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PART I

FUNDAMENTALS AND BASIC APPLICATIONS



In 1955 Fermi, Pasta and Ulam (FPU) (Fermi et al., 1955) and Tsingou (see Douxois, 2008) undertook a numerical study of a one-dimensional anharmonic (nonlinear) lattice. They thought that due to the nonlinear coupling, any smooth initial state would eventually lead to an equipartition of energy, i.e., a smooth state would eventually lead to a state whose harmonics would have equal energies. In fact, they did not see this in their calculations. What they found is that the solution nearly recurred and the energy remained in the lower modes.

To quote them (Fermi et al., 1955):

The results of our computations show features which were, from beginning to end, surprising to us. Instead of a gradual, continuous flow of energy from the first mode to the higher modes, ... the energy is exchanged, essentially, among only a few. ... There seems to be little if any tendency toward equipartition of energy among all the degrees of freedom at a given time. In other words, the systems certainly do not show mixing.

Their model consisted of a nonlinear spring–mass system (see Figure 1.1) with the force law: $F(\Delta) = -k(\Delta + \alpha \Delta^2)$, where Δ is the displacement between the masses, k > 0 is constant, and α is the nonlinear coefficient. Using Newton's second law and the above nonlinear force law, one obtains the following equation governing the longitudinal displacements:

$$m\ddot{y}_{i} = k \left[(y_{i+1} - y_{i}) + \alpha (y_{i+1} - y_{i})^{2} \right] - k \left[(y_{i} - y_{i-1}) + \alpha (y_{i} - y_{i-1})^{2} \right],$$

where i = 1, ..., N - 1, y_i are the longitudinal displacements of the *i*th mass, and (`) = d/dt. Rewriting the right-hand side leads to

$$m\ddot{y}_{i} = k(y_{i+1} - 2y_{i} + y_{i-1}) + k\alpha \left[(y_{i+1} - y_{i})^{2} - (y_{i} - y_{i-1})^{2} \right],$$

which can be further rewritten as

$$\frac{m}{k}\ddot{y}_{i} = \hat{\delta}^{2}y_{i} + \alpha \left[(y_{i+1} - y_{i})^{2} - (y_{i} - y_{i-1})^{2} \right],$$
(1.1)





where the operator $\hat{\delta}^2 y_i$ is defined as

$$\hat{\delta}^2 y_i \equiv (y_{i+1} - 2y_i + y_{i-1}).$$

Equation (1.1) is referred to as the FPU equation. Note that if $\alpha = 0$, then (1.1) reduces to the discrete wave equation

$$\frac{m}{k}\ddot{y}_i = \hat{\delta}^2 y_i$$

The boundary conditions are usually chosen to be either fixed displacements, i.e., $y_0(t) = y_N(t) = 0$; or as periodic ones, $y_0(t) = y_N(t)$ and $\dot{y}_0(t) = \dot{y}_N(t)$; the initial conditions are given for $y_i(t = 0)$ and $\dot{y}_i(t = 0)$. Fermi, Pasta and Ulam chose N = 65 and the sinusoidal initial condition

$$y_i(t=0) = \sin\left(\frac{i\pi}{N}\right), \qquad \dot{y}_i(t=0) = 0, \qquad i = 1, 2, \dots, N-1,$$

with periodic boundary conditions.

The numerical calculations of Fermi, Pasta and Ulam were also pioneering in the sense that they carried out one of the first computer studies of nonlinear wave phenomena. Given the primitive state of computing in the 1950s it was a truly remarkable achievement!

