of the next (i.e.,

cubic) term in the potential function  $V$ . That is, we are now going to assume that we have a slightly anharmonic lattice, with potential function  $V(y) = \frac{k}{2}y^2 + \frac{\alpha}{3}y^3$ , so the force is  $F(y) = -ky - \alpha y^2$ , and  $F_i = k(x_{i+1} + x_{i-1} - 2x_i)[1 + \alpha(x_{i+1} - x_{i-1})]$ , and Newton's Equations now take the form:

$$(FPU) \quad \ddot{x}_i = c^2 \left( \frac{x_{i+1} + x_{i-1} - 2x_i}{h^2} \right) [1 + \alpha(x_{i+1} - x_{i-1})].$$

which we will refer to as the Fermi-Pasta-Ulam lattice equations, after the three mathematicians and physicists who studied it numerically in 1955, using one of the first digital computers.

Finding a good continuum limit for this non-linear lattice is a lot more sophisticated than one might at first expect after the easy time we had with the linear case. In fact the approach to the limit has to be handled with considerable skill to avoid inconsistent results, and it involves several non-obvious steps.

As before we let  $u(x, t)$  denote the function measuring the displacement at time  $t$  of the particle with equilibrium position  $x$ , so if  $x = p_i$  then, by definition,  $x_i(t) = u(x, t)$ ,  $x_{i+1}(t) = u(x+h, t)$ , and  $x_{i-1}(t) = u(x-h, t)$ . Of course  $\ddot{x}_i = u_{tt}(x, t)$  and, as noted earlier, Taylor's Theorem with remainder gives

$$\begin{aligned} \frac{x_{i+1} + x_{i-1} - 2x_i}{h^2} &= \frac{u(x+h, t) + u(x-h, t) - 2u(x, t)}{h^2} \\ &= u_{xx}(x, t) + \left(\frac{h^2}{12}\right)u_{xxxx}(x, t) + O(h^4). \end{aligned}$$

By a similar computation

$$\alpha(x_{i+1} - x_{i-1}) = (2\alpha h)u_x(x, t) + \left(\frac{\alpha h^3}{3}\right)u_{xxx}(x, t) + O(h^5),$$

so substitution in (FPU) gives

$$\left(\frac{1}{c^2}\right)u_{tt} - u_{xx} = (2\alpha h)u_x u_{xx} + \left(\frac{h^2}{12}\right)u_{xxxx} + O(h^4).$$

As a first attempt to derive a continuum description for the FPU lattice in the non-linear case, it is tempting to just let  $h$  approach zero and assume that  $2\alpha h$  converges to a limit  $\epsilon$ . This would give the PDE

$$u_{tt} = c^2(1 + \epsilon u_x)u_{xx}$$

as our continuum limit for the FPU Lattice equations and the non-linear generalization of the wave equation. But this leads to a serious problem. This equation is familiar in applied mathematics—it was studied by Rayleigh in the last century—and it is easy to see from examples that its solutions develop discontinuities (shocks) after a time on the order of  $(\epsilon c)^{-1}$ , which is considerably shorter than the time scale of the almost periods observed in the Fermi-Pasta-Ulam experiments. It was Zabusky who realized that the correct approach was to retain the term of order  $h^2$  and study the equation

$$(ZK) \quad \left(\frac{1}{c^2}\right)u_{tt} - u_{xx} = (2\alpha h)u_x u_{xx} + \left(\frac{h^2}{12}\right)u_{xxxx}.$$



If we differentiate this equation with respect to  $x$  and make the substitution  $v = u_x$ , we see that it reduces to the more familiar Boussinesq equation

$$\left(\frac{1}{c^2}\right)v_{tt} = v_{xx} + \alpha h \frac{\partial^2(v^2)}{\partial x^2} + \left(\frac{h^2}{12}\right)v_{xxxx},$$

(The effect of the fourth order term is to add dispersion to the equation, and this smooths out incipient shocks before they can develop.)

It is important to realize that, since  $h \neq 0$ , (ZK) cannot logically be considered a true continuum limit of the FPU lattice. It should rather be regarded as an asymptotic approximation to the lattice model that works for small lattice spacing  $h$  (and hence large  $N$ ). Nevertheless, we shall now see how to pass from (ZK) to a true continuum description of the FPU lattice.

The next step is to notice that, with  $\alpha$  and  $h$  small, solutions of (ZK) should behave qualitatively like solutions of the linear wave equation  $u_{tt} = c^2 u_{xx}$ , and increasingly so as  $\alpha$  and  $h$  tend to zero. Now the general solution of the linear wave equation is of course  $u(x, t) = f(x + ct) + g(x - ct)$ , i.e., the sum of an arbitrary left moving traveling wave and an arbitrary right moving traveling wave, both moving with speed  $c$ . Recall that it is customary to simplify the analysis in the linear case by treating each kind of wave separately, and we would like to do the same here. That is, we would like to look for solutions  $u(x, t)$  that behave more and more like (say) right moving traveling waves of velocity  $c$ —and for longer and longer periods of time—as  $\alpha$  and  $h$  tend to zero.

