Computational Physics

Problem Solving with Computers

RUBIN H. LANDAU

Professor of Physics
Oregon State University

MANUEL JOSÉ PÁEZ MEJÍA

Professor of Physics
University of Antioquia

Contributors

Hans Kowallik and Henri Jansen

28

Solitons, the KdeV Equation ⊙

In this and the next chapter we look at soliton solutions of nonlinear wave equations. We have marked these chapters as optional because the material is more advanced and the techniques rather subtle. Nevertheless, we recommend that everyone at least read through these chapters because the material is fascinating and because the computer has been absolutely essential in the discovery and understanding of solitons. In recognition of the possible newness of this material to many students, we give additional background and explanatory materials.

28.1 INTRODUCTION

Up until now we have been dealing with *linear* partial differential equations. As is valid for ordinary differential equations, finding analytic solutions of linear equations is simplified by the principle of linear superposition, which tells us that the sum of two solutions is also a solution. When the description of a physical system is made more realistic by including higher-order effects, there frequently result nonlinear effects that may produce some unusual properties (as we are about to see). In most cases the nonlinear equations are no more difficult to solve numerically than linear equations, which is in contrast to trying to solve nonlinear equations analytically.
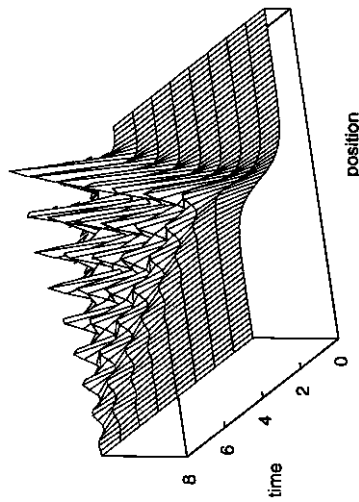
Fig. 28.1 A solution of the KdeV equation describing the behavior of shallow water waves. The single two-level waveform at time zero progressively breaks up into eight solitons as time increases. The taller solitons are then seen to be narrower and faster in their motion to the right.

28.2   PROBLEM: SOLITONS

Your **problem** is to discover whether nonlinear and dispersive systems can support waves with particle-like properties. While a logical response is that systems with dispersion have solutions that broaden in time and thereby lose their identity, consider Fig. 28.1 and the following experimental observation as the **problem** you need to explain. In 1834, J. Scott Russell observed **a** phenomenon on the Edinburgh–Glasgow canal [Russ 44]:

I was observing the motion of a boat which was rapidly drawn along a narrow channel by a pair of horses, when the boat suddenly stopped—not so the mass of water in the channel which it had put in motion; it accumulated round the prow of the vessel in a state of violent agitation, then suddenly leaving it behind, rolled forward with great velocity, assuming the form of a large solitary elevation, a rounded, smooth and well-defined heap of water, which continued its course along the channel apparently without change of form or diminution of speed. I followed it on horseback, and overtook it still rolling on at a rate of some eight or nine miles an hour, preserving its original figure some thirty feet long and a foot to a foot and a half in height. Its height gradually diminished, and after a chase of one or two miles I lost it in the windings of the channel. Such, in the month of August 1834, was my first chance interview with that singular and beautiful phenomenon ....

Russell went on to produce these solitary waves in a laboratory and empirically deduced that their speed c is related to the depth h of the water in the canal and to the amplitude A of the wave by
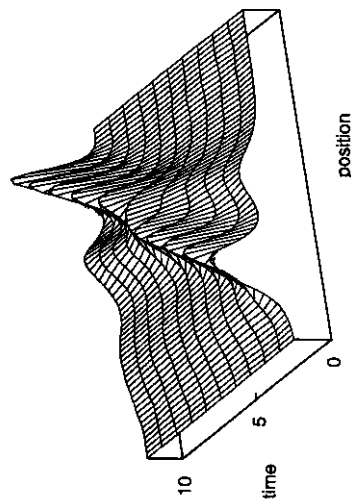
$$c^2 = g(h + A), \qquad (28.1)$$

Fig. 28.2 Two shallow-water solitary waves crossing each other. The taller soliton, on the left at $t = 0$, catches up with the shorter one and overtakes it at $t \simeq 5$. The taller soliton is narrower because a soliton's height times its squared width is approximately constant. The taller soliton is faster because a soliton's height times its squared speed is approximately constant.

where g is the acceleration due to the gravity. Equation (28.1) implies an effect not found for linear systems, namely, that the waves with greater amplitudes travel faster than those with smaller amplitudes. Notice that this is different from *dispersion* in which waves of different wavelengths have different velocities. The former effect is illustrated in Fig. 28.2, where we see a tall soliton catching up with and passing through a short one. Russell also noticed that an initial, arbitrary waveform set in motion in the channel evolves into two or more waves that move at different velocities and progressively move apart until they form individual solitary waves. This effect is illustrated in Fig. 28.1, where we see a single step-like wave breaking up into approximately eight solitons (this shows why these eight solitons are considered the normal modes for this nonlinear systems).

