LATTICE MODELS

Martin A. Guest

Lattice models are examples of systems of ordinary differential equations. They appear naturally in physics and they provide very good experimental material for mathematics. We shall use them to illustrate some standard (and less standard) mathematical techniques for solving differential equations. At the same time we shall consider some philosophical questions:

What kinds of differential equations are there?

For example, it is well known that linear equations behave very differently to nonlinear equations. But are there other qualities that can be used to distinguish different types of differential equations ?

How can geometry (differential geometry, manifold theory) be used to study and solve differential equations?

The Euclidean geometry of $\mathbf{R}^n$ is obviously relevant. But what about other manifolds and other Riemannian metrics, or more sophisticated geometrical structures?

Is there a way to recognise or visualize the "integrability" of differential equations?

For example, when the solution is a curve in $\mathbf{R}^2$ or $\mathbf{R}^3$, we can visualize it directly. Sometimes we can "see " analytic properties of the solution, such as whether it is bounded or smooth. But how about solutions in higher dimensional Euclidean space, or in more complicated manifolds?

We shall not answer these vague and difficult questions in the lectures. But we shall use lattice models to illustrate that the questions are important, and to give some partial answers.

Many of the examples mentioned in the lectures can be found in 3D-XplorMath ([3DXM]). Alternatively, many of them can be produced "by hand" using software such as Maple,

NCTS-NSF Workshop on Differential Equations, Surface Theory, and Mathematical Visualization, NCTS Taiwan, February-March 2003

Mathematica, or Matlab.

We shall use the following terminology:

[3DXM:ODE:ODE(1D):X] means: in the 3D-XplorMath software, in the ODE category, in the ODE(1D) subcategory, look at — or make some choices for — the object called X.

PROBLEM means: something to think about. It may be easy or hard; computers may or may not be helpful.

PROJECT means: a computer project, to be done using software such as Maple, Mathematica, or Matlab.

§1 The differential equation zoo

Before discussing lattice models, we shall look at some simpler systems of ordinary differential equations.

Systems of linear equations.

Consider the system

$$y_1' = ay_1 + by_2$$
$$y_2' = cy_1 + dy_2$$

of two linear first order differential equations for the (real) functions $y_1(t), y_2(t)$, where a, b, c, d are (real) constants. In matrix form we can write this system as $Y' = AY$, where

$$Y = \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}, \quad A = \begin{pmatrix} a & b \\ c & d \end{pmatrix}.$$

The unique solution with $y_1(0) = \alpha, y_2(0) = \beta$ can be written down very tidily as

$$Y = e^{tA} \begin{pmatrix} \alpha \\ \beta \end{pmatrix}.$$

A more computational, and more informative, method is to make a linear change of variables:

$$Z = PY$$

where P is an invertible 2×2 matrix. We obtain

$$Z' = PAP^{-1}Z,$$

and we can choose the matrix P so that PAP^{-1} has the simplest possible form. For example, if A is symmetric ($A^t = A$), then, by linear algebra, we may choose P such that PAP^{-1} is diagonal. This reveals a little bit of geometry, as the columns v_1, v_2 of the matrix P^{-1} are the eigenvectors of the original matrix A:

$$P^{-1} = \begin{pmatrix} | & | \\ v_1 & v_2 \\ | & | \end{pmatrix} \quad \text{satisfies} \quad AP^{-1} = P^{-1} \begin{pmatrix} \lambda_1 & 0 \\ & \\ 0 & \lambda_2 \end{pmatrix} = \begin{pmatrix} | & | \\ \lambda_1 v_1 & \lambda_2 v_2 \\ | & | \end{pmatrix}$$

The directions of these eigenvectors are visible if one looks at the graphs of the curves $(y(t), y'(t))$ in (y_1, y_2)-space.

[3DXM:ODE:ODE(2D)-1st Order:USER]

Note that a second order equation

$$y'' + py' + qy = 0$$

gives rise to a system of the above type, by the standard device of introducing $y_1 = y$, $y_2 = y'$, so that

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -q & -p \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}.$$

In particular, the famous equation $y'' = -ky$ (with $k > 0$) can be solved this way. It has $y = \sin\sqrt{k}t$ and $y = \cos\sqrt{k}t$ as independent solutions. In both cases, however, the graph of the curve $(y(t), y'(t))$ is a circle, and the eigenvectors cannot be "seen", because they are not real (the matrix A is not symmetric).

The different possibilities are determined by the Jordan normal form of the matrix A: for any A, we can find P with

$$PAP^{-1} = \begin{pmatrix} \lambda_1 & \mu \\ 0 & \lambda_2 \end{pmatrix},$$

and the different kinds of pictures correspond to (1) $\mu = 0$ and λ_1, λ_2 real, (2) $\mu = 0$ and $\lambda_1, \lambda_2 = \bar{\lambda}_1$ non-real, (3) $\mu \neq 0$, $\lambda_1 = \lambda_2$, all real.

Slightly more interesting pictures appear when one looks at the graphs of solutions $Y(t)$ of the second order system

$$Y'' = AY.$$

This is of course equivalent to a four-dimensional first order system, and there is a unique solution when the initial values of Y and Y' are specified.

[3DXM:ODE:ODE(2D)-2nd Order:USER]

PROBLEM: Explain these pictures !

The equation $y'' = -ky$ represents simple harmonic motion in physics, and an idea from physics leads to another method of solving the equation. Namely, if we define

$$K = \frac{1}{2}y'^2 \quad \text{(kinetic energy)}$$
$$U = \frac{k}{2}y^2 \quad \text{(potential energy)}$$

then we see that the total energy (or Hamiltonian) $H = K + U$ is a "conserved quantity":

$$\frac{d}{dt}K = y'y'' + kyy' = y'(-ky) + kyy' = 0.$$

That is, if y is a solution of the diffferential equation, then H is constant, i.e. $\frac{1}{2}y'^2 + \frac{k}{2}y^2 = C$ for some C. But then we have a *first* order equation which can be solved directly by integration (by "quadrature").

Generalizing this to the system $Y'' = AY$, we see that

$$H = \frac{1}{2}y_1'^2 + \frac{1}{2}y_2'^2 + U$$

is a conserved quantity if $ay_1 + by_2 = -\frac{\partial U}{\partial y_1}$ and $cy_1 + dy_2 = -\frac{\partial U}{\partial y_2}$. This condition is satisfied if $b = c$ (i.e. A is symmetric), in which case $U = -\frac{1}{2}(ay_1^2 + 2by_1y_2 + dy_2^2)$.

We can look for conserved quantities for any system of equations, even when there is no obvious physical quantity that seems likely to be conserved, and even when the system itself has no obvious physical meaning. (If this direction of thinking does not worry you, you are a mathematician!) We can go on to ask whether it is possible to have more than one conserved quantity, and, if so, how many essentially different ones.

PROBLEM: How many conserved quantities can the system $Y'' = AY$ have?

We shall see that systems of nonlinear equations offer more challenging problems.

Systems of nonlinear equations.

The pendulum equation $y'' = -k\sin y$ is a familiar example of a nonlinear equation from physics.

[3DXM:ODE:ODE(1D)-2nd Order:Pendulum] or

[3DXM:ODE:ODE(2D)-1st Order:Pendulum]

For small values of y, $\sin y$ is near to y, so the situation is similar to the case of $y'' = -ky$. For general y, the total energy $H = \frac{1}{2}y'^2 - k\cos y$ is a conserved quantity, so we can reduce

the equation to a first order equation and then express the solution as an integral. (The integral gives an elliptic function, but we have no objections to this.)

More generally, consider the system

$$y_1'' = F_1(y_1, y_2)$$
$$y_2'' = F_2(y_1, y_2)$$

where F_1, F_2 are (not necessarily linear) functions. In this situation

$$H = \frac{1}{2}{y_1'}^2 + \frac{1}{2}{y_2'}^2 + U$$

is a conserved quantity if $F_1(y_1, y_2) = -\frac{\partial U}{\partial y_1}$ and $F_2(y_1, y_2) = -\frac{\partial U}{\partial y_2}$. A necessary condition for the existence of such a function U is $\frac{\partial F_1}{\partial y_2} = \frac{\partial F_2}{\partial y_1}$. If F_1, F_2 are defined on the entire (y_1, y_2)-plane $\mathbf{R}^2$ (or more generally, on a simply connected region containing the solutions in question), this condition is sufficient for the existence of U.

