Waves in Nonlinear Lattice

Morikazu Toda*)

Department of Applied Physics, Faculty of Science Tokyo University of Education, Tokyo

In this article waves in nonlinear lattice or in nonlinear medium are studied. One of the aims is to seek for the point of view to deal with the great majority of phenomena related to nonlinear waves in general. For one dimensional nonlinear lattice analytic and computer-experimental treatments have been developed. It has been found that a certain kind of pulse-like waves (solitons) is the fundamental motion in nonlinear lattice vibration. If two or more solitons collide, they interact nonlinearly, pass through one another and, when they separate, return to their original forms. Thus solitons are conserved and behave like particles.

§1. Introduction

The problem of wave motion in nonlinear media is interesting not only as purely mechanical problem, but also in connection with many physical phenomena such as shallow water-waves, plasma waves and heat conduction in crystal lattices. Since nonlinear phenomena have infinite variety compared with linear cases, it seems quite important to find the way to extend our pattern of thinking as to make it possible to understand the essence of nonlinear world.

Vibration of a system of particles joined by harmonic springs can be described by superposition of normal modes which are mutually independent. For instance, if we excite a normal mode, its energy is not transferred to other normal modes. The system of harmonic oscillations never reaches the state of thermal equilibrium, and is non-ergodic. Although the harmonic oscillator models give good results for the problems such as the specific heat and other equilibrium properties of crystals, the nonlinear terms ignored in these models have been considered by many people to play an essential role in the problem of approach to thermal equilibrium. However, since the nonlinear terms make calculation insurmountably complex, it is usually assumed that the nonlinear terms guarantee the ergodicity of the system and its approach to thermal equilibrium. Fermi, Pasta and Ulam (FPU)¹⁾ intended to verify this expectation by computer experiments. But contrary to their expectation the one-dimensional nonlinear lattice showed recurrence phenomena. Ford,²⁾ Jackson³⁾ and others further examined the same problem, and it was clarified that one-dimensional nonlinear lattices marvellously sustain the characters of linear lattices.

^{*)} Present address: Institute for Optical Research, Tokyo University of Education.

Now, one-dimensional nonlinear lattice can be considered as the model of nonlinear continuous medium, which can be obtained as a limit of long wave length or of small distance between particles of the lattice. If the deformation of the springs is small, the Hooke's law or the linear term will suffice. So for a little larger deformation, we may write the force of the spring as [linear term] + [nonlinear term]. When the nonlinear term is absent, in virtue of the superposition principle, we can analyze the general motion of the system in terms of suitable fundamental motion. As such, we usually use normal modes represented by sinusoidal waves. In the case of continuous harmonic medium, where dispersion phenomenon is absent, since arbitrary waves are propagated with the same speed keeping their initial wave forms, we can also take, for example, a suitable set of pulse-like waves as the fundamental motion, and express the general wave as the superposition of such pulses.

If the nonlinear term is regarded as perturbation, the expansion in terms of the normal modes yields the so-called secular terms which increases indefinitely with time. If we try to avoid such a kind of fault, as in the theory of nonlinear oscillations, we are led to unreasonably complicated analysis which lacks any sound mathematical basis. In place of such perturbational methods, some other ways must be sought for in order to develop new pattern of thinking essential to nonlinear problems.

Although any concept cannot, of course, be almighty as to cover all the nonliner phenomena, the concept of soliton, which will be described below, seems to have very wide applicability at least in the case of one-dimensional waves. A soliton is a pulse-like wave which travels through nonlinear media without changing its wave form. Its speed depends in general on the height of the pulse. When two solitons approach, they interact, pass through each other, and return to their initial forms. Thus soliton behave like stable particles and seems to be the fundamental motion in nonlinear wave propagation.

§2. Equation of motion of nonlinear lattice

2-1 Finite lattice

First we consider a finite uniform one-dimensional nonlinear lattice, which consists of N particles of mass m connected by nonlinear springs. We assume that the lattice is fixed at the left end, label the particles as $n=1, 2, \dots, N$ from left to right and assume pressure p applied on the right end particle (n=N). If the potential energy of a spring is denoted by $\phi(r)$, and its derivative by $\phi'(r) = d\phi/dr$, where r stands for the elongation of the spring over its natural length, the equation of motion can be written as

$$m\ddot{y}_{n} = -\phi'(y_{n} - y_{n-1}) + \phi'(y_{n+1} - y_{n}),$$

$$m\ddot{y}_{N} = -\phi'(y_{N} - y_{N-1}) - p, \qquad (n = 1, 2, \dots, N-1)$$
(2·1)

where y_n denotes the displacement of the *n*-th particle measured from the equilibrium position for p=0. Naturally $y_0=0$, and the mutual displacement of adjacent particle, or the elongation of the *n*-th spring, is given by

$$r_{n} = y_{n} - y_{n-1}, \qquad (2 \cdot 2)$$

or conversely

$$y_n = r_1 + r_2 + \dots + r_n. \tag{2.3}$$

The momentum s_n conjugate to r_n is, by definition,⁵⁾

$$s_n = \frac{\partial T}{\partial \dot{r}},\tag{2.4}$$

where T is the kinetic energy

$$T = \sum_{n=1}^{N} \frac{m}{2} \dot{y}_{n}^{2} \tag{2.5}$$

with

$$\dot{y}_n = \dot{r}_1 + \dot{r}_2 + \dots + \dot{r}_n. \tag{2.6}$$

Thus it is seen that

$$m\dot{y}_n = s_n - s_{n+1}, \quad s_{N+1} = 0.$$
 (2.7)

Since the pressure p can be considered to be due to the potential energy py_N , the hamiltonian of the system can be written as

$$H = \frac{1}{2m} \sum_{n=1}^{N} (s_n - s_{n+1})^2 + \sum_{n=1}^{N} {\{\phi(r_n) + pr_n\}}.$$
 (2.8)

Therefore the canonical equations of motion are given by

$$\dot{r}_{n} = \frac{1}{m} (2s_{n} - s_{n-1} - s_{n+1}), \qquad (2.9)$$

$$\dot{s}_n = -\{\phi'(r_n) + p\}.$$
 (2.9')

If we eliminate s_n , we get

$$m\ddot{r}_{s} = \phi'(r_{s-1}) + \phi'(r_{s+1}) - 2\phi'(r_{s}),$$
 (2·10)

$$\phi'(r_{N+1}) = -p \tag{2.10'}$$

which are equivalent to Eq. $(2 \cdot 1)$.