28.3   THEORY: THE KORTEWEG-DE VRIES EQUATION

We want to understand these unusual water waves that occur in shallow, narrow channels such as canals [Abar 93, Tab 89]. The description of this "heap of water" was by [KdeV 95] in terms of the partial differential equation:

$$\frac{\partial u(x,t)}{\partial t} + \varepsilon u(x,t)\,\frac{\partial u(x,t)}{\partial x} + \mu\,\frac{\partial^3 u(x,t)}{\partial x^3} = 0. \qquad (28.2)$$

With a little hindsight it's possible to deduce the basic physics in (28.2)

by inspection. There is a nonlinear term, $\varepsilon u \partial u/\partial t$, where the usual wave equation has a $c\partial u/\partial t$ term. This means that as long as u does not change too much, the waves propagate with a speed proportional to εu. In turn, this means that those parts of the wave that have a larger disturbance u move faster. This can lead to a sharpening of the wave and ultimately a *shock* wave. In contrast, the $\partial^3 u/\partial x^3$ term in (28.2) produces dispersive broadening that, for the proper conditions, can exactly compensate the narrowing caused by the nonlinear term.

Korteweg and deVries (KdeV) solved (28.2) and proved that the speed given by Russell, (28.1), is, in fact, correct. In more recent times, the KdeV equation was rediscovered 70 years later by [Z&K 65] who solved it numerically and discovered that a $\cos x/L$ initial condition broke up into eight solitary waves, similar to that shown in Fig. 28.1. They also found that those parts of the wave with larger amplitudes move faster than do those parts with smaller amplitudes, which is why the higher peaks tend to be on the right in Fig. 28.1. As if wonders never cease, Zabusky and Kruskal also observed from their numerical solution that the faster peaks actually passed through the slower one unscathed, as we can see in Fig. 28.2. Zabusky and Kruskal coined the name *soliton* for the solitary wave, and in the process launched a new branch of mathematics.

Before attempting to solve the KdeV equation, it's valuable to have some inkling of the physics lurking in its assorted parts. We can get that by looking at the equation in the limits in which different terms dominate. We start with the linear wave equation:

$$\frac{\partial u(x,t)}{\partial t} + c\frac{\partial u(x,t)}{\partial x} = 0. \quad (28.3)$$

Here we assign positive propagation velocity c to a wave traveling from left to right. An equation of this sort supports traveling-plane-wave solutions of the form

$$u(x,t) = e^{\pm i(kx - \omega t)}. \quad (28.4)$$

When this $u(x,t)$ is substituted into (28.3), we obtain a *dispersion relation*; that is, a relation between the frequency ω and the wave vector k:

$$\omega = \pm ck, \quad \text{or} \quad \omega^2 = c^2 k^2. \quad (28.5)$$

The second form of (28.5) is fine as long as we remember that $c < 0$ implies a wave traveling from right to left. When a wave obeys a dispersion law such as (28.5), the wave velocity $c = \omega/k$ is independent of frequency ω and we call such wave propagation *dispersionless*.

Let us deduce a wave equation that describes waves traveling with a small amount of *dispersion*; that is, with a frequency that decreases slightly as the
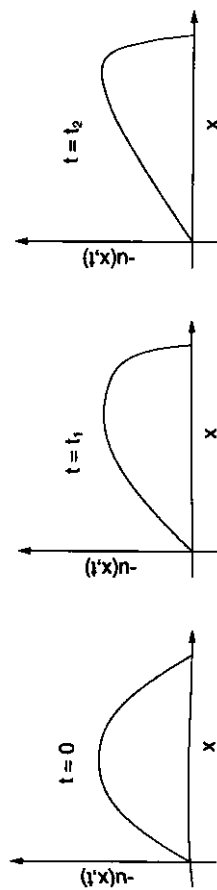
Fig. 28.3   A sketch of a shock wave accumulating as time progresses.

wave number k increases. We postulate

$$\omega^2 \simeq c^2 k^2 - \Gamma k^4, \quad (28.6)$$

where only even powers of k occur to reflect the symmetry in the $\pm x$ direction. There are two forms for the solution:

$$\omega = \pm\sqrt{c^2 k^2 - \Gamma k^4} \simeq \pm ck\left(1 - \frac{\Gamma k^2}{2c^2}\right), \quad (28.7)$$

$$\Rightarrow \quad \omega \simeq \pm ck \mp \beta k^3, \quad (28.8)$$

where β is a constant, and where the upper sign is for waves moving from left to right.