In 1965 Kruskal and Zabusky studied the continuum limit corresponding to the FPU model. To do that, they considered *y* as approximated by a continuous function of the position and time and expanded *y* in a Taylor series,

$$y_{i\pm 1} = y((i\pm 1)l) = y\pm ly_z + \frac{l^2}{2}y_{zz} \pm \frac{l^3}{3!}y_{zzz} + \frac{l^4}{4!}y_{zzzz} + \cdots,$$

where z = il. Setting h = l/L, x = z/L, L = Nl, $t = \tau/(h\omega)$, where τ is non-dimensional time with $\omega = \sqrt{k/m}$, it follows that

$$\frac{\partial}{\partial t} = h\omega \frac{\partial}{\partial \tau}$$

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and using the Taylor series on (1.1) leads to the continuous equation

$$h^{2}y_{\tau\tau} = h^{2}y_{xx} + \frac{h^{4}}{12}y_{xxxx} + \alpha \left[\left(hy_{x} + \frac{h^{2}}{2}y_{xx} + \dots \right)^{2} - \left(hy_{x} - \frac{h^{2}}{2}y_{xx} + \dots \right)^{2} \right].$$

Hence, to leading order, the continuous limit is given by

$$y_{\tau\tau} = y_{xx} + \frac{h^2}{12} y_{xxxx} + \varepsilon y_x y_{xx} + \cdots,$$
 (1.2)

where $\varepsilon = 2\alpha h$ and the higher-order terms are neglected. This equation was derived by Boussinesq in the context of shallow-water waves in 1871 and 1872 (Boussinesq, 1871, 1872)!

There are four cases to consider:

(a) When h² ≪ 1 and |ε| ≪ 1 (read as h² and |ε| are both much less than 1), both the nonlinear term and higher-order derivative term (referred to as the dispersive term) are negligible. Then equation (1.2) reduces to the linear wave equation

$$y_{\tau\tau} = y_{xx}$$

(b) In the small-amplitude limit where $h^2/12 \gg |\varepsilon|$ (or where $\alpha \to 0$ in the FPU model), the nonlinear term is negligible and the correction to (1.2) is governed by the higher-order linear dispersive wave equation

$$y_{\tau\tau} = y_{xx} + \frac{h^2}{12} y_{xxxx}.$$

(c) If $h^2/12 \ll |\varepsilon|$, then the y_{xxxx} term is negligible and (1.2) yields

$$y_{\tau\tau} = y_{xx} + \varepsilon y_x y_{xx},$$

which has, as can be shown from further analysis or indicated by numerical simulation, breaking or multi-valued solutions in finite time. When breaking occurs one must use (1.2) as a more physical model.

(d) In the case of "maximal balance" where $h^2/12 \approx |\varepsilon| \ll 1$, the wave equation is governed by a different equation.

This case of maximal balance is the most interesting case and we will now analyze it in detail.

Let us look for a solution *y* of the form¹

$$y \sim \Phi(X, T; \varepsilon), \qquad X = x - \tau, \qquad T = \frac{\varepsilon \tau}{2}.$$

¹ Later in the book we will see "why".

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It follows that

$$\begin{split} \frac{\partial}{\partial \tau} &= -\frac{\partial}{\partial X} + \frac{\varepsilon}{2} \frac{\partial}{\partial T}, \\ \frac{\partial^2}{\partial \tau^2} &= \left(\frac{\partial}{\partial \tau}\right)^2 = \frac{\partial^2}{\partial X^2} - \varepsilon \frac{\partial}{\partial X \partial T} + \frac{\varepsilon^2}{4} \frac{\partial^2}{\partial T^2}, \\ \frac{\partial}{\partial x} &= \frac{\partial}{\partial X}. \end{split}$$

Substituting these relations into the continuum limit, (1.2) yields

$$\left[\frac{\partial^2 \Phi}{\partial X^2} - \varepsilon \frac{\partial \Phi}{\partial X \partial T} + \frac{\varepsilon^2}{4} \frac{\partial^2 \Phi}{\partial T^2}\right] = \frac{\partial^2 \Phi}{\partial X^2} + \frac{h^2}{12} \frac{\partial^4 \Phi}{\partial X^4} + \varepsilon \frac{\partial \Phi}{\partial X} \frac{\partial^2 \Phi}{\partial X^2}.$$