On the other hand, if Eq. (2.9') is solved for r_n to yield

$$r_{s} = -\frac{1}{m} \chi(\dot{s}_{s}) \tag{2.11}$$

eliminating r_* from Eqs. (2.9) and (2.11), we get

$$\frac{d}{dt}\chi(\dot{s}_{n}) = s_{n-1} + s_{n+1} - 2s_{n}. \qquad (2 \cdot 12)$$

This equation can be interpreted as the equation of motion of a linear chain of particles with "displacements" s_n and "momenta" $\chi(\dot{s}_n)$. In effect, we have interchanged the roles of r_n and s_n , and Eq. (2·12) describes the motion of the "dual lattice".⁵⁾

If we further introduce

$$S_n = \int_0^t s_n dt , \qquad (2 \cdot 13)$$

Eq. $(2\cdot12)$ can be written in a more convenient form:

$$\chi(\ddot{S}_n) = S_{n-1} + S_{n+1} - 2S_n. \tag{2.14}$$

Though the above treatment assumes finite length of the lattice, if we write n-N/2 in place of n and take the limit $N\to\infty$, we get an infinite lattice for which all the above equations are applicable.

2-2 Exponential lattice

In what follows we shall adopt the potential function which has been found to be quite appropriate and convenient. This is of the form⁵

$$\phi(r) = \frac{a}{b}(e^{-br} - 1) + ar,$$
 (ab>0) (2.15)

where the arbitrary additive constant has been chosen in such a way that $\phi(0)=0$. Since r=0 represents the natural state of the spring, $\phi'(0)=0$.

For small |b| we may expand the right-hand side of Eq. (3.1) to yield

$$\phi(r) = \frac{ab}{2} \left(r^2 - \frac{b}{3} r^3 + \cdots \right). \tag{2.16}$$

Thus, for small displacement the spring obeys the Hooke's law with the force constant K=ab. If we keep K=ab finite and take the limit $b\to 0$ we get harmonic system. If we put r=R-D and take limit $b\to \infty$ we will get the system of hard rods of diameter D where the distance between the centers of adjacent rods is represented by R.

If the one-dimensional lattice is subject to a constant pressure p, its effect is equivalent to that of the additional term pr in the potential energy (cf. Eq. $(2 \cdot 8)$). That is, we have only to replace $\phi(r)$ by

$$\phi(r) + pr = \frac{a}{b}e^{-br} + (a+p)r + \text{const}$$

$$= \frac{a'}{b}e^{-br'} + a'r' + \text{const}, \qquad (2.17)$$

where

$$a'=a+p, \qquad (2\cdot 18)$$

and

$$-d = r' - r = \frac{1}{b} \log \frac{a}{a + p} \tag{2.19}$$

represents the contraction of the nonlinear spring due to the pressure.

Therefore, rewriting r' and a' as r and a we can include the effect of the constant pressure in our formalism. In what follows, we will not explicitly deal with the pressure.

In this and the following chapters we want to simplify our notations by replacing r_* and t by dimensionless quantities:

$$br_n \rightarrow r_n$$
, $\sqrt{\frac{ab}{m}}t \rightarrow t$. (2·20)

Then the equation of motion $(2 \cdot 10)$ reduces to

$$\ddot{r}_{n} = 2e^{-r_{n}} - e^{-r_{n-1}} - e^{-r_{n+1}}. \tag{2.21}$$

We may call this lattice the exponential lattice.

Now, let us introduce η_n by

$$e^{-r_n} - 1 = \eta_n \tag{2.22}$$

or by

$$r_n = -\log(1 + \gamma_n). \tag{2.23}$$

Equation (2.21) yields

$$\frac{d^2}{dt^2}\log(1+\eta_n) = \eta_{n-1} + \eta_{n+1} - 2\eta_n. \qquad (2\cdot 24)$$

Further if we introduce $s_n = \int_{-\tau}^{\tau} \eta_n dt$, we have

$$r_n = -\log(1 + \dot{s}_n) \tag{2.25}$$

and we get the following equation, which corresponds to Eq. $(2 \cdot 12)$:

$$\frac{d}{dt}\log(1+\dot{s}_n) = s_{n-1} + s_{n+1} - 2s_n. \tag{2.26}$$

In the right hand side of the above equation, the integral constants have been set equal to zero, which is possible for an appropriate definition of s_n . Alternately if we define $S_n = \int_{-\infty}^{t} s_n dt$, we have

$$r_{s} = -\log(1 + \ddot{S}_{s}) \tag{2.27}$$

which implies that

$$e^{-r_n} - 1 = \ddot{S}_n . \tag{2.28}$$

Then Eq. $(2 \cdot 26)$ yields

$$\log(1+\ddot{S}_n) = S_{n-1} + S_{n+1} - 2S_n \tag{2.29}$$

and from Eq. $(2 \cdot 28)$ we get

$$r_n = 2S_n - S_{n-1} - S_{n+1}. (2.30)$$

In the above equations the integration constant has been chosen appropriately, so as to give the simplest expressions for the relation between r_n and S_n .

Now, we shall describe some properties and particular solutions of our nonlinear lattice.

2-3 Expansion due to vibration

It can be shown that in general motion in the lattice gives rise to expansion (if b>0, and contraction if b<0). We have to show that the average of r_n is positive.

The force on the n-th spring is

$$f_n = -\phi'(r_n) = e^{-br_n} - 1 = \eta_n$$
 (2.31)

The average of the force must vanish if the lattice as a whole is at rest. So, using Eq. $(2 \cdot 22)$ we have

$$\bar{\eta}_n = \overline{e^{-r_n}} - 1 = 0. \tag{2.31'}$$

However the same equation yields

$$r_n = -\log(1 + \eta_n) = -(\eta_n - \frac{1}{2}\eta_n^2 + \cdots).$$
 (2.32)

Therefore we see that for small oscillation

$$\overline{r_n} = \frac{1}{2} \overline{\eta_n^2} \tag{2.33}$$

which indicates that the lattice expands as it vibrates.

If we assume thermal equilibrium, the law of equipartition of energy can be used to estimate the effect of thermal motion in the weakly nonlinear lattice. Since in the usual units, the force constant of the spring is K=ab and the elongation is r_n/b , the equipartition of energy can be written as

$$\frac{ab}{2}\overline{\left(\frac{r_{\text{n}}}{b}\right)^2} = \frac{k_B T}{2}, \qquad (2.34)$$

where k_B is the Boltzman constant. Using Eq. (2.32) or $r_n \cong -\eta_n$, we find that $\eta_n^2 = (b/a)k_B T$, and therefore that

$$\frac{\overline{r_n}}{h} = \frac{1}{2a} k_B T. \tag{2.35}$$

This gives the thermal expansion of the system and is in accordance with the result given by the conventional statistical mechanics.