If plane-wave solutions like (28.4) arise from a wave equation, then we see that the ω term of the dispersion relation arises from a first-order time derivative, that the ck term arises from a first-order space derivative, and that the k^3 term arises from a third-order space derivative. As can be verified by substitution, the wave equation needed to produce the dispersion relation (28.8) is

$$\frac{\partial u(x,t)}{\partial t} + c\frac{\partial u(x,t)}{\partial x} + \beta\frac{\partial^3 u(x,t)}{\partial x^3} = 0. \quad (28.9)$$

Already we have a form close to the KdeV equation.

Next let us examine the small $\partial^3 u/\partial x^3$ limit of the the KdeV equation,

$$\frac{\partial u}{\partial t} + \varepsilon u\frac{\partial u}{\partial x} \simeq 0. \quad (28.10)$$

Equation (28.10), which for small u is almost a linear equation, is an equation of the type that produces *shock waves* [Tab 89]. This is sketched in Fig. 28.3 for $\epsilon = -6$. This tells us that the nonlinear term in the KdeV equation introduces the possibility of shock waves into the solution.

28.4 METHOD, ANALYTIC

The trick in analytic approaches to these types of nonlinear equations is to look for steady-state solutions that have the form of a traveling wave; that is, with a specific dependence on x and t:

$$u(x,t) = f(\xi = x - ct).$$ (28.11)

The traveling-wave form (28.11) means that if we move with a constant speed c, we see a constant phase (yet the speed depends on the magnitude of u). There is no guarantee that this form of a solution exists, but if we are lucky, this substitution converts the partial differential equation into an ordinary differential equation that we can solve. If we take the KdeV equation and make the substitution (28.11), we obtain the ODE

$$\frac{d^3 f}{dt^3} - 6f\frac{df}{dt} - c\frac{df}{dt} = 0.$$ (28.12)

While solving this differential equation may still be somewhat of a challenge, mathematicians are good at that sort of thing and have come up with the inverse solution

$$\xi - \xi_0 = \int \frac{df}{\sqrt{2(f^3 + \frac{1}{2}cf^2 + df + e)}},$$ (28.13)

where d and e are integration constants. If we demand as boundary conditions that f, f', and $f'' \to 0$ as $\xi \to \pm\infty$, we can invert (28.13) to obtain the solution

$$u(x,t) = \frac{-c}{2}\operatorname{sech}^2\left[\frac{1}{2}\sqrt{c}(x - ct - \xi_0)\right].$$ (28.14)

We see in (28.14) an amplitude that is proportional to the wave speed c, and a sech^2 function which gives a single lump-like wave. This is a typical mathematical form for a soliton.

28.5 METHOD, NUMERIC: FINITE DIFFERENCE

The KdeV equation is solved numerically using a centered, finite-difference scheme. The time derivative is expressed as a difference centered at t:

$$\frac{\partial u(x,t)}{\partial t} \simeq \frac{u(x,t+\Delta t) - u(x,t-\Delta t)}{2\Delta t},$$ (28.15)

and we solve the equation on a spacetime grid:

$$x = i\Delta x, \quad t = j\Delta t.$$ (28.16)

In terms of the discrete variables, the expansions of $u(x,t+\Delta t)$ and $u(x,t-\Delta t)$ in Taylor series gives

$$\frac{\partial u}{\partial t}(i,j) \simeq \frac{u(i,j+1) - u(i,j-1)}{2\Delta t},$$ (28.17)

where terms of order $\mathcal{O}(\Delta t)^5$ are neglected. Similarly, the x derivative is

$$\frac{\partial u}{\partial x}(i,j) \simeq \frac{u(i+1,j) - u(i-1,j)}{2\Delta x}$$ (28.18)