Unfortunately it is hopeless to expect conserved quantities in general. This is easy to believe, but not easy to prove. In fact, the existence of systems with no conserved quantities is related to the existence of "chaotic" systems, such as the famous Lorenz attractor.

[3DXM:ODE:ODE(3D)-1st Order:Lorenz]

We shall not discuss chaotic systems, except to say that they are the opposite extreme from systems with many conserved quantities. It is important to keep in mind that "chaotic" is not the same as "nonlinear" (the pendulum is an example of a nonlinear system which has "many conserved quantities").

If one looks at the graphs of solutions $Y(t)$ of the second order nonlinear system

$$Y'' = AY + \text{ nonlinear term}$$

one can see how the nonlinear term disturbs the simple geometry of the linear case.

[3DXM:ODE:ODE(2D)-2nd Order:USER]

PROBLEM: How are the pictures affected by whether the "potential function" U exists?

Other candidates for conserved quantities.

Let us return to the linear system $Y'' = AY$, briefly. We shall assume that $A = A^t$, so that PAP^{-1} is diagonal, with eigenvalues λ_1, λ_2, for a certain matrix P. We have seen that the total energy H is a conserved quantity. It can be written

$$H = \frac{1}{2}\begin{pmatrix} y_1' & y_2' \end{pmatrix}\begin{pmatrix} y_1' \\ y_2' \end{pmatrix} - \frac{1}{2}\begin{pmatrix} y_1 & y_2 \end{pmatrix}\begin{pmatrix} a & b \\ b & d \end{pmatrix}\begin{pmatrix} y_1 \\ y_2 \end{pmatrix} = \frac{1}{2}{Y'}^t Y' - \frac{1}{2}Y^t AY$$

and when we make the change of variables $Y = P^{-1}Z$ we obtain

$$H = \frac{1}{2}Z'^t Z' - \frac{1}{2}Z^t PAP^{-1}Z = \frac{1}{2}Z'^t Z' - \frac{1}{2}Z^t \begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} Z.$$

Since

$$\begin{pmatrix} \lambda_1 & 0 \\ 0 & \lambda_2 \end{pmatrix} = \begin{pmatrix} \lambda_1 & 0 \\ 0 & 0 \end{pmatrix} + \begin{pmatrix} 0 & 0 \\ 0 & \lambda_2 \end{pmatrix}$$

we have a very natural decomposition of H as

$$H = H_1 + H_2 = \frac{1}{2}(z_1'^2 - \lambda_1 z_1^2) \; + \; \frac{1}{2}(z_2'^2 - \lambda_1 z_2^2).$$

Both H_1 and H_2 are conserved quantities as well: we have decomposed the problem $Y'' = AY$ into two separate problems $z_i'' = \lambda_1 z_i$, $i = 1, 2$, and the total energy of each of these separate problems is conserved. This decomposition is called the decomposition into *normal modes.* The system is said to be in the i-th mode if $z_j \equiv 0$ for all $j \neq i$. (A typical solution of the system can be regarded as being in a combination of the normal modes.) The conserved quantity $H_i = \frac{1}{2}(z_i'^2 - \lambda_i z_i^2)$ is called the *energy of the i-th normal mode.*

Now, this kind of separation will not be possible for a nonlinear system such as $Y'' = AY +$ nonlinear term. (Indeed, it is not possible even for the *linear* system $Y'' = AY$ for a general matrix A.) As a slight generalization of the linear case, let us consider the system $Y'' = -\nabla U$ where

$$-2U \quad = \quad ay_1^2 + 2by_1y_2 + dy_2^2 \quad + \quad ey_1^3 + fy_1^2y_2 + gy_1y_2^2 + hy_2^3$$

(thus the nonlinear term in the differential equation is quadratic). A linear change of variable in this case cannot be expected to decompose both the quadratic term *and* the cubic term of U in an equitable way.

One way around this difficulty is to forget the analysis of the linear case, and divide up the total energy in any reasonably symmetrical way, for example

$$H_1 = \frac{1}{2}y_1'^2 + ay_1^2 + by_1y_2 + y_1(ey_1^2 + \frac{1}{2}fy_1y_2 + \frac{1}{2}gy_2^2)$$
$$H_2 = \frac{1}{2}y_2'^2 + by_1y_2 + dy_2^2 + y_2(\frac{1}{2}fy_1^2 + \frac{1}{2}gy_1y_2 + hy_2^2)$$

If we are lucky, H_1 and H_2 will be conserved quantities. If not, we can ask how H_1 and H_2 they vary, for example whether they satisfy diffferential equations which are simpler than the original system.

An interesting aspect of this "artificial" procedure is that, if we are dealing with a solution in which y_1, y_2 remain small, then the contributions of the nonlinearity (the cubic terms of H_1, H_2) are very small indeed. So the question of how to divide up the cubic

terms of H might be irrelevant, and we may as well use the same H_1, H_2 as in the linear case, i.e. the energies of the normal modes:

$$H_1 = \frac{1}{2}({z_1'}^2 - \lambda_1 z_1^2)$$
$$H_2 = \frac{1}{2}({z_2'}^2 - \lambda_1 z_2^2).$$

PROJECT 1: Use a computer to study the following questions. In each case, consider whether the solution Y remains small or not. Take A to be a 2×2 or 3×3 matrix. (1) Let A be a matrix which is *not* symmetric. Consider the system $Y'' = AY$ for several such A. What happens to the energies $H_i = \frac{1}{2}({z_i'}^2 - \lambda_i z_i^2)$ of the normal modes? (2) Let A be a symmetric matrix. Consider some examples of systems of the form $Y'' = AY +$ nonlinear term. What happens to the energies $H_i = \frac{1}{2}({z_i'}^2 - \lambda_i z_i^2)$ of the normal modes? $\square$

Without any experimental evidence or physical intuition, it is difficult to guess what will happen, as various scenarios are plausible. The energies of the normal modes might remain approximately constant, or they might vary in a simple and predictable way, or one of them might eventually dominate the others, or they might vary "randomly", etc. In any case, the kind of behaviour should reflect some underlying mathematical structure of the system.

There are various factors to consider when we perform computer experiments to observe the energies of the normal modes:

(i) Accidental mathematical (or physical) special features of the particular system.

(ii) The accuracy of the approximation of the nonlinear system by the linear system (and the accuracy of the approximation of the respective normal modes).

(iii) Numerical error in the computer calculations.

(iv) The possibility of misinterpretation of the experimental results (e.g. by running the experiment for too short a time).

In other words, we have to be very careful.

The Fermi-Pasta-Ulam experiment.

Physical intuition was the driving force in the experimental calculations of Fermi, Pasta and Ulam when they used one of the first electronic computers, in 1954, to investigate the behaviour of the energies of the normal modes of a certain nonlinear system of differential equations. Their system was a model for a collection of particles, and they expected that the effect of the nonlinearity would be "thermalization": the energies of the normal modes vary unpredictably at first, but eventually they all settle down (roughly speaking) to the

same stable value. This is the kind of "random" behaviour expected in thermodynamics, at least.

But it did not happen!

The energies of the normal modes varied in a complicated way, but certainly not randomly. The experimenters found this behaviour amazing, and could not explain it. Over the next 20 years, a tremendous amount of mathematics was discovered in attempts to understand the situation. A detailed historical account of this story, and how it led to such an unexpected mathematical revolution, can be found in [We].

In the next section we will introduce the Fermi-Pasta-Ulam system and various related "lattice models".

§2 Lattice models

The motion of a collection of N particles, interconnected by springs, is governed by Newton's equations, a system of second order ordinary differential equations for N functions $y_1, \ldots, y_N$. If the springs satisfy Hooke's law, the system is linear; it can be written in the form $Y'' = AY$ for some matrix A, and the matrix is necessarily symmetric. In general, when Hooke's law does not hold, additional nonlinear terms are present.

This kind of system (linear or nonlinear) is called a lattice model. It differs from the examples in §1 only because of its physical interpretation: we are tempted to take N to be large, and to think of a "lattice" of particles.

We shall consider a one-dimensional lattice, where N particles of unit mass lie on a straight line, and we shall denote their positions by

$$Y_1(t),\ Y_2(t),\ \ldots,\ Y_N(t)$$

at time t.

We shall assume that the force in the spring connecting Y_i to Y_{i+1} depends upon the extension of the spring from an equilibrium position of the whole lattice in which $Y_i = e_i$. Let $y_i = Y_i - e_i$ be the displacement of Y_i from its equilibrium position e_i. Then the extension of the spring at time t is $y_{i+1}(t) - y_i(t)$, and our assumption can be written

$$\text{force on } Y_i \text{ from the spring connecting } Y_i \text{ to } Y_{i+1} \ = \ T(y_{i+1} - y_i)$$

for some function T (we assume the same function T applies to all springs). The force on Y_{i+1} from the same spring will be $-T(y_{i+1} - y_i)$.