§3. Particular solutions

3-1 Soliton

In this section we describe particular solutions of Eqs. (2.21), (2.26) and (2.29) for r_n , s_n and S_n .

First we note the solution which represents a soliton,

$$e^{-r_*} - 1 = \beta^2 \operatorname{sech}^2(\alpha n \mp \beta t), \tag{3.1}$$

$$s_n = -\beta \tanh(\alpha n \mp \beta t), \tag{3.2}$$

$$S_n = \log \cosh(\alpha n \mp \beta t) + \text{const},$$
 (3.3)

where

$$\beta = \sinh \alpha$$
. (3.4)

The velocity, β/α , increases with the height of the pulse.

3-2 Collision of two solitons⁶⁾

The state with two solitons can be represented by

$$S_{n} = \log\{\cosh(\kappa n - \beta t) + B\cosh(\mu n - \gamma t + \delta)\} + \text{const}, \qquad (3.5)$$

where β , γ and β are functions of κ and μ , and δ is an arbitrary constant. While Eq. (3.5) gives the state with a soliton when $\kappa = \mu$, it represents two-soliton state when $\kappa \neq \mu$.

There are two cases. One of them is the case two solitons are running in the opposite directions, and the other is the case they are running in the same direction.

(i) The solution representing the state with two solitons running in the opposite directions is given by

$$\beta = 2 \sinh \frac{\mu}{2} \cosh \frac{\kappa}{2},$$

$$r = 2 \sinh \frac{\kappa}{2} \cosh \frac{\mu}{2},$$

$$B = \cosh(\kappa/2)/\cosh(\mu/2).$$
(3.6)

For $t \rightarrow -\infty$, the asymptotic form of the wave is

$$e^{-r_n} - 1 = \beta_i^2 \operatorname{sech}^2(\alpha_i n - \beta_i t + h), \qquad i = 1, 2,$$
 (3.7)

and for $t\rightarrow\infty$, it is

$$e^{-r_n} - 1 = \beta_i^2 \operatorname{sech}^2(\alpha_i n - \beta_i t - h), \qquad (3 \cdot 8)$$

where

$$\alpha_{i} = \frac{\kappa \pm \mu}{2}, \quad \beta_{i} = \frac{\beta \pm \gamma}{2},$$

$$e^{-k} = \sqrt{Be^{-\delta}}.$$
(3.9)

In the above asymptotic forms i=1 and 2 represent two solitons.

(ii) The state in which two solitons are running in the same direction is described by

$$\beta = 2 \sinh \frac{\kappa}{2} \cosh \frac{\mu}{2},$$

$$\gamma = 2 \sinh \frac{\mu}{2} \cosh \frac{\kappa}{2},$$

$$B = \sinh(\kappa/2)/\sinh(\mu/2).$$
(3·10)

Asymptotic forms for $t \to \pm \infty$ are also given by the same equations as Eqs. (3.7) to (3.9).

3-3 Wave train

There is another type of particular solutions which represent periodic wave or wave train. This can be written as⁵⁾

$$e^{-r_{\pi}} - 1 = (2K\nu)^{2} \left[dn^{2} \left\{ 2 \left(\nu t \mp \frac{n}{A} \right) K \right\} - \frac{E}{K} \right],$$
 (3.11)

where the frequency and the wave length Λ satisfy the dispersion relation

$$2K\nu = \left(\frac{1}{\sin^2 \frac{2K}{4}} - 1 + \frac{E}{K}\right)^{-1/2}.$$
 (3·12)

In the above formula sn and dn are the Jacobian elliptic functions, and K and E are the complete elliptic integrals of the first and the second kind respectively. These are all of the same modulus which we shall denote by $k(0 \le k \le 1)$. If we write the modulus k in these functions,

$$K=K(k),$$
 $E=E(k),$
 $\operatorname{sn} x=\operatorname{sn}(x,k),$ $\operatorname{dn} x=\sqrt{1-k^2\operatorname{sn}^2x}=\operatorname{dn}(x,k).$

The function $dn^2(2xK) - E/K$ is a periodic function of x with the period 1, and its Fourier expansion is

$$dn^{2}(2xK) - \frac{E}{K} = \frac{\pi^{2}}{K^{2}} \sum_{l=1}^{\infty} \frac{l \cos 2\pi l x}{\sinh(\pi l K'/K)}, \qquad (3.13)$$

where

$$K' = K(k'), \qquad k' = \sqrt{1 - k^2}.$$
 (3.14)

We see from the above formula that the average over a period of the right hand side of Eq. (3·13) or of Eq. (3·11) vanishes. This implies, as easily seen from the form of the function e^{-br} , that the lattice expands as a whole: $\bar{r}_n > 0$. This is in accordance with the argument in §2–3 that the lattice expands in general when it vibrates.

If the modulus k is very small, K' is very large and we may use the approximation for $k^2 \leqslant 1$ that

$$\exp(-\pi K'/K) \simeq k^2/16$$
,
 $K \simeq \frac{\pi}{2}$,
 $\sin x \simeq \sin x$. (3.15)

Then Eqs. $(3 \cdot 11)$ and $(3 \cdot 12)$ reduce to

$$r_n \simeq -\frac{\omega^2 k^2}{8} \cos\left(\omega t \mp \frac{2\pi n}{4}\right),$$
 (3.16)

$$\omega \simeq 2\sin\frac{\pi}{\Lambda}. \tag{3.17}$$

Therefore, for small modulus k, the wave train reduces to sinusoidal wave whose amplitude is proportional to k^2 . We see that the solution $(3\cdot11)$ contains all the normal modes of the linear lattice vibration as the limit of small amplitude. In the same limit, we have

$$s_n \cong \frac{\omega k^2}{8} \sin \left(\omega t \mp \frac{2\pi n}{4} \right), \qquad (3.18)$$

$$\eta_n = \dot{s}_n \simeq \frac{\omega^2 k^2}{8} \cos \left(\omega t \mp \frac{2\pi n}{4} \right). \tag{3.19}$$

3-4 Relation between the wave train and solitons

If the modulus k approaches to 1, the amplitude of the wave train or the height of the spikes gets larger, and the wave train takes the form of a sequence of pulse-like waves.