To approximate $\partial^3 u(x,t)/\partial x^3$, we expand $u(x,t)$ to $\mathcal{O}(\Delta t)^5$ about the four points $u(x \pm 2\Delta x, t)$ and $u(x \pm \Delta x, t)$. A typical expansion is

$$u(x \pm \Delta x, t) \simeq u(x,t) \pm (\Delta x)\frac{\partial u}{\partial x} + \frac{(\Delta x)^2}{2!}\frac{\partial^2 u}{\partial^2 x} \pm \frac{(\Delta x)^3}{3!}\frac{\partial^3 u}{\partial x^3},$$ (28.19)

which we can solve for $\partial^3 u(x,t)/\partial x^3$. Finally, the factor $u(x,t)$ in the second term in (28.2) is taken as the average of the three values centered at (i,j) in a row (for time t or index j):

$$u(i,j) \simeq \frac{u(i+1,j) + u(i,j) + u(i-1,j)}{3}.$$ (28.20)

After substituting all of these expansions, we obtain the finite-difference form of the KdeV equation:

$$\boxed{\begin{aligned}
u(i,j+1) \simeq\ & u(i,j-1) - \frac{\epsilon}{3}\frac{\Delta t}{\Delta x}[u(i+1,j) + u(i,j) + u(i-1,j)] \\
& \times [u(i+1,j) - u(i-1,j)]] - \mu\frac{\Delta t}{(\Delta x)^3} \\
& \times [u(i+2,j) + 2u(i-1,j) - 2u(i+1,j) - u(i-2,j)].
\end{aligned}}$$ (28.21)

To apply this algorithm, we need to know $u(x,t)$ at present and past times to predict future times. We note that the solution for initial time $u(i,1)$ is known for all positions i because the initial condition on $u(x,t=0)$ is some known function of x. To find $u(i,2)$, we use a noncentered scheme in which we expand $u(x,t)$ keeping only two terms for the time derivative:

$$\begin{aligned}
u(i,2) \simeq\ & u(i,1) \\
& -\frac{\epsilon}{6}\frac{\Delta t}{\Delta x}[u(i+1,1) + u(i,1) + u(i-1,1)][u(i+1,1) - u(i-1,1)] \\
& -\frac{\mu}{2}\frac{\Delta t}{(\Delta x)^3}[u(i+2,1) + 2u(i-1,1) - 2u(i+1,1) - u(i-2,1)].
\end{aligned}$$ (28.22)

The keen observer will note that there are still some undefined columns of points, namely, $u(1,j)$, $u(2,j)$, $u(N_{max}-1,j)$, and $u(N_{max},j)$, where N_{max} is the total number of grid points. A simple technique for determining their values is to assume that $u(1,2)=1$ and $u(N_{max},2)=0$. To obtain $u(2,2)$ and $u(N_{max}-1,2)$, assume that $u(i+2,2)=u(i+1,2)$ and $u(i-2,2)=u(i-1,2)$ [avoid $u(i+2,2)$ for $i=N_{max}-1$, and $u(i-2,2)=u(i-1,2)$ for $i=2$]. To carry out these steps, approximate (28.22) so that

$$u(i+2,2)+2u(i-1,2)-2u(i+1,1)-u(i-2,2)\to u(i-1,2)-u(i+1,2). \quad (28.23)$$

The stability condition for this method of solution is

$$\frac{\Delta t}{\Delta x}\left[\epsilon|u|+4\frac{\mu}{(\Delta x)^2}\right]\le 1 \quad \text{(stability)}. \quad (28.24)$$

The truncation error is:

$$\mathcal{E}(u)=O[(\Delta t)^3]+O[\Delta t(\Delta x)^2]. \quad (28.25)$$

These last two equations are illuminating. They show that smaller time and space steps do lead to smaller truncation error, but, as discussed in Chapter 3, Errors and Uncertainties in Computations, not necessarily smaller total error because roundoff error increases with more steps. We also see that a progressive decrease of the space steps, or even of both space and time steps, will ultimately lead to instability. Care and experimentation are clearly required.

28.6   IMPLEMENTATION: KDEV SOLITONS, SOLITON.F (.C)

Modify or run the program given on the diskette and Web that solves the KdeV equation (28.2) for the initial condition:

$$u(x,t=0)=\frac{1}{2}\left[1-\tanh\left(\frac{x-25}{5}\right)\right], \quad (28.26)$$

with parameters $\epsilon=0.2$ and $\mu=0.1$. Start with $\Delta x=0.4$ and $\Delta t=0.1$. These constants are chosen to satisfy (28.24) with $|u|=1$.