When $1 < i < N$, Newton's equation for Y_i is

$$(Y_i'' =)\ y_i'' = T(y_{i+1} - y_i) - T(y_i - y_{i-1}),$$

and in the special case when Hooke's law holds, so that $T(y) = ky$ for some positive constant k, it is

$$y_i'' = ky_{i-1} - 2ky_i + ky_{i+1}.$$

For the cases $i = 1$ and $i = N$, the equations are similar, but with appropriate "boundary conditions" (which we shall discuss later).

For the initial positions we take $y_i(0) = a_i$, with $e_1 + a_1 < e_2 + a_2 < \cdots < e_N + a_N$. For the initial velocities we take $Y_i'(0) = y_i'(0) = v_i$. Of course we might modify our assumptions later, but for the moment we are thinking of the motion of a one-dimensional string of particles after it has been disturbed slightly from an equilibrium position. Intuition suggests that the particles will move in a complicated way, but not very far from the equilibrium position — if the initial velocities are small, and if $T(y)$ is approximately ky.

In this situation, it seems very plausible that "thermalization" will occur: when N is large, the interactions will be so complicated that, eventually, the particles will all be jiggling slightly in a very similar fashion. After a sufficiently long time, any unusually active particle will be "damped" by its neighbours.

Of course, in the linear case, this does not happen. From §1, we know (as the coefficient matrix A is symmetric) that the motion of the string will be simple harmonic motion in disguise. But in the nonlinear case, the interactions should be truly complicated. This was the motivation for the experiment of Fermi, Pasta and Ulam (and in fact their goal was to measure the rate of thermalization — they were confident that thermalization would occur!)

[3DXM:ODE:Lattice Models:FERMI-PASTA-ULAM,USER]

PROJECT 2: Write a program to carry out the Fermi-Pasta-Ulam experiment. In that experiment, the function T was $T(y) = y + 0.3y^2$, but you can try other functions as well. You can vary the parameter 0.3 too. You can try various boundary conditions, for example $y_1 = y_N = 0$ or $y_1 = y_N$. □

To formulate precise questions about such lattices, let us consider first some examples where just two particles move.

Two particles, free ends.

In this case the equations are

$$y_1'' = T(y_2 - y_1)$$
$$y_2'' = -T(y_2 - y_1)$$

and these are equivalent to the simpler system

$$(y_1 + y_2)'' = 0$$
$$(y_1 - y_2)'' = 2T(y_2 - y_1).$$

Let assume that $T(y) = ky+$ nonlinear terms. The matrix system is

$$\begin{pmatrix} y_1 + y_2 \\ y_1 - y_2 \end{pmatrix}'' = \begin{pmatrix} 0 & 0 \\ 0 & -2k \end{pmatrix} \begin{pmatrix} y_1 + y_2 \\ y_1 - y_2 \end{pmatrix} + \text{ nonlinear terms}$$

and a suitable coordinate change is $z_1 = y_1 + y_2, z_2 = y_1 - y_2$. The energies H_1, H_2 of the normal modes are defined as in §1.

For example, in the case $T(y) = ky$, the general solution is

$$y_1 + y_2 = At + B, \quad y_1 - y_2 = C\cos\sqrt{2k}t + D\sin\sqrt{2k}t$$

We can identify two special kinds of solution:

(1) $y_1 + y_2 = At + B, \quad y_1 - y_2 = 0$

This is motion in the first normal mode. The distance between the particles remains constant ($Y_2 - Y_1 = e_2 - e_1 + y_2 - y_1 = e_2 - e_1$) and the whole spring slides along the line, with constant velocity.

(2) $y_1 - y_2 = C\cos\sqrt{2k}t + D\sin\sqrt{2k}t, \quad y_1 + y_2 = 0$

This is motion in the second normal mode. The centre of the spring remains fixed, and the particles move with equal and opposite simple harmonic motion. Evidently

$$H_1(t) = \text{ constant } \times A^2$$
$$H_2(t) = \text{ constant } \times k(C^2 + D^2)$$

and these are indeed independent of t — they are conserved quantities of the linear system.

As a nonlinear example, let $T(y) = \sin y$. Then we may choose $z_1 = y_1 + y_2$, $z_2 = y_1 - y_2$ as before. We have $y_1 + y_2 = At + B$ as in the previous example. But $y_1 - y_2$ is more complicated, and H_2 is not independent of t. (Nevertheless, H_2 is a periodic function — it behaves "predictably"— and for small values of $y_1 - y_2$ it is approximately constant.)

Four particles, both ends fixed.

Consider Y_0, Y_1, Y_2, Y_3 with $Y_0(t) = e_0$, $Y_1(t) = e_1$ for all t. In this case the equations for the middle two particles are

$$y_1'' = T(y_2 - y_1) - T(y_1 - y_0)$$
$$y_2'' = T(y_3 - y_2) - T(y_2 - y_1)$$

with $y_0 = y_3 = 0$. In the linear case ($T(y) = ky$) we obtain

$$y_1'' = -2ky_1 + ky_2$$
$$y_2'' = ky_1 - 2ky_2.$$

i.e.

$$(y_1 + y_2)'' = -k(y_1 + y_2)$$
$$(y_1 - y_2)'' = -3k(y_1 - y_2).$$

The normal mode solutions are

(1) $y1 + y_2 = A\cos\sqrt{k}t + B\sin\sqrt{k}t, \quad y_1 - y_2 = 0$

(2) $y_1 - y_2 = C\cos\sqrt{3k}t + D\sin\sqrt{3k}t, \quad y_1 + y_2 = 0$

and the general solution is a linear combination of the two; it can be described as simple harmonic motion of frequency $\sqrt{k}$ with a simple harmonic forcing term of frequency $\sqrt{3}k$ (or vice versa).

A comparison.

In both of the above examples, for any function T (assumed smooth on $\mathbf{R}^2$), we have a system of the form

$$y_1'' = F_1(y_1, y_2)$$
$$y_2'' = F_2(y_1, y_2)$$

with $\frac{\partial F_1}{\partial y_2} = \frac{\partial F_2}{\partial y_1}$. Therefore we have a total energy function H, and this is a conserved quantity. In both examples, when $T(y) = ky$, we have $H = H_1 + H_2$, and the energies H_1, H_2 of the normal modes are also conserved quantities. But when T is nonlinear, there is an important difference. In the first example, H_1 is a conserved quantity, hence $H - H_1$ is also a conserved quantity (but not H_2). In the second example, neither H_1 nor H_2 is a conserved quantity, in general; the existence of other conserved quantities (besides H) is not clear.

Examples of systems of N particles.

Let us return to the situation of a large number of particles. We shall generalize the second example above by considering $N + 2$ particles, with the end particles fixed:

$$y_1'' = T(y_2 - y_1) - T(y_1)$$
$$y_2'' = T(y_3 - y_2) - T(y_2 - y_1)$$
$$\cdots$$
$$y_{N-1}'' = T(y_N - y_{N-1}) - T(y_{N-1} - y_{N-2})$$
$$y_N'' = T(-y_N) - T(y_N - y_{N-1})$$

Let us assume that the initial velocities are all zero, and that the initial positions are given by the "shape function" $s : \{1, \ldots, N\} \to \mathbf{R}$, $s(i) = y_i(0) = a_i$.

We shall consider the following four forces:

(I) $T(y) = y$ (linear case)

(II) $T(y) = y + 0.3y^2$ (Fermi-Pasta-Ulam)

(III) $T(y) = y + 100y^3 + 5y^4 + 5y^5$ ("arbitrary" nonlinear case)

(IV) $T(y) = 1 - e^{-y} = y - \frac{1}{2}y^2 + \frac{1}{6}y^3 - \ldots$ (Toda)

[3DXM:ODE:Lattice Models:USER,FERMI-PASTA-ULAM,USER,TODA ...

When N is large, computer simulations of the motion of the lattice are not very revealing. All four examples seem to exhibit similar behaviour. It is more useful to plot the positions of the particles on a vertical axis, using the horizontal axis to list the particles.

... ACTION:SET LATTICE PARAMETERS:TRANSVERSE DISPLAY ...

