

LECTURE 3: THE KORTEWEG-DE VRIES EQUATION (CONTINUATION)

The twentieth century. The experiments of Fermi-Pasta-Ulam and Zabusky-Kruskal. In the 1950's, Enrico Fermi, John Pasta, and Stan Ulam were interested in the question of how *thermalization* occurs in solid-state physics. A simple model for a solid material is a chain of identical particles (of mass m) connected to nearest neighbors by identical springs (with restoring force $F(\Delta)$ where Δ is the length of the spring). Thus, Newton's second law says

$$m \frac{d^2 x_n}{dt^2} = F(\Delta_0 + x_{n+1} - x_n) - F(\Delta_0 + x_n - x_{n-1})$$

where Δ_0 is the equilibrium displacement of the particles. In the linear case, Hooke's law says that for some constant $k > 0$, $F(\Delta) = k\Delta$, and the system becomes

$$m \frac{d^2 x_n}{dt^2} = k(x_{n+1} - 2x_n + x_{n-1}).$$

The problem appears complicated, but it is easily solved by Fourier theory. Multiply through by e^{-ipn} and sum over n assuming that x_n decays to zero for large n :

$$m \frac{d^2}{dt^2} \sum_{n=-\infty}^{\infty} x_n e^{-ipn} = 2k(\cos(p) - 1) \sum_{n=-\infty}^{\infty} x_n e^{-ipn}.$$

The sums are the Fourier coefficients:

$$\hat{x}(p) := \sum_{n=-\infty}^{\infty} x_n e^{-ipn}.$$

They depend on t through the $x_n(t)$. It is easy to solve in closed form for the Fourier coefficients:

$$\hat{x}(p) = A(p) \cos(\omega(p)t) + B(p) \sin(\omega(p)t)$$

where the frequency is

$$\omega(p) = \sqrt{\frac{2k}{m}(1 - \cos(p))},$$

and $A(p)$ and $B(p)$ are arbitrary constants. The quantity $A(p)^2 + B(p)^2$ is usually interpreted as the *energy in mode p* (as the total squared L^2 norm is the sum or integral of these quantities by Plancherel). There are two observations here:

- On the basis of physical reasoning of statistical thermodynamics, one expects that as the system evolves in time, it should evolve toward *equipartition* in which the energy is divided more or less equally among all of the modes.
- But the equation of motion shows that all $\hat{x}(p)$ are *uncoupled* from each other; indeed this is the very definition of what is meant by a *normal mode*. Therefore unless the initial condition is already in equipartition, the system can never evolve into such a state!

Fermi, Pasta, and Ulam sought to explain the observed equipartition by breaking the feature of the simple Hooke's law model that leads to the decoupling of the modes. They made the springs nonlinear. They used an expression of the form

$$F(\Delta) = k\Delta + \alpha\Delta^3$$

and performed numerical integration of the ODEs for the $x_n(t)$ on one of the first computers, the MANIAC at Los Alamos. They used an initial condition in which all of the energy was in the first few Fourier modes. At a sequence of times $t = t_k$ they computed the Fourier coefficients $\hat{x}(p, t_k)$ from the output of their program. As expected, the energy leaked from mode to mode. But what surprised them was that after some time (not too long) most of the energy spilled back into the first few modes! It was as if the nonlinearity they put into the problem only "temporarily" thermalized the material.

Later in 1965, Zabusky and Kruskal revisited this problem from the point of view of partial differential equations. They assumed that the particle positions $x_n(t)$ could be considered to be samples of a smooth function $v(x, t)$: $x_n(t) = v(nh, t)$ for some small lattice spacing h . Taking the limit $h \rightarrow 0$ in an appropriate

frame of reference moving with constant velocity, they derived as a *continuum limit* equation for a function $u(x, t)$ related to v the KdV equation

$$u_t + uu_x + \epsilon^2 u_{xxx} = 0.$$

where ϵ is proportional to h . They carried out numerical simulations of this partial differential equation with initial data similar to FPU's.

You can carry out Zabusky and Kruskal's numerical experiment and also view the dynamics corresponding power spectra $A(p)^2 + B(p)^2$ using the Mathematica notebook `ZabuskyKruskal.nb`.

The pulses shed by the evolution were identified in shape by Zabusky and Kruskal as the solitary waves we obtained earlier. But they also noted the fact that these shapes survived multiple collisions with each other, and it was they who coined the term *solitons* to describe these robust objects.

Mathematical structure within the KdV equation.