It is not difficult to make precise sense out of this requirement. Suppose that  $y(\xi, \tau)$  is a smooth function of two real variables such that the map  $\tau \mapsto y(\cdot, \tau)$  is uniformly continuous from  $\mathbf{R}$  into the bounded functions on  $\mathbf{R}$  with the sup norm—i.e., given  $\epsilon > 0$  there is a positive  $\delta$  such that  $|\tau - \tau_0| < \delta$  implies  $|y(\xi, \tau) - y(\xi, \tau_0)| < \epsilon$ . Then for  $|t - t_0| < T = \delta/(\alpha h c)$  we have  $|\alpha h c t - \alpha h c t_0| < \delta$ , so  $|y(x - ct, \alpha h c t) - y(x - ct, \alpha h c t_0)| < \epsilon$ . In other words, the function  $u(x, t) = y(x - ct, \alpha h c t)$  is uniformly approximated by the traveling wave  $u^0(x, t) = y(x - ct, \alpha h c t_0)$  on the interval  $|t - t_0| < T$  (and of course  $T \rightarrow \infty$  as  $\alpha$  and  $h$  tend to zero). To restate this a little more picturesquely,  $u(x, t) = y(x - ct, \alpha h c t)$  is approximately a traveling wave whose shape gradually changes in time. Notice that if  $y(\xi, \tau)$  is periodic or almost periodic in  $\tau$ , the gradually changing shape of the approximate traveling wave will also be periodic or almost periodic.

To apply this observation, we define new variables  $\xi = x - ct$  and  $\tau = (\alpha h)ct$ . Then by the chain rule,  $\partial^k/\partial x^k = \partial^k/\partial \xi^k$ ,  $\partial/\partial t = -c(\partial/\partial \xi - (\alpha h)\partial/\partial \tau)$ , and  $\partial^2/\partial t^2 = c^2(\partial^2/\partial \xi^2 - (2\alpha h)\partial^2/\partial \xi \partial \tau) + (\alpha h)^2 \partial^2/\partial \tau^2$ .

Thus in these new coordinates the wave operator transforms to:

$$\frac{1}{c^2} \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x^2} = -2\alpha h \frac{\partial^2}{\partial \xi \partial \tau} + (\alpha h)^2 \frac{\partial^2}{\partial \tau^2},$$

so substituting  $u(x, t) = y(\xi, \tau)$  in (ZK) (and dividing by  $-2\alpha h$ ) gives:

$$y_{\xi\tau} - \left(\frac{\alpha h}{2}\right)y_{\tau\tau} = -y_{\xi}y_{\xi\xi} - \left(\frac{h}{24\alpha}\right)y_{\xi\xi\xi\xi},$$

and, at last, we are prepared to pass to the continuum limit. We assume that  $\alpha$  and  $h$  tend to zero at the same rate, i.e., that as  $h$  tends to zero, the quotient  $h/\alpha$  tends to a positive

limit, and we define  $\delta = \lim_{h \rightarrow 0} \sqrt{h/(24\alpha)}$ . Then  $\alpha h = O(h^2)$ , so letting  $h$  approach zero gives  $y_{\xi\tau} + y_{\xi}y_{\xi\xi} + \delta^2 y_{\xi\xi\xi} = 0$ . Finally, making the substitution  $v = y_{\xi}$  we arrive at the KdV equation:

$$(KdV) \quad v_{\tau} + vv_{\xi} + \delta^2 v_{\xi\xi\xi} = 0.$$

**Remark.** Note that if we re-scale the independent variables by  $\tau \rightarrow \beta\tau$  and  $\xi \rightarrow \gamma\xi$ , then the KdV equation becomes:

$$v_{\tau} + \left(\frac{\beta}{\gamma}\right)vv_{\xi} + \left(\frac{\beta}{\gamma^3}\right)\delta^2 v_{\xi\xi\xi} = 0,$$

so by appropriate choice of  $\beta$  and  $\gamma$  we can obtain any equation of the form  $v_{\tau} + \lambda vv_{\xi} + \mu v_{\xi\xi\xi} = 0$ , and any such equation is referred to as “the KdV equation”. A commonly used choice that is convenient for many purposes is  $v_{\tau} + 6vv_{\xi} + v_{\xi\xi\xi} = 0$ , although the form  $v_{\tau} - 6vv_{\xi} + v_{\xi\xi\xi} = 0$  (obtained by replacing  $v$  by  $-v$ ) is equally common. We will use both these forms.