The initial positions of the particles are indicated by the graph of the shape function s in this case. Defining $s(0) = s(N + 1) = 0$ corresponds to fixing the ends of the lattice.

... ACTION:SET LATTICE PARAMETERS:INITIAL SHAPE,ZERO BOUNDARY CONDITION]

The energies $H_1, \ldots, H_N$ of the normal modes can be indicated in a similar way. In case (1) they remain constant of course (the values being determined by the initial conditions). In cases (2)-(4) they do not remain constant. But there is a significant diffference between case (3) and cases (2),(4): in the latter two cases, the normal modes appear to be approximately periodic. This is the phenomenon that Fermi, Pasta and Ulam found surprising.

Before we try to analyse these different kinds of nonlinear behaviour, let us briefly dispose of the linear case, (1). Only the messiness of the explicit solutions distinguishes this from the case $N = 2$ — the system behaves like N simple harmonic oscillators, which are uncoupled by the normal coordinates. First, the matrix form $Y'' = AY$ of the system is

$$\begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \cdots \\ y_N \end{pmatrix}'' = \begin{pmatrix} -2 & 1 & 0 & \cdots & 0 \\ 1 & -2 & 1 & \cdots & 0 \\ 0 & 1 & -2 & \cdots & 0 \\ \cdots & \cdots & \cdots & \cdots & \cdots \\ 0 & 0 & 0 & \cdots & -2 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ \cdots \\ y_N \end{pmatrix}$$

An orthogonal matrix P^{-1} whose columns are eigenvectors of A is

$$\sqrt{\tfrac{2}{N+1}}\begin{pmatrix} \sin p & \sin 2p & \sin 3p & \cdots & \sin Np \\ \sin 2p & \sin 4p & \sin 6p & \cdots & \sin 2Np \\ \sin 3p & \sin 6p & \sin 9p & \cdots & \sin 3Np \\ \cdots & \cdots & \cdots & \cdots\cdots & \\ \sin Np & \sin 2Np & \sin 3Np & \cdots & \sin N^2p \end{pmatrix}$$

where $p = \pi/(N+1)$. Note that $P^t = P$, so we have $P = P^{-1} = P^t$. The change of variables $Z = PY$ is

$$z_i = \sqrt{\tfrac{2}{N+1}} \sum_{j=1}^{N} y_j \sin pji$$

The eigenvalues are

$$\lambda_l = 4\sin^2 \frac{lp}{2} = 2\cos lp - 2 = 2\cos\frac{l\pi}{N+1} - 2, \quad l = 1, \ldots, N.$$

Motion in the l-th normal mode is represented by the following solution:

$$z_l = A_l \cos(2t \sin\frac{lp}{2}) + B_l \sin(2t\sin\frac{lp}{2}), \quad z_i = 0 \text{ if } i \neq l.$$

Since we assume $z_l'(0) = 0$, we have $B_l = 0$. Hence

$$\begin{aligned} y_i &= \sqrt{\tfrac{2}{N+1}} \sum_{j=1}^{N} z_j \sin pji \\ &= \sqrt{\tfrac{2}{N+1}}\, A_l \cos(2t\sin\frac{lp}{2}) \sin lpi \\ &= a_i \cos(2t\sin\frac{lp}{2}) \end{aligned}$$

(using the initial condition $y_i(0) = a_i$). Thus, "motion in the l-th normal mode" means that the i-th particle moves with simple harmonic motion of frequency $2\sin\frac{lp}{2}$ and amplitude a_i.

Remark: It is tempting to regard the function $y(i,t) = y_i(t)$ as a "wave" which satisfies the "wave equation" $\partial^2 y/\partial t^2 = \partial^2 y/\partial i^2$, where $\partial^2 y/\partial i^2$ is interpreted as $(y_{i+1} - y_i) - (y_i - y_{i-1})$. It is then natural to use "separation of variables" by trying a solution like $y_i = \sin\alpha i \cos\beta t$. Substituting in the equation, we obtain $\beta^2 = 4\sin^2\frac{\alpha}{2}$. Hence $y_i = \sin\alpha i\cos(2t\sin\alpha)$ is a solution for any α.

§3 The Toda lattice

After the linear case (I), the example which has been most thoroughly investigated is case (IV), the Toda lattice. It was introduced by M. Toda around 1967 (see [To1], [To2]), using a force of the form $T(y) = \alpha(e^{\beta y} - 1)$.

N particles, free ends.

Newton's equations become

$$\begin{aligned} y_1'' &= \alpha e^{\beta(y_2 - y_1)} - \alpha \\ y_i'' &= \alpha e^{\beta(y_{i+1} - y_i)} - \alpha e^{\beta(y_i - y_{i-1})}, \quad 2 \le i \le N-1 \\ y_N'' &= -\alpha e^{\beta(y_N - y_{N-1})} + \alpha \end{aligned}$$

Several remarks are appropriate at this point.

(i) The same equations hold with Y_i instead of y_i.

(ii) Deleting the terms $-\alpha, \alpha$ in the equations for y_1, y_N corresponds to adding a constant "outwards" force of magnitude $-\alpha$ to the first and last particles.

(iii) Replacing y_i by $\lambda y_i + i\mu$ has the effect of replacing α by $e^{\mu}\alpha/\lambda$ and β by $\lambda\beta$. We can rescale α and β by arbitrary positive numbers or by arbitrary negative numbers this way.

By taking $\alpha = \beta = -2$, deleting the constant terms, and replacing $y_1, \ldots, y_N$ by $q_1, \ldots, q_n$, we obtain the following modification (which will be extremely convenient for our calculations). This is usually called "the open Toda lattice" or "the open Toda molecule".

$$\begin{aligned} q_1'' &= -2e^{2(q_1 - q_2)} \\ q_i'' &= -2e^{2(q_i - q_{i+1})} + 2e^{2(q_{i-1} - q_i)} \quad i = 2, \ldots, n-1 \\ q_n'' &= \qquad\qquad 2e^{2(q_{n-1} - q_n)}. \end{aligned}$$

In view of the above remarks, we have made only one serious change: we have introduced an additional (constant) force which will cause the whole lattice to expand. From the differential equation point of view, we are considering an inhomogeneous system instead of a homogeneous one.

The case $n = 2$ is easy to solve "by hand". We have $(q_1 + q_2)'' = 0$ so $q_1 + q_2 = At + B$ (as in §2). It is natural to choose $A = B = 0$; this corresponds to fixing the centre of mass of the spring at the origin. So we can put $q = q_1 = -q_2$ and we have to solve $q'' = -2e^{4q}$. Let us impose the initial conditions $q(0) = a$, $q'(0) = 0$. The quantity $q'^2 + e^{4q}$ is conserved, so we can put $q'^2 + e^{4q} = C$ and integrate to obtain (eventually) $q(t) = a - \frac{1}{2}\log\cosh(2te^{2a})$.

The case $n = 3$, however, seems much more difficult. What we need are more conserved quantities. But where can we find them?

In 1973 H. Flaschka made the following remarkable observation. Let us define $n \times n$ matrices L, M by

$$L = \begin{pmatrix} p_1 & Q_1 & 0 & \dots & 0 & 0 \\ Q_1 & p_2 & Q_2 & \dots & 0 & 0 \\ 0 & Q_2 & p_3 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & p_{n-1} & Q_{n-1} \\ 0 & 0 & 0 & \dots & Q_{n-1} & p_n \end{pmatrix}$$

and

$$M = \begin{pmatrix} 0 & Q_1 & 0 & \dots & 0 & 0 \\ -Q_1 & 0 & Q_2 & \dots & 0 & 0 \\ 0 & -Q_2 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & Q_{n-1} \\ 0 & 0 & 0 & \dots & -Q_{n-1} & 0 \end{pmatrix}$$

where $p_i = q_i'$ and $Q_i = e^{q_i - q_{i+1}}$.

Proposition. *The open Toda lattice is equivalent to the matrix equation $L' = [L, M]$.*

The proof is a straightforward calculation.