Local conservation laws. The KdV equation

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

conserves the *mass functional*

$$m[u] := \int_{-\infty}^{\infty} u(x) dx.$$

This just represents the area of water under the free surface of the fluid. The best way to see that the mass is conserved is to notice that the KdV equation can be written in the form

$$u_t + \left[\frac{1}{2}u^2 + u_{xx} \right]_x = 0.$$

Such an equation, of the form $D_t + F_x = 0$, is called a *local conservation law*. The *conserved local density* is D and its *flux* is F . Every local conservation law implies, under appropriate boundary conditions, the conservation of an integral of D :

$$\frac{d}{dt} \int_a^b D(x) dx + F(b) - F(a) = 0$$

so if F vanishes at the boundary, the integral of D is conserved. Similarly, if u satisfies periodic boundary conditions on some finite interval. It is also easy to show that u^2 is a conserved local density for KdV: begin by multiplying the KdV equation through by $2u$ after which it becomes

$$(u^2)_t + 2u^2u_x + 2uu_{xxx} = 0.$$

Now we want to show that the last two terms comprise the x -derivative of some expression F in u and its derivatives. The first term is clearly a perfect x derivative:

$$2u^2u_x = \left(\frac{2}{3}u^3 \right)_x,$$

but (in my opinion) the term $2uu_{xxx}$ is less obvious. But it too is a perfect derivative:

$$\begin{aligned} 2uu_{xxx} &= 2uu_{xxx} + 2u_xu_{xx} - 2u_xu_{xx} \\ &= (2uu_{xx})_x - (u_x^2)_x \\ &= (2uu_{xx} - u_x^2)_x. \end{aligned}$$

So we have found the local conservation law

$$(u^2)_t + \left(\frac{2}{3}u^3 + 2uu_{xx} - u_x^2 \right)_x = 0$$

which implies that under suitable boundary conditions the integral of u^2 is a conserved quantity. Further conserved local densities also exist, but they must involve x -derivatives of u .

Constants of motion in finite-dimensional systems. Consider a finite-dimensional system of the form

$$\frac{du_j}{dt} = F_j(u_1, \dots, u_N), \quad j = 1, \dots, N.$$

A *conserved quantity* or *constant of the motion* for this system is a function $E(u_1, \dots, u_N)$ defined on the phase space such that whenever $u_j(t)$ satisfy the ODEs, then

$$\frac{d}{dt}E(u_1(t), \dots, u_N(t)) = 0.$$

Thus, the value of the function E as t varies is equal to the value calculated on the initial conditions:

$$E(u_1(t), \dots, u_N(t)) = E(u_1(0), \dots, u_N(0)).$$

This means that it is consistent to restrict the system of ODEs to a level hypersurface given by

$$E(u_1, \dots, u_N) = E_0$$

where E_0 is specified by initial conditions. The existence of one constant of motion reduces the dimension of the system of ODEs by one; in the best case we can solve the above equation for u_N in terms of u_1, \dots, u_{N-1} and E_0 :

$$u_n = G_N(u_1, \dots, u_{N-1}; E_0)$$

and then we have a smaller system governing u_1, \dots, u_{N-1} only:

$$\frac{du_j}{dt} = F_j(u_1, \dots, u_{N-1}, G_N(u_1, \dots, u_{N-1}; E_0)) = \tilde{F}_j(u_1, \dots, u_{N-1}; E_0), \quad j = 1, \dots, N-1.$$

which determines $u_1(t), \dots, u_{N-1}(t)$ from initial conditions and then we get $u_N(t)$ as a function of these and E_0 . The process can be repeated. If we are lucky enough to find $N-1$ constants of motion E_1, \dots, E_{N-1} , then the system will be reduced to a single autonomous nonlinear first-order differential equation:

$$\frac{du_1}{dt} = \tilde{F}_1(u_1; E_{1,0}, E_{2,0}, \dots, E_{N-1,0})$$

which can be solved to determine t as a function of u_1 by separation of variables. Modulo inverting the function $t(u_1)$ to find $u_1(t)$, this procedure solves the system of differential equations in closed form.

Finite-dimensional Hamiltonian systems. Completely integrable systems. If there is more structure, then fewer conserved quantities are needed to solve the problem. A *Hamiltonian* system is one of dimension $2N$ that can be written in the form

$$\frac{d\vec{u}}{dt} = \mathbf{J}\nabla_u H$$

for some function $H(\vec{u})$ called the *Hamiltonian function*; here \mathbf{J} is (for the moment) the matrix (broken into four $N \times N$ blocks)

$$\mathbf{J} = \begin{pmatrix} 0 & \mathbb{I} \\ -\mathbb{I} & 0 \end{pmatrix}.$$

We can write easily an equation for any function $F(u_1, \dots, u_N)$ specified on the phase space, just by using the chain rule:

$$\frac{dF}{dt} = \left\langle \nabla_u F, \frac{d\vec{u}}{dt} \right\rangle = \langle \nabla_u F, \mathbf{J}\nabla_u H \rangle =: \{F, H\}$$

The angle brackets are the usual inner (dot) product, and the expression on the right-hand side defines the *Poisson bracket* between two functions F and H specified on the phase space. It has the following elementary properties:

- Skew symmetry: $\{F, G\} = -\{G, F\}$.
- Bilinearity: $\{F_1 + F_2, G\} = \{F_1, G\} + \{F_2, G\}$.
- Leibnitz rule: $\{F_1 F_2, G\} = F_1 \{F_2, G\} + F_2 \{F_1, G\}$.
- Jacobi identity: $\{F, \{G, H\}\} + \{H, \{F, G\}\} + \{G, \{H, F\}\} = 0$.