Calling $u = \partial \Phi / \partial X$ and dropping the $O(\varepsilon^2)$ terms, leads to the equation studied by Zabusky and Kruskal (1965) and Kruskal (1965)

$$u_T + uu_X + \delta^2 u_{XXX} = 0, (1.3)$$

where $\delta^2 = h^2/12\varepsilon$ and u(X, 0) is the given initial condition. It is important to note that (1.3) is the well-known (nonlinear) Korteweg–de Vries (KdV) equation. It should be remarked that Boussinesq derived (1.3) and other approximate long-wave equations for water waves [e.g., (1.2)] (Boussinesq, 1871, 1872, 1877). Korteweg and de Vries investigated (1.3) in considerable detail and found periodic "cnoidal" wave solutions in the context of long (or shallow) water waves (Korteweg and de Vries, 1895). Before the early 1960s, the KdV equation was primarily of interest only to researchers studying water waves. The KdV equation was not of wide interest to mathematicians during the first half of the twentieth century, since most studies at the time tended to concentrate on linear second-order equations, whereas (1.3) is nonlinear and third order.

Kruskal and Zabusky considered the KdV equation (1.3) with periodic initial values. They initially took δ^2 small with $u(X, 0) = \cos(\pi X)$. When $\delta = 0$ one gets the so-called inviscid Burgers equation,

$$u_T + u u_X = 0,$$

which leads to breaking or a multi-valued solution or shock formation in finite time. The inviscid Burgers equation is discussed further in Chapter 2.

When $\delta^2 \ll 1$, a sharp gradient appears at a finite time, which we denote by $t = t_B$, together with "wiggles" (see the dashed line in Figure 1.2). When $t \gg t_B$, the solution develops many oscillations that eventually separate into a train of solitary-type waves. Each solitary wave is localized in space (see the solid line in Figure 1.2). Subsequently, under further propagation, the solitary waves interact and the solution eventually returns to a state that is similar to Cambridge University Press 978-1-107-01254-7 - Nonlinear Dispersive Waves: Asymptotic Analysis and Solitons Mark J. Ablowitz Excerpt <u>More information</u>



Figure 1.2 Calculations of the KdV equation (1.3), $\delta \approx 0.022$ [from numerical calculations of Zabusky and Kruskal (1965)].

the initial conditions, one which resembles the recurrence phenomenon first observed by FPU in their computations.

An important aspect raised by Kruskal and Zabusky in 1965 was the appearance of the train of solitary waves. To study an individual solitary wave one can look for traveling wave solutions of (1.3); that is, $u = U(\zeta)$, where $\zeta = (X - CT - X_0)$, *C* is the speed of the traveling wave, and X_0 is the phase. Doing so reduces (1.3) to

$$-CU_{\zeta} + UU_{\zeta} + \delta^2 U_{\zeta\zeta\zeta} = 0.$$

To look for a solitary wave we take $U \to U_{\infty}$ as $|\zeta| \to \infty$. First integrate this equation once to find

$$\delta^2 U_{\zeta\zeta} + \frac{U^2}{2} - CU = \frac{E_1}{6},$$

where E_1 is a constant of integration. Multiplying by U_{ζ} and integrating again leads to

$$\frac{\delta^2}{2}U_{\zeta}^2 + \frac{U^3}{6} - C\frac{U^2}{2} = \frac{E_1}{6}U + \frac{E_2}{6},$$

where E_2 is another constant of integration. Thus, one obtains the equation

$$\frac{\delta^2}{2}U_\zeta^2 = \frac{1}{6}P_3(U)$$

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Figure 1.3 Solitons can exist when $\beta < U < \gamma$.