Equations of this type are called Lax equations. The Lax equation immediately gives n conserved quantities:

Corollary. *Each eigenvalue of (the symmetric matrix) L is a conserved quantity for the open Toda lattice.*

Proof. It follows from the Lax equation that $(\operatorname{trace} L^k)' = 0$ for any k. $\square$

Let us compute the conserved quantities for the case $n = 3$. Writing

$$L = \begin{pmatrix} p_1 & Q_1 & 0 \\ Q_1 & p_2 & Q_2 \\ 0 & Q_2 & p_3 \end{pmatrix} = \begin{pmatrix} s_1 & t_1 & 0 \\ t_1 & s_2 & t_2 \\ 0 & t_2 & s_3 \end{pmatrix},$$

and computing the characteristic polynomial $\det(L - \lambda I)$, we obtain the following conserved quantities (these are, up to sign, the symmetric functions of the eigenvalues):

$$s_1 + s_2 + s_3$$
$$s_1 s_2 + s_2 s_3 + s_3 s_1 - t_1^2 - t_2^2$$
$$s_1 s_2 s_3 - s_1 t_2^2 - s_3 t_1^2$$

Of course the first one is trivial — it is identically zero if we use the normalization $q_1 + q_2 + q_3 = 0$ as in the case $n = 2$. The second one is essentially the same as the total energy. The third one is new.

Having two independent conserved quantities allows us to solve the system (for the independent variables q_1, q_2, say), just as we used one conserved quantity to solve the system for q_1 in the case $n = 2$. The calculations are messy but the answer is explicit. Let the initial conditions be

$$V = L(0) = \begin{pmatrix} 0 & v_1 & 0 \\ v_1 & 0 & v_2 \\ 0 & v_2 & 0 \end{pmatrix}.$$

Then

$$\begin{aligned} q_1(t) &= q_1(0) + \frac{1}{2}\log\frac{\alpha(t)}{\beta(t)} \\ q_2(t) &= q_2(0) + \frac{1}{2}\log\frac{\beta(t)}{\gamma(t)} \\ q_3(t) &= q_3(0) + \frac{1}{2}\log\frac{\gamma(t)}{\alpha(t)} \end{aligned}$$

where

$$\begin{aligned} \alpha(t) &= v_1^2 + v_2^2 \\ \beta(t) &= v_1^2 \cosh\, 2t\sqrt{v_1^2+v_2^2} + v_2^2 \\ \gamma(t) &= v_1^2 + v_2^2 \cosh\, 2t\sqrt{v_1^2+v_2^2} \end{aligned}$$

and

$$q_1(0) = \frac{2}{3}\log v_1 + \frac{1}{3}\log v_2, \quad q_2(0) = -\frac{1}{3}\log v_1 + \frac{1}{3}\log v_2, \quad q_3(0) = -\frac{1}{3}\log v_1 - \frac{2}{3}\log v_2.$$

You may feel suspicious: surely the Lax equation $\dot{L} = [L, M]$ came first, then the Toda lattice? But this is not correct. Toda invented the Toda lattice by contemplating addition formulae for elliptic functions. Computer simulations by J. Ford, D. Stoddard, and J. Turner ([FST]) *suggested* that the Toda lattice with $n = 3$ and $n = 6$ might have additional conserved quantities. Then M. Hénon found the conserved quantities for the general case ([He]). Only after this did H. Flaschka find the Lax equation.

The only deceitfulness in the above account of the case $n = 3$ is that there is a much easier way of finding the explicit solution than using the conserved quantities.

Proposition. *The solution of the open Toda lattice $L' = [L, M]$ with $L(0) = V$ is given by the following explicit formula:*

$$L(t) = (\exp\, tV)_1^{-1} V (\exp\, tV)_1.$$

The notation X_1, for an $n \times n$ real invertible matrix X, denotes the matrix which is obtained by orthogonalizing the columns of X, by the Gram-Schmidt procedure, starting from the last column.

Incidentally, this formula gives another proof of the fact that the eigenvalues of L are independent of t, because

$$\det(L(t) - \lambda I) = \det((\exp tV)_1^{-1} V (\exp tV)_1 - \lambda I) = \det(V - \lambda I).$$

For the (easy!) proof of the proposition, and further explanation and references, see [Gu].

Finally we shall mention several other kinds of Toda lattice. (We shall sheepishly ignore the original version without the artificial expansion forces.) All of them possess "many conserved quantities" and can be solved explicitly, but the formulae are much more complicated than for the open Toda lattice.

$N + 2$ particles, both ends fixed.

This is:

$$\begin{aligned} q_1'' &= -2e^{2(q_1 - q_2)} + 2e^{-2q_1} \\ q_i'' &= -2e^{2(q_i - q_{i+1})} + 2e^{2(q_{i-1} - q_i)} \quad i = 2, \dots, n-1 \\ q_n'' &= -2e^{2q_n} \qquad + 2e^{2(q_{n-1} - q_n)}. \end{aligned}$$

We shall not investigate it any further, as it is a special case of the next version.

$N + 1$ particles, periodic.

This is:

$$q_i'' = -2e^{2(q_i - q_{i+1})} + 2e^{2(q_{i-1} - q_i)} \quad i \in \mathbf{Z} \bmod n$$

(the previous case is given by imposing the condition $q_{in} = 0$ for all i).

For $n = 2$ we obtain $q'' = -2e^{4q} + 2e^{-4q}$. The total energy $\frac{1}{2}q'^2 + \cosh 4q$ is a conserved quantity, and the equation can be integrated in terms of elliptic functions.

For any n there are $n - 1$ independent nontrivial conserved quantities, and they arise from a Lax equation $L' = [L, M]$ as in the case of the open Toda lattice. For the periodic Toda lattice we have to take

$$L = \begin{pmatrix} p_1 & Q_1 & 0 & \dots & 0 & Q_n \\ Q_1 & p_2 & Q_2 & \dots & 0 & 0 \\ 0 & Q_2 & p_3 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & p_{n-1} & Q_{n-1} \\ Q_n & 0 & 0 & \dots & Q_{n-1} & p_n \end{pmatrix}$$

and

$$M = \begin{pmatrix} 0 & Q_1 & 0 & \dots & 0 & -Q_n \\ -Q_1 & 0 & Q_2 & \dots & 0 & 0 \\ 0 & -Q_2 & 0 & \dots & 0 & 0 \\ \vdots & \vdots & \vdots & & \vdots & \vdots \\ 0 & 0 & 0 & \dots & 0 & Q_{n-1} \\ Q_n & 0 & 0 & \dots & -Q_{n-1} & 0 \end{pmatrix}.$$

As in the case of the open Toda lattice, the conserved quantities can be used to solve the periodic Toda lattice explicitly. This is done in [To1], but as Toda himself says (Chapter 25):

"The method is very difficult to understand, and so complicated that lectures on this problem are usually not so well accepted (I feel that some simpler method will be found in the future). Readers are requested to read through the following chapters dealing with cyclic lattices without gettting stuck on minor points."

In fact, more conceptual methods were found later, analogous to the formula $L(t) = (\exp tV)_1^{-1} V (\exp tV)_1$ above (but they are hardly "simpler", as they involve infinite dimensional Lie algebras).

Infinitely many particles.

The infinite Toda lattice is:

$$q_i'' = -2e^{2(q_i - q_{i+1})} + 2e^{2(q_{i-1} - q_i)} \quad i \in \mathbf{Z}$$

(the periodic case is given by imposing the condition $q_i = q_{i+n}$ for all i).

We shall discuss this case separately, later on.

§4 Some explanations

The kind of examples and phenomena that we have seen in §1-§3 have led, directly or indirectly, to important advances in mathematics. We shall mention three of these topics and illustrate them using our examples.

Completely integrable Hamiltonian systems.

As explained in [Pa], Newton's equations (using coordinates $q_1, \dots, q_n$ for the configuration space $\mathcal{C}$) can be expressed using coordinates $q_1, \dots, q_n, p_1, \dots, p_n$ for the tangent space $T\mathcal{C}$. The resulting equations are called Hamilton's equations.

Let H be the total energy function. Regarded as a function from $T\mathcal{C}$ to $\mathbf{R}$, it is called the Hamiltonian function. Then the condition that a function $F : T\mathcal{C} \to \mathbf{R}$ is a conserved quantity — namely $\frac{d}{dt}F(q_1, \ldots, q_n, p_1, \ldots, p_n) = 0$ for any solution $(q_1(t), \ldots, q_n(t))$ — can be expressed as $\{H, F\} = 0$.

The Arnold-Liouville theorem says that if

(1) $F_1, \ldots, F_n$ are (functionally independent) conserved quantities, and

(2) $\{F_i, F_j\} = 0$ for all i, j,

then there exist new "action-angle" variables $\hat{q}_1, \ldots, \hat{q}_n, \hat{p}_1, \ldots, \hat{p}_n$ such that Hamilton's equations are

$$(\hat{q}_i)' = \text{ constant}, \quad (\hat{p}_i)' = 0.$$

The solution of this system is that each $\hat{q}_i(t)$ must be a linear function of t. So, if we can find the new coordinates explicitly, we can find the solution to the original system explicitly.