1. Define a 2-D array $u(131,3)$ with the the first index corresponding to the position x and the second to the time t. With our choice of parameters, the maximum value for x is $130\times0.4=52$.

2. Initialize the time to $t=0$ and assign values to $u(i,1)$ using (28.26).

3. Assign values to $u(i,2)$, i=3, 4, ..., 129 corresponding to the next time interval. Use (28.22) to advance the time, but note that you cannot start at $i=1$ nor end at $i=131$ because (28.22) would include $u(132,2)$

and (u,132), which are beyond the limits of the array.

4. Increment the time and assume that $u(1,2)=1$ and $u(131,2)=0$. To obtain $u(2,2)$ and $u(130,2)$, assume that $u(i+2,2)=u(i+1,2)$ and $u(i-2,2)=u(i-1,2)$. Avoid $u(i+2,2)$ for i=130, and $u(i-2,2)$ for i=2. To do this, approximate (28.22) so that (28.23) is satisfied.

5. Increment time and compute $u(i,j)$ for j=3 and for i=3, 4, ..., 129, using equation (28.21). Again follow the same procedures to obtain the missing array elements $u(2,j)$ and $u(130,j)$ [set $u(1,j)=1.0$ and $u(131,j)=0$]. As you print out the numbers during the iterations, you will be convinced that it was a good choice.

6. Set $u(i,1)=u(i,2)$ and $u(i,2)=u(i,3)$ for all i. In this way you are ready to find the next $u(i,j)$ in terms of the previous two rows.

7. Repeat the previous two steps some 2000 times. Write your solution out to a file after every ~250 iterations.

28.7   ASSESSMENT: VISUALIZATION

1. Use your favorite graphics tool to plot your results as a 3-D graph of disturbance u versus position and versus time.

2. Observe the wave profile as a function of time and try to confirm Russell's observation that a taller soliton travels faster than a smaller one.

28.8   EXPLORATION: TWO SOLITONS CROSSING

Explore what happens when a tall soliton collides with a short one. Do they bounce off each other? Do they go through each other? Do they interfere? Do they destroy each other? Does the tall soliton still move faster than the short one after collision? (One result we obtained is shown in Fig. 28.2.) Start off by placing a tall soliton of height 0.8 at $x=12$, and a smaller soliton in front of it at $x=26$:

$$u(x,t=0)=0.8\left[1-\tanh^2\left(\frac{3x}{12}-3\right)\right]+0.3\left[1-\tanh^2\left(\frac{4.5x}{26}-4.5\right)\right]. \quad (28.27)$$

The procedure is now similar to the example.

1. The KdeV equation (28.2) now has the constants $\mu=0.1$, $\epsilon=0.2$, $\Delta=0.029$, and the numerical algorithm has step sizes $\Delta x=0.4$, $\Delta t=0.1$.

2. Establish the initial condition (28.27).

3. Try 4000 time steps with printouts every 400 iterations.

28.9   EXPLORATION: PHASE-SPACE BEHAVIOR

Construct phase-space plots of the KdeV equation for various parameter values. Note that only very specific sets of parameters produce solitons. In particular, by correlating the behavior of the solutions with your phase-space plots, show that the soliton solutions correspond to the *separatrix* solutions to the KdeV equation.

28.10   EXPLORATION: SHOCK WAVES

Study the solutions of the simple PDE (28.10) and show that it produces shock waves.

29

Sine–Gordon Solitons ⊙

This chapter extends the optional study of solitons that began in the previous chapter. Here we concentrate on 2-D solitons or *pulsons* as might occur in field-theoretic models for elementary particles, or as disturbances in an non-linear elastic medium. We base our implementations on the work of a number of sources [C&L 81, C&O 78, Argy 91].

29.1   PROBLEM 1: ELEMENTARY PARTICLES FROM FIELD EQUATIONS

For field theory to produce what we normally think of as particles, we need solutions to the field equations that are confined to a region of space for a long time and that do not radiate away their energy. Your **problem** is to see if something as singular and individual as an elementary particle can occur as the solution of a wave equation.

29.2   THEORY: PULSON BEHAVIOR OF CIRCULAR RING SOLITONS

There arises in field theories the wave equation for mesons:

$$\nabla^2 u(\mathbf{x}, t) - \frac{\partial^2 u(\mathbf{x}, t)}{\partial t^2} = m^2 u(\mathbf{x}, t) + g^2 u^3(\mathbf{x}, t). \tag{29.1}$$