Let us recapitulate the relationship between the FPU Lattice and the KdV equation. Given a solution  $x_i(t)$  of the FPU Lattice we get a function  $u(x, t)$  by interpolation—i.e.,  $u(ih, t) = x_i(t)$ ,  $i = 0, \dots, N$ . For small lattice spacing  $h$  and non-linearity parameter  $\alpha$  there will be solutions  $x_i(t)$  so that the corresponding  $u(x, t)$  will be an approximate right moving traveling wave with slowly varying shape, i.e., it will be of the form  $u(x, t) = y(x - ct, \alpha hct)$  for some smooth function  $y(\xi, \tau)$ , and the function  $v(\xi, \tau) = y_{\xi}(\xi, \tau)$  will satisfy the KdV equation  $v_{\tau} + vv_{\xi} + \delta^2 v_{\xi\xi\xi} = 0$ , where  $\delta^2 = h/(24\alpha)$ .

# Appendix C

## Solving Wave Equations Numerically: The Pseudospectral Method

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### Introduction.

So-called pseudospectral methods, for the numerical integration of evolution equations, use discrete Fourier transforms instead of finite differencing to evaluate spatial derivatives (an excellent early article is [FW]). A surprising fact is that these methods often work very well for nonlinear equations. The time-stepping for pseudospectral methods is accomplished by a classical differencing scheme that can in principle be either explicit or implicit, but for the usual stability reasons, an implicit method such as Crank-Nicolson (the trapezoidal rule) is usually preferred. However, when the equation is nonlinear, the solution of the implicit equations that arise can present a problem. One approach is to employ split-stepping; use Crank-Nicolson plus Gaussian elimination for the linear terms, but fall back to an explicit method for the nonlinear terms. An alternative approach (pioneered in [WMGS] and that we refer to as the WMGS method) is to treat the linear and nonlinear terms together, write the implicit equation in fixed-point form, and then solve it by an iteration scheme.

WGMS originally developed their method to solve the initial value problems for the KdV and KP equations with periodic boundary conditions, and we became aware of their technique via [S], in which D. H. Sattinger reports on a modified WGMS method for solving the KdV equation developed in collaboration with Yi Li. In this paper, we will discuss a generalization of the WGMS algorithm to treat the initial value problem for a fairly broad class of evolutionary PDE that are “weakly nonlinear”, in the sense that their nonlinear terms are a lower order perturbation of the linear part (see below for a precise definition) and we will prove a convergence theorem for the iteration method that is at the heart of the WGMS algorithm.

### Weakly Nonlinear PDE of Evolution.

Let  $U$  denote a finite dimensional complex inner product space and  $V$  a vector space of  $U$ -valued functions on  $\mathbf{R}$ . Usually we will work in a fixed orthonormal basis  $(e_1, \dots, e_n)$  for  $U$  and use it to identify  $U$  with  $\mathbf{C}^n$ , so that elements  $u$  of  $V$  can be considered as  $n$ -tuples  $(u^1, \dots, u^n)$  of complex-valued functions. (If  $n = 1$  we shall say we are in the *scalar case* and we then identify  $u$  with  $u^1$ .)

We will specify  $V$  more precisely later, but the elements of  $V$  will admit derivatives up to a certain order, and they will in most cases be required to be  $2\pi$ -periodic, in which case we shall also consider them as functions on the unit circle in the complex plane. If  $u(t)$  is a curve in  $V$  we will also write  $u(x, t)$  for  $u(t)(x)$ . As usual we think of  $t$  as denoting time and  $x$  as space. We denote by  $D$  the differentiation operator  $\frac{\partial}{\partial x}$  and we also write  $u_x^i = Du^i$ ,  $u_{xx}^i = D^2u^i$ , etc., and of course  $u_t = \frac{\partial u}{\partial t}$ .

We will be considering “evolution equations” of the form  $u_t = F(u)$ , where  $F : V \rightarrow V$  should be thought of as a vector field on  $V$ , and its form will be a smooth function (usually polynomial) of the  $u^i$  and their derivatives,  $Du^j, D^2u^k, \dots$ . Usually  $F(u)$  will be the sum of a “dominant” linear differential operator, and a nonlinear part that we can consider as a “small

perturbation” of this linear part. By a linear differential operator on  $V$  we will always mean an operator of the form  $u \mapsto \mathcal{L}(u) = (\mathcal{L}^1(u), \dots, \mathcal{L}^n(u))$  where  $\mathcal{L}^i(u) = \sum_{j=1}^n \mathcal{L}_j^i(D)u^j$ . Here each  $\mathcal{L}_j^i(X)$  is a polynomial with constant coefficients in an indeterminate  $X$ . In the scalar case  $\mathcal{L}(u) = \mathcal{L}(D)u$  and we will often use  $\mathcal{L}(D)u$  to denote  $\mathcal{L}(u)$  in the general case too.