In principle, by making use of the conserved quantities, the new coordinates can be found explicitly "by quadrature" (although in practice the calculations might be complicated). We have already seen several examples of this procedure. The simplest example is

$$y'' = -ky.$$

Here $n = 1$ and y is a coordinate for the configuration space. Let us take $y_1 = y$ and "$y_2 = y'$" as coordinates for the tangent space. The total energy function is $H = \frac{1}{2}y'^2 + \frac{1}{2}ky^2$, and the Hamiltonian function is $H = \frac{1}{2}y_2^2 + \frac{1}{2}ky_1^2$. Hamilton's equations

$$y_1' = \frac{\partial H}{\partial y_2}, \quad y_2' = -\frac{\partial H}{\partial y_1}$$

are the familiar first order system

$$\begin{pmatrix} y_1 \\ y_2 \end{pmatrix}' = \begin{pmatrix} 0 & 1 \\ -k & 0 \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \end{pmatrix}.$$

We already know how to solve this system, but let us see what lies behind the Arnold-Liouville theorem in this case. Observing that the Hamiltonian function can be written

$$H = (\tfrac{1}{\sqrt{2}}y_2)^2 + (\tfrac{\sqrt{k}}{\sqrt{2}}y_1)^2,$$

let us introduce

$$r = \sqrt{(\tfrac{1}{\sqrt{2}}y_2)^2 + (\tfrac{\sqrt{k}}{\sqrt{2}}y_1)^2}, \quad \theta = \tan^{-1}\frac{\frac{\sqrt{k}}{\sqrt{2}}y_1}{\frac{1}{\sqrt{2}}y_2}.$$

Then (a calculation shows that) Hamilton's equations take the expected form

$$\theta' = \text{ constant}, \quad r' = 0$$

This simple example illustrates the reason why n conserved quantities (rather than $2n$) are sufficient, and (more or less) why the new variables are called action-angle variables.

Another aspect of the Arnold-Liouville theorem — and one which is easier to visualize — is the fact that, if the Hamiltonian function is a proper function (hence $H^{-1}(c)$ is compact, for any c), the solution to the system must lie on a torus in $T\mathcal{C}$. The n conserved quantities describe an n-dimensional torus in $T\mathcal{C}$ and the n "angles" are local coordinates on this torus. There are two possible kinds of solution: either periodic (a circle) or almost periodic (a "line of irrational slope" on a torus of dimension at least two).

[3DXM:ODE:ODE(2D)-2nd Order:USER]

This explains very clearly the behaviour of a linear system $Y'' = AY$ where A is a symmetric $n \times n$ matrix. There are n conserved quantities (the energies H_i of the normal modes) and it is easy to verify that $\{H_i, H_j\} = 0$. The solution is given by linear motion on an n-dimensional torus in $\mathbf{R}^n \times \mathbf{R}^n$. Using the normal mode coordinates $Z = PY$ we can introduce action-angle coordinates as in the simple example above.

PROBLEM: What can we say about $Y'' = AY$ when A is not symmetric?

Now let us look at our lattice models in the light of the Arnold-Liouville theorem.

(I) $T(y) = y$ (linear case)

(II) $T(y) = y + 0.3y^2$ (Fermi-Pasta-Ulam)

(III) $T(y) = y + 100y^3 + 5y^4 + 5y^5$ ("arbitrary" nonlinear case)

(IV) $T(y) = 1 - e^{-y} = y - \frac{1}{2}y^2 + \frac{1}{6}y^3 - \dots$ (Toda)

The linear case is covered by the remarks above.

The Toda lattice (at least, for suitable boundary conditions) turns out to be an example of a completely integrable Hamiltonian system, i.e. a system to which the Arnold-Liouville theorem applies. (We found the "maximum" number of conserved quantities in §3. For the proof of $\{F_i, F_j\} = 0$, and for more information, see [Gu].) This explains the almost periodic behaviour of the energies of the normal modes of the Toda lattice, because the energies of the normal modes are defined in terms of the solutions, and the solutions are almost periodic.

Regarding cases (II) and (III), we have not yet seen any conserved quantities beyond the total energy, but we have seen that the two systems behave very differently. The Fermi-Pasta-Ulam lattice *appears* almost periodic, while the "arbitrary" lattice *appears* to

thermalize. Therefore it is reasonable to conjecture that case (II) is completely integrable and case (III) is ergodic. (As explained in [Pa], ergodic systems are in some sense the opposite extreme to completely integrable Hamiltonian systems. In particular, they possess exactly the "minimum" number of conserved quantities, namely one.)

Since case (III) is an artificial example, we shall abandon it at this point. From now on we shall look for further evidence concerning the behaviour of the Fermi-Pasta-Ulam lattice.

Is it an integrable system or not?

The Kolmogorov-Arnold-Moser theory.

The KAM theory (see [Pa], [We]) predicts that it is possible for a nonlinear system to behave like an integrable system if it is sufficiently close to an integrable system. This "obvious" statement was very surprising when it was discovered, because the slightest (nonlinear) perturbation of an integrable system had been expected to be ergodic.

This means that we have two rather different posssible explanations for the behaviour of the Fermi-Pasta-Ulam lattice:

— it might be completely integrable, or

— it might be sufficiently close (in the sense of KAM) to a completely integrable system.

In fact, there is a very good candidate for the second explanation: the Toda lattice. To explain this, let us return to the general equations of the Toda lattice with force $T(y) = \alpha(e^{\beta y} - 1)$.

Writing $k = \alpha\beta$, we have

$$\begin{aligned} T(y) &= \alpha\beta y + \frac{1}{2!}\alpha\beta^2 y^2 + \frac{1}{3!}\alpha\beta^3 y^3 + \dots \\ &= ky + \frac{1}{2!}k\beta y^2 + \frac{1}{3!}k\beta^2 y^3 + \dots \end{aligned}$$

so we must take $k > 0$ in order to have Hooke's law near $y = 0$. Let us choose $k = 1$ for simplicity. Then the quadratic approximation is

$$T(y) \approx y + \frac{1}{2}\beta y^2$$

and we have two essentially distinct cases:

(a) $\alpha, \beta < 0$. For $\beta = -0.6$ we obtain $T(y) \approx y - 0.3y^2$,

(b) $\alpha, \beta > 0$. For $\beta = 0.6$ we obtain $T(y) \approx y + 0.3y^2$, i.e. the Fermi-Pasta-Ulam case.

The physical interpretation of these two cases can be expressed as follows. For a small expansion of the spring ($y > 0$), the restoring force (T) is greater in case (b); for a small compression of the spring ($y < 0$), the repulsive force (i.e. the magnitude of $-T$) is greater in case (a). It is also possible to express this by comparing the potential energy functions. We consider the system consisting of the lattice points Y_i and Y_{i+1} and the spring between them, and we write $y = y_i - y_{i-1}$. Then we define a potential function U by

$$y'' = -U'(y)$$

In other words, since $y'' = -2T(y)$ here, we have $T(y) = \frac{1}{2}U'(y)$. Hence

$$\frac{1}{2}U(y) \approx \text{ constant } + \frac{1}{2}y^2 + \frac{1}{6}\beta y^3$$

The difference between (a) and (b) corresponds to the asymmetry in the potential function near the stable equilibrium point $y = 0$.

The Fermi-Pasta-Ulam lattice is, therefore, approximated up to second order by the Toda lattice with $\alpha = k/0.6$, $\beta = 0.6$. This would be consistent with the KAM theory and the (apparent) almost periodicty of the energies of the normal modes. In this sense, we have "explained" the Fermi-Pasta-Ulam experimental observations, but there remains the question of whether the system is completely integrable.

Soliton theory.

A different kind of explanation of the Fermi-Pasta-Ulam observations comes from soliton theory. Solitons are exceptionally stable solutions of the KdV equation (a nonlinear generalization of the wave equation). It can be shown that the Fermi-Pasta-Ulam lattice is a discrete approximation to the KdV equation, or, more precisely, that the KdV equation can be obtained as a certain "continuum limit" of the Fermi-Pasta-Ulam system. Hence, the latter might posess its own soliton solutions, and these might have been the solutions observed by Fermi, Pasta and Ulam.

In [Pa] a simpler case of this phenomenon was described: the wave equation $u_{tt} = c^2 u_{xx}$ can be obtained as a "continuum limit" of the linear lattice equations. We have already noticed (at the end of §2) that the linear lattice admits wave-like solutions; in fact our entire analysis of the linear lattice resembled a discrete version of the method of Fourier series.