where

$$P_3(U) = -U^3 + 3CU^2 + E_1U + E_2.$$

We will study the case when the third-order polynomial $P_3(U)$ can be factorized as $P(U) = -(U - \alpha)(U - \beta)(U - \gamma)$, with $\alpha \le \beta \le \gamma$; i.e., three real roots; when there is only one real root, it can be shown that the solution is unbounded. Since U_{ζ}^2 cannot be negative, one can conclude from the (U_{ζ}^2, U) phase plane diagram (see Figure 1.3) that a real periodic wave can exist only when U is between the roots β and γ , since only in this zone can the solution oscillate. In addition, it is straightforward to derive

$$3C = \alpha + \beta + \gamma, \qquad E_1 = -(\beta \gamma + \alpha \beta + \beta \gamma), \qquad E_2 = \alpha \beta \gamma.$$

Furthermore, the periodic wave solution takes the form

$$U(\zeta) = \beta + (\gamma - \beta)cn^2 \left[\left(\frac{\gamma - \alpha}{12\delta^2} \right)^{1/2} \zeta; m \right],$$

where cn(x; m) is the cosine elliptic function with modulus *m* [see Abramowitz and Stegun (1972) or Byrd and Friedman (1971) for more details about elliptic functions] and

$$m = \frac{\gamma - \beta}{\gamma - \alpha}.$$

The above solution is often called a "cnoidal" wave following the terminology of Korteweg and de Vries (1895).

In the special limit $\beta \rightarrow \alpha$, i.e., when the factorization has a double root (see Figure 1.4), we can integrate directly; it follows that m = 1, $C = (2\alpha + \gamma)/3$, and the solution can be put in the elementary form

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Figure 1.4 The limiting case of a double root ($\alpha = \beta$).



Figure 1.5 Hyperbolic secant solution approaches α as $|\zeta| \to \infty$.

$$U(\zeta) = \alpha + (\gamma - \alpha) \operatorname{sech}^2 \left[\left(\frac{\gamma - \alpha}{12\delta^2} \right)^{1/2} \zeta \right].$$

In this case $U \to \alpha$ as $|\zeta| \to \infty$ (see Figure 1.5).

If $\alpha = 0$ then the solution reduces to

$$U(\zeta) = \gamma \operatorname{sech}^{2}\left[\left(\frac{\gamma}{12\delta^{2}}\right)^{1/2}\zeta\right] = 3C\operatorname{sech}^{2}\left(\frac{\sqrt{C}}{2\delta}\zeta\right) = 12\delta^{2}\kappa^{2}\operatorname{sech}^{2}\kappa\zeta,$$

where $\kappa = \sqrt{C}/2\delta$.

We see that such traveling solitary waves propagate with a speed that increases with the amplitude of the waves. In other words, larger-amplitude waves propagate faster than smaller ones. In a truly important discovery, by studying the numerical simulations of the FPU problem, Zabusky and Kruskal (1965) found that these solitary waves had a special property. Namely the solitary waves of the KdV equation collide "elastically"; i.e., they found that after a

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Figure 1.6 "Elastic" collision of two solitons.

large solitary wave overtakes a small solitary wave their respective amplitudes and velocities tend to the amplitude and speed they had before the collision. This suggests that the speeds and amplitudes are invariants of the motion. In fact, the only noticeable change due to the interaction is a phase shift from where the wave would have been if there were no interaction. For example, in Figures 1.6 and 1.7 we see that the smaller soliton is retarded in time whereas the larger one is pushed forward. Zabusky and Kruskal called these elastically interacting waves "solitons". Further, they conjectured that this property of the collisions was the reason for the recurrence phenomenon observed by FPU.²

Subsequent research has shown that solitary waves with this elastic interaction property, i.e., solitons, are associated with a much larger class of equations than just the KdV equation. This has to do with the connection of solitons with nonlinear wave equations that are exactly solvable by the technique of the inverse scattering transform (IST). Integrable systems and IST are briefly covered in Chapters 8 and 9. It should also be mentioned that the term soliton has taken on a much wider scope than the original notion of Zabusky and Kruskal: in many branches of physics a soliton represents a solitary or localized type of wave. When we discuss a soliton in the original sense of Zabusky and Kruskal we will relate solitons to the special aspects of the underlying equation and its solutions.

² The detailed analysis of the recurrence phenomenon is quite intricate and will not be studied here.