The simplest kind of nonlinear operator that we shall consider is a zero order nonlinear operator, by which we will mean a map of the form  $u \mapsto G(u) = (G^1(u), \dots, G^n(u))$ , where  $G^i(u)(x) = G^i(u^1(x), \dots, u^n(x))$  and  $G^i(Y_1, \dots, Y_n)$  is either a constant coefficient polynomial on  $\mathbf{C}^n$  or more generally an entire function of these variables (i.e., given by a power series that converges for all values of  $(Y_1, \dots, Y_n)$ ). Of course, care must be taken to make sure that if  $u \in V$  then also  $G(u) \in V$ . When we come to the rigorous proofs, we will assume that  $V$  is one of the Sobolev Hilbert spaces  $H^m(\mathbf{R}, U)$  for  $m > \frac{1}{2}$ , and since it is well-known that  $H^m(\mathbf{R}, \mathbf{C})$  is a Banach algebras, it follows easily that  $G$  is a smooth map of  $H^m(\mathbf{R}, U)$  to itself. The most general kind of nonlinearity that we will consider will be one that can be factored into a composition of the form  $M(D)G(u)$  where  $M(D)$  is a linear differential operator as above and  $G(u)$  is a zero order nonlinearity.

If  $L(X) = \sum_{m=1}^{\ell} a_m X^m$  is a complex polynomial, then the differential operator  $L(D)$  is called *formally skew-adjoint* if  $\langle L(D)u_1, u_2 \rangle = -\langle u_1, L(D)u_2 \rangle$  whenever  $u_1$  and  $u_2$  are smooth maps of  $\mathbf{R}$  into  $U$  with compact support. Here  $\langle u, v \rangle$  denotes the  $L^2$  inner product, i.e.,  $\langle u, v \rangle := \int_{-\infty}^{\infty} \langle u(x), v(x) \rangle dx$ . Integration by parts shows that  $D$  is skew-adjoint. Moreover an odd power of a formally skew-adjoint operator (and  $i$  times an even power) is clearly again formally skew-adjoint, so it follows that  $L(D)$  is formally skew-adjoint if and only if the coefficients  $a_m$  are real for  $m$  odd and imaginary for  $m$  even, i.e., if and only if  $L(ik)$  is imaginary for all real  $k$ , and it is this last condition that we shall use.

**Definition** A system of partial differential equation of the form:

$$(WNWE) \quad u_t^i = L^i(D)u^i + M^i G^i(u).$$

is called a *weakly nonlinear wave equation* if:

- 1) Each  $L^i(D)$  is a formally skew-adjoint operator and the polynomials  $L^i(X)$  all have the same degree,  $\ell$ ,
- 2) degree  $M^i(X) < \ell$ ,
- 3)  $G^i(0) = 0$ , so that  $u(x, t) \equiv 0$  is a solution of (WNWE).

In what follows we will denote the minimum difference,  $\ell - \text{degree } M^i(X)$ , by  $q$ . For the most part, we will be dealing with the case  $n = 1$ , in which case we put  $L = L^1$  and  $M = M_1^1$ , so  $\ell = \text{degree } L$  and  $q = \text{degree } L - \text{degree } M$ , and a weakly nonlinear wave equation has the form:

$$(WNWE) \quad u_t = L(D)u + M(D)G(u).$$

Two important examples are the Korteweg-deVries Equation:

$$(KdV) \quad u_t = -u_{xxx} - uu_x = -D^3u - \frac{1}{2}D(u^2),$$

and the Nonlinear Schrödinger Equation:

$$(NLS) \quad u_t = iu_{xx} + i|u|^2u = iD^2u + i|u|^2u.$$

In the former case we have  $L(X) = -X^3$ ,  $M(X) = -\frac{1}{2}X$ ,  $G(X) = X^2$ , and in the latter,  $L(X) = iX^2$ ,  $M(X) = i$ ,  $G(X) = |X|^2X$ .

In the next section we will see that the Sine-Gordon Equation:

$$(SGE) \quad u_{tt} = u_{xx} + \sin u$$

also can be regarded as a weakly nonlinear wave equation.

### The Sine-Gordon Equation

A natural reduction of the linear wave equation to a system of first order PDE is  $\frac{\partial u}{\partial t} = \frac{\partial v}{\partial x}$ ,  $\frac{\partial v}{\partial t} = \frac{\partial u}{\partial x}$ . in fact,  $\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t} \frac{\partial}{\partial x} v = \frac{\partial}{\partial x} \frac{\partial}{\partial t} v = \frac{\partial^2 v}{\partial x^2} u$ .