This can be understood if we note the identity

$$\mathrm{dn^2}(2xK) - \frac{E}{K} = \left(\frac{\pi}{2K'}\right)^2 \sum_{l=-\infty}^{\infty} \mathrm{sech^2}\left\{\frac{\pi K}{K'}(x-l)\right\} - \frac{\pi}{2KK'} \qquad (3\cdot20)$$

so that the wave train can be expressed as

$$e^{-r_{\pi}} - 1 = \sum_{l=-\infty}^{\infty} \beta^{2} \operatorname{sech}^{2} \{\beta t - \alpha (n - \Lambda l)\} - 2\beta \nu$$
 (3.21)

with

$$\alpha = \frac{\pi K}{K' \Lambda}, \quad \beta = \frac{\pi K}{K'} \nu.$$
 (3.22)

The right-hand side of Eq. (3·21) represents a sequence of infinite pulses at equal intervals of Λ , and with a downward shift of $2\beta\nu$. Each pulse is a sech²-wave and, as is seen in the next section, it is indeed a soliton: The wave train is a sequence of solitons progressing equidistantly. These solitons are mutually interacting, not independent of each other, and their speed is given by the dispersion relation of the wave train (Eq. (3·12)).

If we take the limit α =finite, $\Lambda \rightarrow \infty$, $k\rightarrow 1$, in Eq. (3·21), the wave train reduces to a soliton in an infinite lattice.

§4. Wave train and elliptic &-functions

4-1 Wave train in terms of ϑ_0

The elliptic ϑ -function, $\vartheta_0(x)$, has the period of 1 and satisfies the relation $^{7)}$

$$\frac{\vartheta_0(x+y)\vartheta_0(x-y)}{\lceil \vartheta_0(x)\rceil^2} = C\left\{1 + \nu^2 \frac{d^2}{dx^2} \log \vartheta_0(x)\right\}, \qquad (4\cdot 1)$$

where

$$C = C(y) = \left[\frac{\vartheta_0(y)}{\vartheta_0(0)}\right]^2 \left\{1 - \left(1 - \frac{E}{K}\right) \operatorname{sn}^2(2Ky)\right\}, \tag{4.2}$$

$$\nu^{2} = \nu^{2}(y) = \frac{\operatorname{sn}^{2}(2Ky)}{(2K)^{2} \left\{ 1 - \left(1 - \frac{E}{K} \right) \operatorname{sn}^{2}(2Ky) \right\}} . \tag{4.3}$$

Comparing Eq. (4·1) with Eq. (2·29), we find a special solution of the form

$$S_n = \log \left[\vartheta_0 \left(\nu t - \frac{n}{\Lambda} \right) / C^{n^2/2} \right], \tag{4.4}$$

where $y=1/\Lambda$, or

$$C = \left[\frac{\vartheta_0(1/\Lambda)}{\vartheta_0(0)} \right]^2 \left\{ 1 - \left(1 - \frac{E}{K} \right) \operatorname{sn}^2(2K/\Lambda) \right\}, \tag{4.5}$$

$$(2K\nu)^{2} = \left(\frac{1}{\operatorname{sn}^{2}} - 1 + \frac{E}{K}\right)^{-1}.$$
 (4.6)

This solution represents the same wave train we have been discussing in the preceding section. We can show this by using the relation between the ϑ -function and the Jacobian Z-function, or zn-function:

$$s_{n} = \dot{S}_{n} = \nu \frac{\vartheta_{0}' \left(\nu t - \frac{n}{\Lambda}\right)}{\vartheta_{0} \left(\nu t - \frac{n}{\Lambda}\right)}$$
$$= 2K\nu Z \left\{ 2\left(\nu t - \frac{n}{\Lambda}\right)K\right\}, \tag{4.7}$$

where Z(u) is related to dn by

$$Z(u) = \int_0^u \left(dn^2 u - \frac{E}{K} \right) du. \tag{4.8}$$

Therefore,

$$e^{-r_n} - 1 = \dot{S}_n = (2K\nu)^2 \left[dn^2 \left\{ 2\left(\nu t - \frac{n}{A}\right)K \right\} - \frac{E}{K} \right]$$
 (4.9)

coincides with Eq. (3.11), i.e. the wave train described in the preceding section.

Now, to see the amount of elongation due to vibration we take a part of the lattice which contains N particles such that N is a multiple of the wave length Λ . In other words, we think Λ to be, or very close to, a rational number and N includes an integral number of the wave length Λ . Then we have $r_{N+1}=r_1$; that is, the lattice is cyclic. The length of this part of the lattice is

$$\begin{split} r_1 + r_2 + \cdots + r_N &= (2S_1 - S_0 - S_2) + (2S_2 - S_1 - S_3) + \cdots + (2S_N - S_{N-1} - S_{N+1}) \\ &= (S_N - S_{N+1}) - (S_0 - S_1) \\ &= \log \left[\frac{\vartheta_0 \left(\nu t - \frac{N}{A} \right)}{\vartheta_0 \left(\nu t - \frac{1}{A} \right)} - \frac{\vartheta_0 \left(\nu t - \frac{1}{A} \right)}{\vartheta_0 (\nu t)} - \frac{C^{(N+1)^{2/2}}}{C^{N^{2/2}} C^{1/2}} \right] \\ &= N \log C. \end{split}$$

$$(4 \cdot 10)$$

We have used the fact that N/Λ is an integer and ϑ_0 is a periodic function with the period of 1, so that

$$\begin{split} &\vartheta_0\!\left(\nu t\!-\!\frac{N}{\varLambda}\right)\!=\!\vartheta_0\!\left(\nu t\right)\;,\\ &\vartheta_0\!\left(\nu t\!-\!\frac{N\!+\!1}{\varLambda}\right)\!=\!\vartheta_0\!\left(\nu t\!-\!\frac{1}{\varLambda}\right). \end{split}$$

It is therefore shown that the average length of the spring is given by

$$\bar{r} = \log C$$
. (4.11)

For small amplitude $(k^2 \le 1)$, expanding the right hand side of Eq. (4.5) in powers of k^2 (cf. Appendix I), we get

$$\log C \simeq \frac{k^2}{16} \sin^4 \frac{\pi}{4} \,. \tag{4.12}$$

Thus we have verified the fact that the lattice expands when it vibrates. Equation $(4\cdot12)$ is in accordance with the result using Eqs. $(2\cdot33)$, $(3\cdot17)$ and $(3\cdot19)$.