It is very natural, therefore, to look for "soliton solutions" of nonlinear lattice systems, such as those of Fermi-Pasta-Ulam and Toda. The Toda lattice does in fact admit soliton solutions (seee [To1], in the sense that these solutions are given by explicit formulae and have analogous properties to soliton solutions of the KdV equation. On the other hand, it is not clear how to find soliton solutions of the Fermi-Pasta-Ulam lattice, since we have no explicit formulae.

M. Kruskal and N. Zabusky ([Kr-Za]) were the first to demonstrate the relation between the Fermi-Pasta-Ulam lattice and the KdV equation, and they performed a numerical experiment with the KdV equation which exhibited the same almost-periodic behaviour, quantitively as well as qualitatively. This provided further strong evidence for the "special" nature of the Fermi-Pasta-Ulam lattice. It also led to the vigorous development of soliton theory which continues to this day.

§5 The Hénon-Heiles system

As a model for the motion of a star in a certain kind of galaxy, M. Hénon and C. Heiles ([He-He]) considered the following Hamiltonian function:

$$H(q_1, q_2) = \frac{1}{2}(p_1^2 + p_2^2) + \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3}q_2^3.$$

Thus, Hamilton's equations or Newton's equations are equivalent to the following system:

$$q_1'' = -\frac{\partial H}{\partial q_1} = -q_1 - 2q_1 q_2$$
$$q_2'' = -\frac{\partial H}{\partial q_2} = -q_2 - q_1^2 + q_2^2$$

By construction, H is a conserved quantity. Hénon and Heiles asked themselves the question: is this system completely integrable? Or, at least, is there a second conserved quantity?

They performed computer experiments to observe the solutions for various initial conditions with the same value of H. If the system is completely integrable, then (by the Arnold-Liouville theorem) the solution $(q_1(t), q_2(t), q_1'(t), q_2'(t))$ is a "linear flow" on a two-dimensional torus in $\mathbf{R}^4$. If there is a second conserved quantity F, then (even if $\{H, F\}$ is not zero) the solution should lie on a two-dimensional surface of the form $H^{-1}(\text{constant}) \cap F^{-1}(\text{constant})$ in $\mathbf{R}^4$. If H is the only conserved quantity, then the solution is likely to be ergodic, wandering over a three-dimensional subset $H^{-1}(\text{constant})$.

Instead of looking at a projection of the solution on $\mathbf{R}^2$ or $\mathbf{R}^3$, they examined the *intersection* of the solution with a suitable $\mathbf{R}^2$. To be precise, they chose the (q_2, p_2)-plane in $\mathbf{R}^4$ and computed the intersection points of the solution with this plane. (This idea is due to Poincaré.)

PROJECT 3: Write a program to carrry out the Hénon-Heiles experiment. Use the program to investigate other systems (linear and nonlinear). □

The results of the experiment with low values of H suggested motion on a two-dimensional surface. However, for higher values of H, the intersection points seemed to appear randomly, suggested ergodic motion on a three-dimensional subspace of $\mathbf{R}^4$. This "proves" that a second conserved quantity cannnot exist, because the second conserved quantity would constrain the motion to a two-dimensional surface for any value of H.

PROBLEM: Is it possible to convert this "computer proof" into a mathematical proof?

A physical explanation of these results can be obtained from the properties of the potential energy

$$U(q_1, q_2) = \frac{1}{2}(q_1^2 + q_2^2) + q_1^2 q_2 - \frac{1}{3}q_2^3.$$

The point $(0, 0)$ is a stable equilibrium point, and for small values of the total energy the solution must remain near to $(0, 0)$, with (approximately) simple harmonic motion. This gives an impression of complete integrability in the computer experiments. But for higher total energy, the solution can "escape" from the region around $(0, 0)$.

[3DXM:SURFACE:USER]

This phenomenon can also be observed by plotting the solution curve $(q_1(t), q_2(t))$ in the usual way, i.e. by *projecting* onto the (q_1, q_2)-plane.

[3DXM:ODE:ODE(2D)-1st Order:USER]

However, the advantage of the Poincaré method is that it is can be used to observe how the ergodic behaviour begins — how order turns into chaos. For more information on this, see [To1] and [We].

Our main reason for mentioning the Hénon-Heiles system is that it is related to the Toda and Fermi-Pasta-Ulam lattices in the case of three particles with periodic boundary conditions. We shall explain this briefly, following [To1].

Let us begin with the Toda system, using the general force $T(y) = \alpha(e^{\beta y} - 1)$. It is easy to verify that the total energy function is

$$H = \frac{1}{2}({y_1'}^2 + {y_2'}^2 + {y_3'}^2) + \frac{\alpha}{\beta}(e^{\beta(y_3 - y_2)} + e^{\beta(y_2 - y_1)} + e^{\beta(y_1 - y_3)}).$$

The "linearized system" is

$$\begin{aligned} y_1'' &= k(y_2 - 2y_1 + y_3) \\ y_2'' &= k(y_3 - 2y_2 + y_1) \\ y_3'' &= k(y_1 - 2y_3 + y_2) \end{aligned}$$

where $k = \alpha\beta$ as usual. This corresponds to the total energy function

$$H = \frac{1}{2}({y_1'}^2 + {y_2'}^2 + {y_3'}^2) + \frac{1}{2}k((y_3 - y_2)^2 + (y_2 - y_1)^2 + (y_1 - y_3)^2)$$

(we have omitted the constant term $3\alpha/\beta$ as it has no effect on the system.) The eigenvalues of the coeficient matrix are $-3k, -3k, 0$.

Let us take $k = 1$ for simplicity. Then suitable coordinates z_1, z_2, z_3 for the normal modes are given by

$$\begin{pmatrix} z_1 \\ z_2 \\ z_3 \end{pmatrix} = \begin{pmatrix} 1/\sqrt{6} & -\sqrt{2}/\sqrt{3} & 1/\sqrt{6} \\ 1/\sqrt{2} & 0 & -1/\sqrt{2} \\ 1/\sqrt{3} & 1/\sqrt{3} & 1/\sqrt{3} \end{pmatrix} \begin{pmatrix} y_1 \\ y_2 \\ y_3 \end{pmatrix}$$

and we obtain

$$H = \frac{1}{2}({z_1'}^2 + {z_2'}^2 + {z_3'}^2) + \frac{3}{2}(z_1^2 + z_2^2)$$

The coordinate $z_3 = (y_1+y_2+y_3)/\sqrt{3}$ does not appear — it is an ignorable coordinate (see [Pa]) so z_3 and ${z_3}'$ must be constant. (We have already made this observation directly, in §2.) Therefore we can omit the term z_3' too, and conclude that the total energy function

$$\frac{1}{2}({z_1'}^2 + {z_2'}^2) + \frac{3}{2}(z_1^2 + z_2^2)$$

governs the first order approximation of the Toda system.

Next, the cubic term

$$\frac{1}{6}\,\frac{\alpha}{\beta}\,\beta^3((y_3 - y_2)^3 + (y_2 - y_1)^3 + (y_1 - y_3)^3)$$

is equal to

$$\frac{3\beta}{2\sqrt{2}}(z_1^2 z_2 - \frac{1}{3}z_2^3),$$

so we can say that the total energy function

$$\frac{1}{2}({z_1'}^2 + {z_2'}^2) + \frac{3}{2}(z_1^2 + z_2^2) + \frac{3\beta}{2\sqrt{2}}(z_1^2 z_2 - \frac{1}{3}z_2^3)$$

governs the second order approximation of the Toda system. If we put $\beta = 2\sqrt{2}$ (and rescale the time variable) this gives exactly the Hénon-Heiles system.

To quote Toda ([To1], page 256)

"That the H-H system turned out to be equivalent to the [Toda] lattice was entirely accidental; a very strange happening indeed."

Since we already know that the second order approximation of the Toda system gives the Fermi-Pasta-Ulam system, the computer observations of Hénon and Heiles "prove" that the Fermi-Pasta-Ulam system is not completely integrable !