This suggests that to find a representation of Sine-Gordon as a weakly nonlinear wave equation, we should start with systems of the form  $\frac{\partial u}{\partial t} = \frac{\partial v}{\partial x} + F(u, v)$ ,  $\frac{\partial v}{\partial t} = \frac{\partial u}{\partial x} + G(u, v)$  or  $\frac{\partial}{\partial t}(u, v) = L(u, v) + (F(u, v), G(u, v))$  where  $F$  and  $G$  are entire functions on  $\mathbf{C} \times \mathbf{C}$ , and of course  $F(0, 0) = G(0, 0) = 0$ . We will next show that with appropriate choice of  $F$  and  $G$  we do indeed get Sine-Gordon, and moreover that essentially the only other equations of the form  $u_{tt} = u_{xx} + \Gamma(u)$  that arise in this way are the Klein-Gordon equation,  $u_{tt} = u_{xx} + u$ , and the Sinh-Gordon equation  $u_{tt} = u_{xx} + \sinh u$ .

Starting out as above,  $\frac{\partial^2 u}{\partial t^2} = \frac{\partial}{\partial t}(\frac{\partial v}{\partial x} + F(u, v)) = \frac{\partial}{\partial x} \frac{\partial v}{\partial t} + F_1 \frac{\partial u}{\partial t} + F_2 \frac{\partial v}{\partial t} = \frac{\partial^2 u}{\partial x^2} + (F_1 F + F_2 G) + \frac{\partial u}{\partial x}(G_1 + F_2) + \frac{\partial v}{\partial x}(G_2 + F_1)$ . For the latter to be of the form  $u_{tt} = u_{xx} + \Gamma(u)$  we must have  $\frac{\partial}{\partial v}(F_1 F + F_2 G) = 0$ ,  $G_1 = -F_2$ , and  $G_2 = -F_1$ , in which case  $u_{tt} = u_{xx} + \Gamma(u)$  with  $\Gamma = F_1 F + F_2 G$ .

Next note that these conditions on  $F$  and  $G$  give  $F_{11} = -G_{21} = -G_{12} = F_{22}$ , or in other words,  $F$  is a solution of the one-dimensional wave equation, and hence a sum of a left moving wave and a right-moving wave:  $F(u, v) = h(u+v) + k(u-v)$ . Then using  $G_1 = -F_2$ , and  $G_2 = -F_1$  it follows that  $G(u, v) = k(u-v) - h(u+v)$ , where  $h(0) = k(0) = 0$  in order to make  $F(0, 0) = G(0, 0) = 0$ . The condition  $\frac{\partial}{\partial v}(F_1 F + F_2 G) = 0$  now gives  $\frac{\partial}{\partial v}(h'(u+v)k(u-v) + h(u+v)k'(u-v)) = 0$  or  $h''(u+v)k(u-v) = h(u+v)k''(u-v)$ , or  $\frac{h''(u+v)}{h(u+v)} = \frac{k''(u-v)}{k(u-v)}$ . Since  $u+v$  and  $u-v$  are coordinates, the only way the last relation can hold identically is for both sides to be a constant  $\lambda$ , i.e.  $h'' = \lambda h$  and  $k'' = \lambda k$ .

If  $\lambda$  is negative, say  $\lambda = -\omega^2$ , then since  $h(0) = k(0) = 0$ , it follows that  $h(u) = A \sin(\omega u)$  and  $k(u) = B \sin(\omega u)$ . If we choose  $\omega = \frac{1}{2}$  and  $A = B = 1$  we get  $F(u, v) = \sin(\frac{u}{2} + \frac{v}{2}) + \sin(\frac{u}{2} - \frac{v}{2}) = 2 \sin \frac{u}{2} \cos \frac{v}{2}$  and similarly  $G(u, v) = -2 \cos \frac{u}{2} \sin \frac{v}{2}$ , and this gives the system of partial differential equations  $\frac{\partial u}{\partial t} = \frac{\partial v}{\partial x} + 2 \sin \frac{u}{2} \cos \frac{v}{2}$ ,  $\frac{\partial v}{\partial t} = \frac{\partial u}{\partial x} - 2 \cos \frac{u}{2} \sin \frac{v}{2}$ , and we will leave it to the reader to check that if  $(u, v)$  is a solution of this system, then  $u$  is a solution of the Sine-Gordon equation. (Other choices of  $A, B$ , and  $\omega$  lead to equations that can be transformed to the Sine-Gordon equation by a simple re-scaling of independent and dependent variables. Similarly taking  $\lambda = 0$  gives the Klein-Gordon equation, and  $\lambda$  positive gives Sinh-Gordon.)