4-2 Decomposition of a wave train

 $\vartheta_0(x)$ is defined in product form as

$$\vartheta_0(x) = \vartheta_0(x, q) = \phi(q) \prod_{r=1}^{\infty} (1 - 2q^{2r-1}\cos 2\pi x + q^{4r-2}),$$
 (4·13)

where

$$\phi(q) = \prod_{r=1}^{\infty} (1 - q^{2r}). \tag{4.14}$$

The parameter q is related to the modulus k by the relation

$$q = e^{-\pi K'/K} . \tag{4.15}$$

Now, since

$$(1 - 2q_1\cos 2\pi x + q_1^2)(1 - 2q_1\cos 2\pi(x \pm \frac{1}{2}) \pm q_1^2) = 1 - 2q_1^2\cos 4\pi x + q_1^4,$$

$$(4 \cdot 16)$$

 $\vartheta_0(2x, q^2)$ can be written as

$$\vartheta_0(2x, q^2) = \varphi(q)\vartheta_0(x, q)\vartheta_0(x \pm \frac{1}{2}, q), \qquad (4.17)$$

where $\varphi(q)$ is a functional of q. This identity gives the following decomposition of a wave train into two wave trains:

$$S_{n}\left(\nu t - \frac{n}{A}\right) = \log \vartheta_{0}\left(\nu t - \frac{n}{A}, q\right) + \text{const}$$

$$= \log \vartheta_{0}\left(\frac{\nu}{2}t - \frac{n}{2A}, \sqrt{q}\right) + \log \vartheta_{0}\left(\frac{\nu}{2}t - \frac{n+A}{2A}, \sqrt{q}\right)$$

$$= S'_{n}\left(\frac{\nu}{2}t - \frac{n}{2A}\right) + S'_{n}\left(\frac{\nu}{2}t - \frac{n+A}{2A}\right), \tag{4.18}$$

or, in terms of $e^{-r_n}-1$,

$$e^{-r_{\bullet}} - 1 = \left\{ 2K(k)\nu \right\}^{2} \left[\operatorname{dn}^{2} \left\{ 2\left(\nu t - \frac{n}{A}\right)K(k), k \right\} - \frac{E(k)}{K(k)} \right]$$

$$= \left\{ K(\kappa)\nu \right\}^{2} \left[\operatorname{dn}^{2} \left\{ \left(\nu t - \frac{n}{A}\right)K(\kappa), \kappa \right\} - \frac{E(\kappa)}{K(\kappa)} \right]$$

$$+ \left\{ K(\kappa)\nu \right\}^{2} \left[\operatorname{dn}^{2} \left\{ \left(\nu t - \frac{n}{A} - 1\right)K(\kappa), \kappa \right\} - \frac{E(\kappa)}{K(\kappa)} \right], \quad (4 \cdot 19)$$

where the moduli k and κ are related by

$$\frac{K(k')}{2K(k)} = \frac{K(\kappa')}{K(\kappa)}. \qquad (k' = \sqrt{1 - k^2}, \quad \kappa' = \sqrt{1 - \kappa^2})$$
 (4·20)

Equation $(4\cdot19)$ shows that the wave train with the wave length Λ can be decomposed into two wave trains, component waves, each with the wave length 2Λ and progressing at the distance Λ . This means, conversely, that wave trains of the same form, with the wave length 2Λ and set at a distance Λ , can be superposed to yield a wave train. The speed of the wave train is determined by the dispersion relation of the resultant wave and not by that of the component waves. In general, the speed of a wave is controlled by the presence of other waves. This is one of the characters of nonlinear decomposition and superposition of nonlinear waves.

Each of the component wave with the wave length 2Λ can be further decomposed into waves each with the wave length 4Λ , and so forth. Or, more generally, we can decompose a wave train into three, or four, or into any integral number of wave trains. This can be verified by a extension of Eq. $(4\cdot17)$, that is, by the relation

$$\vartheta_0(lx, q') = \frac{\phi(q')}{\{\phi(q)\}'} \prod_{s=0}^{l-1} \vartheta_0\left(x + \frac{s}{l}, q\right). \tag{4.21}$$

Using this relation we get

$$\begin{split} e^{-r_{\kappa}} - 1 &= \{2K(k)\nu\}^{2} \left[\operatorname{dn}^{2} \left\{ 2\left(\nu t - \frac{n}{\Lambda}\right) K(k), k \right\} - \frac{E(k)}{K(k)} \right] \\ &= \left\{ 2K(\kappa) \frac{\nu}{l} \right\}^{2} \sum_{s=0}^{l-1} \left[\operatorname{dn}^{2} \left\{ 2\left(\frac{\nu}{l} t - \frac{n}{l\Lambda} + \frac{s}{l}\right) K(\kappa), \kappa \right\} - \frac{E(\kappa)}{K(\kappa)} \right] \end{split}$$

$$(4 \cdot 22)$$

with

$$\frac{K(k')}{lK(k)} = \frac{K(\kappa')}{K(\kappa)}.$$
 (4.23)

This decomposition means that the wave train with the wave length Λ can be considered as a superposition of l wave trains each with the wave length $l\Lambda$ and set equidistantly at the distance Λ .

If we take the limit $l \to \infty$ we see that $\kappa \to 1$ and Eq. (4·22) reduces to Eq. (3·21) as it should. A wave train can be considered as a superposition of pulse like waves, which, as will be seen in what follows, are actually solitons.

4-3 Solitons and wave trains in a ring (Cyclic boundary condition)

Though we have treated a wave train as if it is in an infinite lattice $(-\infty < n < \infty)$, we can consider such a periodic wave as a wave in a ring $(0 \le n \le N)$ whose length is an integral multiple of the wave length, i.e. N/A=integer. Therefore, we can superpose or decompose a wave train under

periodic boundary condition in a similar manner as we have done in an infinite lattice. We have only to renew the labels appropriately; that is, in place of the labels $(\cdots, -1, 0, 1, \cdots, N, N+1, \cdots)$, we have $(\cdots, N-1, N, 1, \cdots, N, 1, \cdots)$.

We consider a ring of N particles $n=1, 2, \dots, N$. n=0 means n=N, and $r_{N+1}=r_1$, or $r_{N+n}=r_n$.