§6 Geometry

We have seen (in §3) the explicit solution of the Toda system

$$\begin{aligned} q_1'' &= -2e^{2(q_1-q_2)} \\ q_i'' &= -2e^{2(q_i-q_{i+1})} + 2e^{2(q_{i-1}-q_i)} \quad i = 2,\dots,n-1 \\ q_n'' &= \qquad\qquad 2e^{2(q_{n-1}-q_n)}. \end{aligned}$$

It is complicated (and the solutions to the other versions of the Toda lattice are even worse). On the other hand, the Arnold-Liouville theorem tells us that there is a simple geometrical picture of the solution, namely a linear flow on an $(n-1)$-dimensional torus in $\mathbf{R}^{2n-2}$. (This is not quite correct for the above system, because the conserved quantities are not proper functions, and so we have a flow on an affine space instead of a torus.) But the Arnold-Liouville theorem is virtually useless for computations.

It is natural to ask whether there are other geometrical descriptions of the solutions, more concrete than the Arnold-Liouville picture but less intimidating than a formula for the functions q_i. We shall discuss one such description, due to J. Moser ([Mo]). It uses the theory of homogeneous spaces (real projective spaces, in the case of the system above) and it leads to very interesting new questions.

Recall that the system can be formulated as a Lax equation $L' = [L, M]$ with initial condition $L(0) = V$, and that the solution is given by

$$L(t) = (\exp tV)_1^{-1} V (\exp tV)_1$$

where X_1 means the matrix obtained by orthogonalizing the columns of X, by the Gram-Schmidt procedure, starting from the last column. As we remarked in §3, this formula shows immediately that the eigenvalues $\lambda_1, \dots, \lambda_n$ of $L(t)$ are constant. On the other hand, the *eigenvectors* of $L(t)$ are *not* constant, and it is interesting to consider their behaviour.

The eigenvalues are determined by the initial condition: since V is a symmetric matrix there exists an orthogonal matrix P such that

$$PVP^{-1} = \begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix} = \Lambda \text{ (say)}$$

This means that the columns of P^{-1} (the rows of P) are eigenvectors of V.

Let us write $u = (\exp tV)_1$ so that

$$L = u^{-1} V u = (Pu)^{-1} \Lambda (Pu).$$

It follows that the columns of $(Pu)^{-1}$ (the rows of Pu) are eigenvectors of L, i.e. our object of study.

We have

$$\begin{aligned} Pu &= P(\exp\, tV)_1 \\ &= (P \exp\, tV)_1 \\ &= (P(\exp\, tV)P^{-1}P)_1 \\ &= ((\exp\, tPVP^{-1})P)_1 \\ &= ((\exp\, t\Lambda)P)_1. \end{aligned}$$

Now, it is possible to show by explicit calculation that L is determined by the last column of Pu. But the last column of $((\exp\, t\Lambda)P)_1$ is easy to calculate; it is simply the normalization of the last column of $(\exp\, t\Lambda)P$. Let us write

$$P = \begin{pmatrix} & & r_1 \\ & & \\ & & r_n \end{pmatrix}$$

so that

$$(\exp\, t\Lambda)P = \begin{pmatrix} & & e^{\lambda_1 t} r_1 \\ & & \vdots \\ & & e^{\lambda_n t} r_n \end{pmatrix}.$$

Then the last column of $((\exp\, t\Lambda)P)_1$ is

$$\begin{pmatrix} e^{\lambda_1 t} r_1 / \sqrt{\sum_i e^{2\lambda_i t} r_i^2} \\ \\ \vdots \\ \\ e^{\lambda_n t} r_n / \sqrt{\sum_i e^{2\lambda_i t} r_i^2} \end{pmatrix}$$

To avoid the inconvenient normalization we can work in the real projective space $\mathbf{R}P^{n-1}$ instead of $\mathbf{R}^n$. With the usual homogeneous coordinates for $\mathbf{R}P^{n-1}$, we obtain the formula

$$[e^{\lambda_1 t} r_1;\, \ldots\, ; e^{\lambda_n t} r_n]$$

for the solution of the Toda lattice.

What does this formula mean? Essentially we have made a coordinate change, from the original q_i, p_i to λ_i, r_i. This is another manifestation of the Arnold-Liouville action-angle coordinates — the "linearity" of the solution is apparent — but it is more concrete. Even better, we may be able to use the geometry of the space $\mathbf{R}P^{n-1}$ to study the behaviour of the solutions of the Toda system.

Indeed, Moser used the "Schubert decomposition" of $\mathbf{R}P^{n-1}$ to study the "scattering theory" of the system. Physically, the phenomenon of scattering arises because of the constant expansion of the lattice (see §3). As $t \to \infty$ or $t \to -\infty$ the solutions are asymptotically linear, and their derivatives (the velocities of the particles in the lattice) are asymptotically constant. We can regard the system as a device which relates the velocities at ∞ to the velocities at $-\infty$.

PROJECT 4: Write a program to estimate the "velocities at ∞" and the "velocities at $-\infty$" for the above version of the Toda lattice. What do you observe? Can you explain this (in the three particle case) by looking at the explicit solutions in §3? Can you explain it by looking at the solution in $\mathbf{R}P^{n-1}$? $\square$

The concept of scattering plays an important role in many other integrable systems with noncompact phase space, and in some cases provides a method of solving the system. The geometrical method can also be useful in the study of integrable systems with compact phase space — it provides a more concrete version of the Arnold-Liouville theorem.

§7 Some conclusions

The Fermi-Pasta-Ulam lattice was one of the first mathematical research problems to be attacked by computer, almost 50 years ago. The surprising results of that experiment led to tremendous progress in the theory of differential equations. The experiment could not have been done without using a computer, and many of the new concepts arising from such experiments (integrable systems, solitons, ergodicity and chaos) can be visualized much more satisfactorily with the aid of computers. It seems clear that computers will greatly expand the frontiers of mathematics in the next 50 years. But the road will not be easy: computer experiments have to be carefully formulated, continually checked for accuracy, and correctly interpreted.

We have discussed the Fermi-Pasta-Ulam lattice as one of our main examples, and we have — by a combination of mathematical arguments and computer experiments — reached some important conclusions:

— it is a second-order approximation to a completely integrable system (the Toda lattice)

— it exhibits almost periodic motion for "low" total energy (this is merely an experimental observation, but it is consistent with KAM theory and soliton theory)

— it is (almost certainly!) not completely integrable.

On the other hand, our attempts to reach these conclusions suggest further questions. For example, the behaviour of the energies of the normal modes deserves a much more detailed description than simply "almost periodic".

PROBLEM: At the beginning of this course we asked three very general questions about differential equations. Have these lectures provided any answers?

What kinds of differential equations are there?

???

How can geometry (differential geometry, manifold theory) be used to study and solve differential equations?

???

Is there a way to recognise or visualize the "integrability" of differential equations?

???

References

[3DXM] *http://rsp.math.brandeis.edu/3D-XplorMath/.*

[FST] J. Ford, D. Stoddard, and J. Turner, *On the integrability of the Toda lattice*, Prog. Theoret. Phys. **50** (1973), 1547–1560.

[Gu] M.A. Guest, *Harmonic Maps, Loop Groups, and Integrable Systems*, Cambridge Univ. Press, 1997.

[He-He] M. Hénon and C. Heiles, *The applicability of the third integral of motion: some numerical experiments*, Astron. J. **69** (1964), 73–79.

[He] M. Hénon, *Integrals of the Toda lattice*, Phys. Rev. B **9** (1974), 1921– 1923.

[Kr-Za] N. Zabusky and M. Kruskal, *Interaction of solitons in a collisionless plasma and the recurrence of initial states*, Phys. Rev. Lett. **15** (1965), 240–243.

[Mo] J. Moser, *Finitely many mass points on the line under the influence of an exponential potential — an integrable system*, Lecture Notes in Physics **38** (1975), 467–497.

[Pa] R. Palais, *Equations of evolution*, this Workshop.

[To1] M. Toda, *Nonlinear Waves and Solitons.*, Mathematics and its Applications, 5, Kluwer, 1989.

[To2] M. Toda, *Theory of Nonlinear Lattices*, Springer Series in Solid-State Sciences, 20, Springer-Verlag, 1989.

[We] T.P. Weissert, *The Genesis of Simulation in Dynamics. Pursuing the Fermi-Pasta-Ulam Problem.*, Springer, 1997.

Department of Mathematics, Graduate School of Science, Tokyo Metropolitan University, Minami-Ohsawa 1-1, Hachioji-shi, Tokyo 192-0397, Japan

martin@math.metro-u.ac.jp

14 March 2003

CORRECTED VERSIONS OF THESE NOTES WILL BE AVAILABLE IN THE FUTURE AT: http://www.comp.metro-u.ac.jp/˜martin

PLEASE SEND YOUR SUGGESTIONS OR CORRECTIONS!