While this system of PDE for  $u$  and  $v$  is not in the form (WNWE), if we define  $u^1 = u + v$  and  $u^2 = u - v$ , then  $u^1$  and  $u^2$  satisfy:

$$\begin{aligned} u_t^1 &= +u_x^1 + 2 \sin\left(\frac{u^1}{2} - \frac{u^2}{2}\right), \\ u_t^2 &= -u_x^2 + 2 \sin\left(\frac{u^1}{2} + \frac{u^2}{2}\right). \end{aligned}$$

which is manifestly in the form (WNWE), with  $L^1(X) = D$ ,  $L^2(X) = -D$ , and  $M^i(X) = 1$ , and moreover we can recover  $u$  from  $u^1$  and  $u^2$  by  $u = \frac{u^1 + u^2}{2}$ .

To simplify the exposition, we will from now on assume we are in the scalar case,  $n = 1$  and that  $G$  is a polynomial. The modifications needed for the general case are obvious.

### The Generalized WGMS Method (Heuristics).

Let us assume that for some particular example of (WNEE) we know that there is a unique solution  $u(t)$  with the initial condition  $u(0) \in V$ . Let  $\Delta t$  be close to zero, and let us look for a time-stepping algorithm that, given a sufficiently good approximation to  $u(t)$  as input will produce an approximation to  $u(t') = u(t + \Delta t)$  as output. If we integrate (WNEE) with respect to  $t$ , from  $t$  to  $t'$ , and use the trapezoidal rule to approximate the integrals on the right hand side, we find:

$$\begin{aligned} u(t') - u(t) &= \frac{\Delta t}{2} L(D)[u(t) + u(t')] \\ &\quad + \frac{\Delta t}{2} M(D)[G(u(t)) + G(u(t'))] \end{aligned}$$

or

$$\begin{aligned} (I - dL(D))u(t') &= (I + dL(D))u(t) \\ &\quad + dM(D)[G(u(t)) + G(u(t'))], \end{aligned}$$

which we can rewrite as:

$$u(t') = Cu(t) + B[G(u(t)) + G(u(t'))]$$

where  $d = \frac{\Delta t}{2}$ ,  $B = \frac{dM(D)}{I - dL(D)}$ , and  $C = \frac{I + dL(D)}{I - dL(D)}$  is the Cayley transform of the skew-adjoint operator  $dL(D)$ . We note that the skew-adjointness of  $L(D)$  assures that  $I - dL(D)$  is invertible, and that  $C$  is a unitary operator. In fact, as we shall see shortly, on the Fourier transform side, both  $C$  and  $B$  become simple multiplication operators, whose properties are obvious from those of the polynomials  $L(X)$  and  $M(X)$ .

Next, for each  $u$  in  $V$ , we define a map  $H_u : V \rightarrow V$  by

$$H_u(w) := Cu + B[G(u) + G(w)],$$

and we note that the equation above becomes  $H_{u(t)}(u(t')) = u(t')$ , i.e.,  $u(t')$ , which is what we are trying to compute, is a fixed-point of  $H_{u(t)}$ .

Now, we permit ourselves a little optimism—we assume that  $u(t')$  is in fact a *contracting* fixed point of  $H_{u(t)}$ . If this is so then, for  $\Delta t$  small,  $u(t)$  will be close to  $u(t')$ , and we can expect that iterating  $H_{u(t)}$  starting at  $u(t)$ , will produce a sequence that converges to  $u(t')$ . This the essence of the WGMS time-stepping algorithm (generalized to WNEE).

For this to work as a numerical method, we must be able to compute  $H_u$  efficiently, and that is where the Fourier Transform comes in. Let us write  $\mathcal{F}$  for the Fourier Transform,

mapping  $V$  isomorphically onto  $\hat{V}$ , and  $\mathcal{F}^{-1}$  for its inverse. We define operators  $\hat{C} = \mathcal{F}C\mathcal{F}^{-1}$  and  $\hat{B} = \mathcal{F}B\mathcal{F}^{-1}$  on  $\hat{V}$ . Then  $\mathcal{F}H_u(w) = \mathcal{F}C\mathcal{F}^{-1}\mathcal{F}(u) + \mathcal{F}B\mathcal{F}^{-1}\mathcal{F}[G(u) + G(w)]$ , so we can rewrite  $H_u$  as:

$$H_u(w) = \mathcal{F}^{-1}(\hat{C}\hat{u} + \hat{B}\mathcal{F}[G(u) + G(w)]),$$

where  $\hat{u} = \mathcal{F}(u)$  is the Fourier Transform of  $u$ .