The solution representing a wave with only a spike in the ring may be called a soliton under the cyclic boundary condition. Such a soliton is given by

$$\begin{split} S_{\mathbf{n}} &= \log \left[\vartheta_{\mathbf{0}} \left(\nu_{\mathbf{s}} t - \frac{n}{\Lambda} \right) \middle/ \left\{ C(1/N) \right\}^{n^2/2} \right], \\ e^{-r_{\mathbf{n}}} &- 1 = \left\{ 2K(\kappa) \nu_{\mathbf{s}} \right\}^2 \left[\operatorname{dn}^2 \left\{ 2 \left(\nu_{\mathbf{s}} t - \frac{n}{N} \right) K(\kappa), \kappa \right\} - \frac{E(\kappa)}{K(\kappa)} \right], \quad (4 \cdot 24) \end{split}$$

where the modulus is written as κ and the frequency as ν_s , which is given by

$$2K(\kappa)\nu_{s} = \left\{ \frac{1}{\operatorname{sn}^{2} \frac{2K(\kappa)}{N}} - 1 + \frac{E(\kappa)}{K(\kappa)} \right\}^{-1/2}.$$
(4.25)

If we set two such solitons so that they are separated from each other by the distance N/2 apart, a wave train with two spikes in the ring is obtained. The modulus k of the wave train is related to the modulus of the solitons by Eq. $(4\cdot20)$, and the frequency or the speed of the wave train is given by Eq. $(4\cdot6)$ with $\Lambda=N/2$.

In general, from the solutions for an infinite lattice, for instance Eq. (4.9), we can make the wave trains in the ring. In the limit of small amplitude, they reduce to the normal modes of the ring in the harmonic limit. Thus the wave train with, say m spikes, may be called the m-th "normal mode" of the nonlinear ring.

However, the nonlinear normal mode has the peculiar character that it can be decomposed into other normal modes as stated above: If the number of spikes is a multiple of some integer l, it can be decomposed into l wave trains, and it can be decomposed into as many solitons in the ring as the number of spikes present. Thus it is seen that the nonlinear "normal modes" are not the fundamental motion, but they are superposition of solitons. Therefore the solitons are to be considered as the fundamental motion of the nonlinear lattice.

A soliton in the ring has a spike where $r_n < 0$ (lattice contracts) and a tail where $r_n > 0$ (lattice elongates). It is given by Eq. (4·24). However, we shall study it for a large ring $(N \gg 1)$.

It is convenient to use Eq. (3·21) with $\Lambda = N$ for such a soliton. If we want to keep the width $\alpha^{-1} = K'N/\pi K$ finite for $N \gg 1$, we have to assume the case $K/K' \gg 1$ or the case where the modulus $k \approx 1$. Thus for $N \gg 1$,

the soliton can be approximated by

$$e^{-r_*} - 1 \cong \beta^2 \operatorname{sech}^2(\beta t - \alpha n) - 2\beta \nu, \quad \left(-\frac{N}{2} \leq n \leq \frac{N}{2}\right)$$
 (4.26)

where $\beta \cong 2K\nu$. However for the limit $k \to 1$, since $\operatorname{sn} x \cong \tanh x$, $E/K \cong 0$, the dispersion relation $(3 \cdot 12)$ yields $(\alpha = 2K/N)$

$$\beta \simeq 2K_{\nu} = \sinh \alpha$$
, (4.27)

which is the dispersion relation for the soliton, its speed being $\beta/\alpha = \sinh \alpha/\alpha$. The first term of Eq. (4·26) represents the spike where the lattice is contracted and the second term represents the tail where it is elongated.

The total change of the length of the ring can be evaluated using Eq. $(4\cdot10)$ or $(4\cdot11)$. In the limit stated above,

$$\frac{\vartheta_0(y)}{\vartheta_0(0)} \cong e^{-\pi K y^2/K'} \cosh\left(\frac{\pi K}{K'}y\right) \qquad \left(y = \frac{1}{N}\right) \qquad (4 \cdot 28)$$

and therefrom

$$C \simeq \exp\left\{\frac{1}{K}\sinh^2\left(\frac{2K}{N}\right) - \frac{4K}{N^2}\right\}. \tag{4.29}$$

The change in the length of the ring is $(\alpha = 2K/N)$

$$R = \sum_{n=1}^{N} r_n = N \log C = 2\alpha \left\{ \left(\frac{\sinh \alpha}{\alpha} \right)^2 - 1 \right\}$$
 (4.30)

which is always positive. It is therefore shown that, although the spike of the soliton represents compression of the lattice, the trough gives small $(\sim 1/N)$ but non-negligible contribution to elongation, and as a whole, the soliton gives elongation of the lattice. In the case of infinite lattice the infinitesimal elongation in the infinitely long trough gives rise to a finite elongation of the lattice given by Eq. $(4\cdot30)$. So we must note the fact that soliton expressed, for instance, by Eqs. $(3\cdot1)$ to $(3\cdot4)$ implies no elongation formally, it should be complemented by the total elongation R given by this equation.

§5. Continuum limit

(Korteweg-de Vries equation)

If the wave form varies slowly compared with the distance between particles, the continuum limit is generally valid. We may apply the operation rule

$$e^{\pm d/dn}f(n) = f(n+1) \tag{5.1}$$

to $r(n,t) = r_n(t)$ and rewrite Eq. (2.21) as

$$\frac{\partial^2 r}{\partial t^2} + \left[2 \sinh \left(\frac{1}{2} \frac{\partial}{\partial n} \right) \right]^2 e^{-r} = 0.$$
 (5·2)

If we neglect higher order derivatives, and higher powers of r, we can rewrite the above equation as

$$\left(\frac{\partial}{\partial t} - 2\sinh\frac{1}{2}\frac{\partial}{\partial n} + \frac{1}{2}\frac{\partial}{\partial n}r\right)\left(\frac{\partial}{\partial t} + 2\sinh\frac{1}{2}\frac{\partial}{\partial n} - \frac{1}{2}r\frac{\partial}{\partial n}\right)r = 0. \quad (5\cdot3)$$

The operators here are to operate on all the terms on the right. Thus for the wave which advance to the right, we have

$$\left(\frac{\partial}{\partial t} + 2\sinh\frac{1}{2}\frac{\partial}{\partial n} - \frac{1}{2}r\frac{\partial}{\partial n}\right)r = 0$$
 (5.3')

or, if we expand sinh,

$$\left(\frac{\partial}{\partial t} + \frac{\partial}{\partial n} - \frac{1}{12} \frac{\partial^3}{\partial n^3} - \frac{1}{2} r \frac{\partial}{\partial n}\right) r = 0.$$
 (5.4)

(For the wave advancing to the left we have to change n by -n.) If we recover the usual unit to see the effect of potential parameters, looking back Eq. $(2 \cdot 20)$, we get

$$\sqrt{\frac{m}{ab}} \frac{\partial r}{\partial t} + \frac{\partial r}{\partial n} - \frac{1}{12} \frac{\partial^3 r}{\partial n^3} - \frac{b}{2} r \frac{\partial r}{\partial n} = 0.$$
 (5.5)

Now, we introduce

$$u = \gamma r$$
, $\tau = \beta \sqrt{\frac{ab}{m}} t$, $\xi = \frac{\mu}{N} \left(n - \sqrt{\frac{ab}{m}} t \right)$ (5.6)

where γ , β , μ and N are constants. Then Eq. (5.5) reduces to

$$\frac{\partial u}{\partial r} + \sigma u \frac{\partial u}{\partial z} + \delta^2 \frac{\partial^3 u}{\partial z^3} = 0 \tag{5.7}$$

with

$$\sigma = -\frac{\mu b}{2\gamma\beta N}, \quad \delta^2 = \frac{\mu^3}{24\beta N^3}. \tag{5.8}$$

Equation (5·7) is the Korteweg-de Vries equation⁸⁾ which is used to describe shallow water wave, plasma wave and nonlinear lattice waves.