These follow immediately from our formula for \mathbf{J} , but in fact we can replace this \mathbf{J} with any matrix function $\mathbf{J} = \mathbf{J}(\vec{u})$ as long as the skew symmetry and Jacobi identity properties hold (the bilinear property and Leibnitz rule hold automatically).

In a Hamiltonian system a function $F(u_1, \dots, u_N)$ is a conserved quantity if

$$\{F, H\} = 0$$

as this is equivalent to $dF/dt = 0$. We say that F “Poisson-commutes” with H . Note that by skew-symmetry, we have $\{H, H\} = 0$, so the Hamiltonian function itself is always a conserved quantity. Every conserved quantity defines a symmetry group for the solutions of a Hamiltonian system. Suppose F is conserved. Then we can find (at least locally) a vector function \vec{u} of two variables t and s such that both

$$\frac{\partial u_j}{\partial t} = \{u_j, H\} \quad \text{and} \quad \frac{\partial u_j}{\partial s} = \{u_j, F\}$$

because the mixed partials commute: taking $\partial/\partial s$ of the first equation and subtracting $\partial/\partial t$ of the second equation should give zero, and indeed:

$$\begin{aligned} \frac{\partial}{\partial s}\{u_j, H\} - \frac{\partial}{\partial t}\{u_j, F\} &= \{\{u_j, H\}, F\} - \{\{u_j, F\}, H\} \\ &= -\{\{H, u_j\}, F\} - \{\{u_j, F\}, H\} \\ &= \{\{F, H\}, u_j\} \\ &= 0. \end{aligned}$$

This gives a symmetry group parametrized by s , because if for $s = 0$ the function $\vec{u}(0, t)$ satisfies $d\vec{u}/dt = \mathbf{J}\nabla H$, then for each $s \in \mathbb{R}$ so does $\vec{u}(s, t)$.

The best situation to be in for a Hamiltonian system of dimension $2N$ is characterized by the Liouville-Arnold theorem:

Theorem 1 (Liouville-Arnold). *Suppose that the functions F_1, \dots, F_N on \mathbb{R}^{2N} satisfy*

$$\{F_j, F_k\} = 0, \quad j, k = 1, \dots, N$$

(we say that they are in involution). Pick \vec{f} and let $M(\vec{f})$ be a common level set of the F_k :

$$M(\vec{f}) = \{\vec{u} \in \mathbb{R}^{2N} : F_k(\vec{u}) = f_k, \quad k = 1, \dots, N\},$$

and suppose that the F_k are independent functions on $M(\vec{f})$. Then

- (1) $M(\vec{f})$ is a smooth manifold, invariant under the dynamics of the Hamiltonian system with Hamiltonian function $H = F_1$.
- (2) If the manifold $M(\vec{f})$ is compact and connected, then it is diffeomorphic to the N -dimensional torus

$$T^N := \{(\varphi_1, \dots, \varphi_N) \pmod{2\pi}\}.$$

- (3) The Hamiltonian system with Hamiltonian function H determines a quasiperiodic motion on $M(\vec{f})$, that is, there exist angular coordinates $(\varphi_1, \dots, \varphi_N)$ on $M(\vec{f})$ such that $d\vec{u}/dt = \mathbf{J}\nabla_u H$ restricted to $M(\vec{f})$ is just

$$\frac{d\varphi_j}{dt} = \omega_j(f_1, \dots, f_N), \quad j = 1, \dots, N.$$

Such a system is said to be completely integrable.

It is clear that in the coordinates $(\varphi_1, \dots, \varphi_N)$ on the torus $M(\vec{f})$ the dynamics can be solved explicitly:

$$\varphi_j(t) = \varphi_j(0) + \omega_j(f_1, \dots, f_N)t \pmod{2\pi}.$$

Note the undistinguished role played by $H = F_1$ in the statement of the theorem. This implies that on the common level set $M(\vec{f})$ we may simultaneously solve all N systems $d\vec{u}/dt = \mathbf{J}\nabla_u F_k$, which all admit restriction to $M(\vec{f})$ and take the same form:

$$\frac{d\varphi_j}{dt_k} = \omega_{jk}(f_1, \dots, f_N), \quad j, k = 1, \dots, N.$$