Assuming that we have a good algorithm for computing  $\mathcal{F}$  and  $\mathcal{F}^{-1}$  (e.g., the Fast Fourier Transform), it is now clear that it is easy and efficient to calculate  $H_u$ , and hence to carry out the iteration. Indeed, calculating  $G(u)$  and  $G(w)$  at a point  $x$  is just a matter of evaluating the polynomial  $G$  at  $u(x)$  and  $w(x)$ . And since  $M(X)$  and  $L(X)$  are constant coefficient polynomials, the operators  $\hat{C}$  and  $\hat{B}$  are diagonal in the Fourier basis  $e_k(x) = e^{ikx}$ , i.e., they are multiplication operators, by the rational functions  $\frac{1+dL(ik)}{1-dL(ik)}$  and  $\frac{dM(ik)}{1-dL(ik)}$  respectively. Since  $L(D)$  is by assumption skew-adjoint,  $L(ik)$  is pure imaginary, so the denominator  $1 - dL(ik)$  does not vanish. Moreover the function  $\frac{1+dL(ik)}{1-dL(ik)}$  clearly takes its values on the unit circle, and since  $L(X)$  has degree greater than  $M(X)$ , it follows that while the nonlinearity  $G(w)$  may push energy into the high frequency modes of the Fourier Transform, multiplication by  $\frac{dM(ik)}{1-dL(ik)}$  acts as a low-pass filter, attenuating these high frequency modes and giving the WGMS method excellent numerical stability.

### Proof that $H_u$ is a Contraction.

In this section we will justify the above optimism by showing that, with a proper choice of the space  $V$ , a suitable restriction of the mapping  $H_u$  does indeed satisfy the hypotheses of the Banach Contraction Theorem provided  $\|u\|$  and  $\Delta t$  are sufficiently small. The space we will choose for  $V$  is the Sobolev Hilbert space  $H^m = H^m(\mathbf{S}^1, V)$ , with  $m > \frac{1}{2}$ . We recall that this is the Hilbert space of all functions  $u$  in  $L^2(\mathbf{S}^1, V)$  such that  $\|u\|_m^2 = \sum_k (1+k^2)^{\frac{m}{2}} |\hat{u}(k)|^2$  is finite, where as before,  $\hat{u}(k)$  are the Fourier coefficients of  $u$ .

The principal property of these spaces that we shall need is that  $H^m(\mathbf{S}^1, \mathbf{R})$  is a commutative Banach algebra under pointwise multiplication when  $m > \frac{1}{2}$  (cf. [A], Theorem 5.23, or [P]). As a first consequence, it follows that if  $P : V \rightarrow V$  is a polynomial mapping, then  $u \mapsto P(u)$  is a map of  $H^m$  to itself, and moreover  $\|P(u)\|_m < C \|u\|_m^r$ , where  $r$  is the degree of  $P$ . We will permit ourselves the abuse of notation of denoting this latter map by  $P$ , and it is now elementary to see that it is Frechet differentiable, and in fact that  $DP_u(v) = P'(u)v$ , where  $P'$  is the derivative of  $P$ . (This will follow if we can show that there is an algebraic identity of the form  $P(X+Y) = P(X) + P'(X)Y + Q(X, Y)Y^2$ , for some polynomial  $Q$  in  $X$  and  $Y$ . But it is clearly enough to check this for monomial  $P$ , in which case it is immediate from the binomial theorem.)

Let us denote by  $B_R$  the ball of radius  $R$  in  $H^m$ . Then as an immediate consequence of the preceding remarks we have:

**Proposition 1.** *For any  $R > 0$  there exist positive constants  $C_1$  and  $C_2$  such that for all  $u$  in  $B_R$ ,  $\|G(u)\|_m < C_1$  and  $\|DG_u\| < C_2$ .*

It will be important for us to have a good estimate of how the norm of  $B$  depends on  $\Delta t$ .

**Proposition 2.** *Given  $T > 0$ , there is a positive constant  $C_3$  such that the norm of the operator  $B$  on  $H^m$  satisfies  $\|B\| < C_3 \Delta t^{\frac{\ell}{2}}$ , for all  $\Delta t < T$ , where  $\ell = \text{degree}(L(X))$  and  $q = \text{degree}(L(X)) - \text{degree}(M(X))$ . Thus  $\lim_{\Delta t \rightarrow 0} \|B\| = 0$ .*

PROOF. It is clear that the Fourier basis  $e_k(x) = e^{ikx}$  is orthogonal with respect to the  $H^m$  inner-product (though not orthonormal, except for the case  $H^0 = L^2$ ). Thus, since all constant coefficient differential operators are diagonalized in this basis, we can compute their norms on  $H^m$  by taking the maximum absolute values of their eigenvalues on the  $e_k$ . In the case of  $B$ , we have already seen that these eigenvalues are  $\frac{dM(ik)}{1-dL(ik)}$ . Since  $d = \frac{\Delta T}{2}$ , to prove the proposition it will suffice to show that  $\frac{dM(ik)}{1-dL(ik)} < C_3 d^{\frac{q}{2}}$  for all real  $k$  and all  $d < 2T$ .