KdV equation has been discussed using various scales, which correspond to suitable choice of the constants α , β , μ and N.

Let us use the units for which $\sigma=1$ in the following discussion.

KdV equation has special solutions representing soliton and wave train respectively. A soliton is given by

$$u = u_{\infty} + A \operatorname{sech}^{2} \tilde{a}(\xi - \tilde{c}\tau),$$
 (5.9)

where

$$\tilde{c} = u_{\infty} + \frac{A}{3}, \quad \tilde{a} = \frac{1}{\delta} \sqrt{\frac{A}{12}}.$$
 (5·10)

This can be derived quite easily as a limit of the lattice soliton given by Eq. $(3\cdot1)$ using the transformation described by Eq. $(5\cdot6)$, and some modification to include u_{∞} , the uniform strain at infinity. In a similar manner, we can derive the state with two solitons of KdV equation from Eq. $(3\cdot5)$. Further, corresponding to the wave train in the lattice we have the wave train of the KdV equation:

$$u = u_{\infty} + A \operatorname{cn}^{2} \tilde{a}(\xi - \tilde{c}\tau), \tag{5.11}$$

where (k is the modulus of the cn-function)

$$\tilde{c} = u_{\infty} + \frac{A}{3} \left(2 - \frac{1}{k^2} \right),$$

$$\tilde{a} = \frac{1}{k\hbar} \sqrt{\frac{A}{12}}.$$
(5·12)

This is called a cnoidal wave.⁸⁾ Equation (5·11) approaches to a soliton, Eq. $(5\cdot9)$, as the modulus k approaches to 1.

It has been shown very useful to consider the eigen-value equation (Schrödinger type equation)⁹⁾

$$6\delta^2 \frac{d^2 \psi^{(I)}}{d\xi^2} - (U - \lambda_I) \psi^{(I)} = 0 \tag{5.13}$$

for the KdV equation ($\sigma=1$), where

$$U = -u, (5.14)$$

since the eigen-value λ_i are independent of time, though u evolves with time according to the KdV equation:⁹⁾

$$\frac{d\lambda_i}{d\tau} = 0. ag{5.15}$$

Such a invariant property of the eigen-values may be used to predict the number and the height of solitons which will emerge out of the initial wave form.

If the initial wave $U(\xi,0)$ is very large, or if δ^2 is very small, there will be many eigen-values, and these may be evaluated by means of the WKB method, or by the "quantum condition" where $\sqrt{12\delta^2}$ replaces \hbar :

$$J = \oint p d\xi = (n + \frac{1}{2}) 2\pi \sqrt{12\delta^2} \qquad (n = 0, 1, 2, \dots) \quad (5 \cdot 16)$$

in which the momentum p is given, in terms of energy, by

$$p = \sqrt{2(E - U)}. \tag{5.17}$$

Therefore the number of eigen-values between E and E+dE can be approximated by

$$\frac{dn}{dE}dE = \frac{dE}{2\pi\sqrt{12\delta^2}} \oint \frac{d\xi}{\rho} . \tag{5.18}$$

For instance, if $U(\xi,0)$ is maximum at $\xi=0$ and symmetric with respect to $\xi=0$, such that

$$U = -U_0 \mathbf{0}(\boldsymbol{\xi}), \tag{5.19}$$

where U_0 is the maximum value at $\xi=0$. Putting

$$\boldsymbol{\phi}(\boldsymbol{\xi}) = \boldsymbol{z}, \quad -\frac{d\boldsymbol{\phi}}{d\boldsymbol{\xi}} = \boldsymbol{\Psi}(\boldsymbol{z}) \tag{5.20}$$

we have

$$\frac{dn}{dE} = \frac{2}{\pi \sqrt{12\delta^2}} \sqrt{\frac{2}{U_0}} \int_0^{\sqrt{1-\frac{|E|}{U_0}}} d\lambda / \Psi \left(\lambda^2 + \frac{|E|}{U_0} \right). \tag{5.21}$$

Since the height of the soliton with the eigen-value $\lambda = E$ is equal to A = 2|E|, we put

$$\eta = \frac{A}{U_0} = 2 \frac{|E|}{U_0} \tag{5.22}$$

and write the number of solitons between η and $\eta + d\eta$ by $f(\eta)d\eta$. We get

$$f(\eta) = \frac{dn}{dE} \frac{dE}{d\eta} = \frac{\sqrt{U_0}}{\pi \sqrt{6\delta^2}} \int_0^{\sqrt{1-\frac{\eta}{2}}} d\lambda / \Psi \left(\lambda^2 + \frac{\eta}{2} \right) \qquad (\eta \le 2)$$

$$= 0. \qquad (\eta \ge 2) \qquad (5.23)$$

This is in accordance with the result given by Karpman.¹⁰⁾
For example, if the initial wave is

$$U(\xi,0) = -U_0 \operatorname{sech}^2 \alpha \xi \tag{5.24}$$

we get

$$f(\eta) = \frac{1}{\alpha} \sqrt{\frac{U_0}{48\eta \delta^2}}.$$
 (5.25)

And the total number of solitons is

$$N = \int_0^2 f(\eta) d\eta = \frac{1}{\alpha} \sqrt{\frac{U_0}{6\delta^2}}.$$
 (5.26)

Whereas the exact eigen-values in this case are

$$\lambda_n = -6\alpha\delta^2 \left(\frac{p}{\alpha} - n\right)^2, \tag{5.27}$$

where we have put

$$U_0 = 6\delta^2 p(p + \alpha). \tag{5.28}$$

If U_0 is very large, the total number of the eigen-values is $N \simeq p/\alpha \simeq \sqrt{U_0/6\delta^2}/\alpha$, in accordance with the above result.