Writing  $L(X) = \sum_{j=0}^{\ell} b_j X^j$  and  $M(X) = \sum_{j=0}^{\ell-q} a_j X^j$ , let us define parametric families of polynomials  $L_c$  and  $M_c$  for  $c \geq 0$  by  $L_c(X) = \sum_{j=0}^{\ell} (c^{\ell-j} b_j) X^j$  and  $M_c(X) = \sum_{j=0}^{\ell-q} (c^{\ell-q-j} a_j) X^j$ . Now note that if we define  $\delta = d^{\frac{1}{2}}$  then (since  $\delta^{\ell-j} (\delta X)^j = dX^j$ ) clearly  $L_{\delta}(\delta X) = dL(X)$ , and similarly  $M_{\delta}(\delta X) = \delta^q dM(X)$ , so  $\frac{dM(ik)}{1-dL(ik)} = \delta^q \frac{M_{\delta}(i\delta k)}{1-L_{\delta}(i\delta k)}$ , and to complete the proof it will suffice to show that the family of rational functions  $R_c(x) = \frac{M_c(ix)}{1-L_c(ix)}$  is uniformly bounded for  $0 \leq c \leq (\Delta T/2)^{\frac{1}{2}}$  and  $x$  real. If  $\tilde{\mathbf{R}}$  is the one-point compactification of  $\mathbf{R}$  and we define  $R_c(\infty) = 0$ , then since the denominator of  $R_c(X)$  never vanishes and has degree greater than the numerator, it follows that  $(c, x) \mapsto R(c, x)$  is continuous and hence bounded on the compact space  $[0, (\Delta T/2)^{\frac{1}{2}}] \times \tilde{\mathbf{R}}$ . ■

**Theorem.** *Given  $R > 0$  there exist positive  $r$  and  $T$  such that  $H_u$  is a contraction mapping of  $B_R$  into itself provided that  $u$  is in  $B_r$  and  $\Delta t < T$ . Moreover there is a uniform contraction constant  $K < 1$  for all such  $u$  and  $\Delta t$ .*

PROOF. From Proposition 1 and the definition of  $H_u$  it follows that  $H_u$  is differentiable on  $H^m$  and that  $D(H_u)_v = B \circ DG_v$ . Then, again by Proposition 1,  $\|D(H_u)_v\| < C_2 \|B\|$  for all  $u$  in  $B_R$ , and so by Proposition 2,  $\|D(H_u)_v\| < C_2 C_3 \Delta t^{\frac{q}{2}}$ . Given  $K < 1$ , if we choose  $T < \left(\frac{K}{C_2 C_3}\right)^{\frac{2}{q}}$  then  $\|D(H_u)_v\| < K$  on the convex set  $B_R$  and hence  $K$  is a contraction constant for  $H_u$  on  $B_R$ , and it remains only to show that if we choose  $r$  sufficiently small, and perhaps a smaller  $T$  then  $H_u$  also maps  $B_R$  into itself for  $u$  in  $B_r$ .

But using the definition of  $H_u$  again, it follows that

$$\|H_u(w)\|_m < \|Cu\|_m + \|B\| (\|G(u)\|_m + \|G(w)\|_m),$$

and recalling that  $C$  is unitary on  $H^m$ , it follows from Propositions 1 and 2 that  $\|H_u(w)\|_m < r + 2C_1 C_3 T^{\frac{q}{2}}$ . Thus  $H_u$  will map  $B_R$  into itself provided  $r + 2C_1 C_3 T^{\frac{q}{2}} < R$ , i.e., provided  $r < R$  and  $T < \left(\frac{R-r}{2C_1 C_3}\right)^{\frac{2}{q}}$ . ■

## Numerics.

There are several types of numerical errors inherent in the WGMS algorithm. The first and most obvious is the error in approximating the integral of the right hand side of the equation using the trapezoidal rule.

A second ‘‘truncation’’ error occurs when we stop the fixed point iteration after a finite number of steps.

In actually implementing the WGMS algorithm to solve an initial value program numerically, one usually chooses an integer  $N$  of the form  $2^e$ , and works in the space  $V_N$  of



“band-limited” functions  $u$  whose Fourier coefficients  $\hat{u}(k)$  vanish for  $|k| > N/2$ . Of course,  $V_N$  is in all the Sobolev spaces. If we start with an initial condition  $u_0$  not actually in  $V_N$  then there will be an aliasing error when the initial Fast Fourier Transform projects it into  $V_N$ . Also, since the WGMS method does not rigorously preserve  $V_N$ , there will be further such errors at each time step.

Of course it is important to investigate the magnitude of these various local errors, see how they propagate, and get a bound for the global error.

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