§6. Recurrence phenomena

Studying the KdV equation by computer-experiment, Zabusky and Kruskal¹¹⁾ found recurrence to initial state. This phenomenon can be interpreted as follows.

Consider the initial wave of the form

$$u|_{\tau=0} = A\cos\pi\xi$$
. $(0 \le \xi \le 2)$ $(6 \cdot 1)$

We take the cyclic boundary-condition $u(\xi) = u(\xi + 2)$. Assuming A to be much smaller than $\sqrt{12\delta^2}$, we expand the potential $U = -u|_{\tau=0}$ as

$$U = -A\cos\pi\xi \cong -A + \frac{A\pi^2}{2}\xi^2 \tag{6.2}$$

to obtain the approximate eigen-values

$$\lambda_n = -A + (n + \frac{1}{2})\sqrt{12\delta^2 A \pi^2}. \tag{6.3}$$

The solitons associated to these eigen-values travel, interact as they collide and pass through one another. If we neglect the acceleration during interaction, solitons will travel independently. The velocities of solitons in the above approximation form an arithmetical series with the common difference

$$\Delta \tilde{c} = \frac{2}{3} \sqrt{12 \delta^2 A \pi^2} \,. \tag{6.4}$$

When these solitons move in the region of length 2, there comes again the state with the same mutual situation as the initial state after the time interval

$$\tau_{R} = \frac{2}{\Delta \tilde{c}} = \frac{\sqrt{3}}{2\pi\sqrt{A}\delta} = \frac{0.364}{\sqrt{A}\delta}.$$
 (6.5)

This is the recurrence time in our approximation. If we put A=1, $\delta=0.0222$ we get the recurrence time $\tau_R=40/\pi$, which is to be compared with the experimental value $\tau_R=30.4/\pi$ observed under the same condition. The discrepancy will be due to the change in speed of solitons during interaction. In actuality, solitons were rather close to each other and therefore not mutually independent in this experiment.

Fermi, Pasta and Ulam¹⁾ found the recurrence of the nonlinear lattice.¹²⁾ In this case computer experiment was done under fixed-end condition.

The relation between the KdV continuum of length 2 to the lattice of length 2N, can be obtained if we refer to Eq. (5.6):

$$\nu = -b, \quad \beta = \frac{1}{2N}, \quad \mu = 1, \quad \delta^2 = 1/12N^2.$$
 (6.6)

Denoting by y_n the displacement of the *n*-th particle in the lattice, we assume the initial condition

$$y_n|_{t=0} = B\sin\frac{\pi n}{N} \tag{6.7}$$

with fixed ends. The stationary wave thus generated may be approximated by the superposition of two progressive waves travelling in opposite directions,

$$y_{\pi}|_{t=0} = \frac{B}{2} \sin \frac{\pi n}{N} \tag{6.8}$$

which corresponds to

$$u_n \approx \gamma \frac{\partial y_n}{\partial n} = -\frac{\pi b B}{N} \cos \pi \xi. \tag{6.9}$$

Therefore if we put

$$A = -\frac{\pi bB}{N} \tag{6.10}$$

Eq. (6.7) takes the same form as Eq. (6.1). Therefore the recurrence time of the lattice is, referring to Eqs. (5.6), (6.6) and (6.5), given by

$$t_{R} = \tau_{R} \frac{2N}{\sqrt{ab/m}} = \frac{3N^{3/2}}{\pi^{3/2}b^{1/2}\sqrt{B}} t_{L}, \qquad (6.11)$$

where $t_L = 2N/\sqrt{ab/m}$ is the time necessary for a wave of extremely long wave length to travel the lattice of length 2N. Equation (6·11) is to be compared with experimental results, which reveals that¹⁸⁾

$$t_{R} = \frac{0.4N^{8/2}}{\sqrt{\alpha B/h}}, \qquad (6.12)$$

where $\alpha = bh/2$ is the nonlinearity constant used FPU, h represents the natural length of a spring, B/h is the initial amplitude measured in units of h. We see that theoretical expectation $(6\cdot11)$ is very close to experimental results $(6\cdot12)$.

Appendix I

Formulas of elliptic functions

Calculations involving elliptic functions are sometimes annoying because

of the lack of suitable tables of formulas. Here we summarize those formulas, which seem appropriate to be listed in connection with the present calculation, including some integrals.

a) Complete elliptic integrals:

$$K = K(k) = \int_{0}^{\pi/2} \frac{d\theta}{\sqrt{1 - k^{2} \sin^{2} \theta}}$$

$$= \int_{0}^{1} \frac{dx}{\sqrt{(1 - x^{2})(1 - k^{2} x^{2})}},$$

$$E = E(k) = \int_{0}^{\pi/2} \sqrt{1 - k^{2} \sin^{2} \theta} \, d\theta$$

$$= \int_{0}^{1} \sqrt{\frac{1 - k^{2} x^{2}}{1 - x^{2}}} \, dx,$$

$$K(k) = \frac{\pi}{2} \left(1 + \frac{1}{4} k^{2} + \frac{9}{64} k^{4} + \cdots \right), \quad (k \le 1)$$

$$E(k) = \frac{\pi}{2} \left(1 - \frac{1}{4} k^{2} - \frac{9}{64} \frac{k^{4}}{3} - \cdots \right), \quad (k \le 1)$$

$$K(k) \to \log \frac{4}{\sqrt{1 - k^{2}}}, \quad E(k) \to 1, \quad (k \to 1)$$

$$K(k') \equiv K', \quad E(k') \equiv E', \quad k' = \sqrt{1 - k^{2}}.$$

b) Jacobian elliptic functions:

$$u = \int_0^{\mathfrak{p}} \frac{d\theta}{\sqrt{1 - k^2 \sin^2 \theta}} = \int_0^{\sin \mathfrak{p}} \frac{dx}{\sqrt{(1 - x^2)(1 - k^2 x^2)}},$$

$$\sin u = \sin \varphi = \sin(u, k),$$

$$\cot u = \cos \varphi = \cot(u, k),$$

$$\det u = \sqrt{1 - k^2 \sin^2 u} = \det(u, k),$$

$$\sin(u, 0) = \sin u, \ \cot(u, 0) = \cos u,$$

$$\sin(u, 1) = \tanh u, \ \cot(u, 1) = \det(u, 1) = \operatorname{sech} u,$$

$$\frac{d}{du} \sin u = \cot u \, \operatorname{dn} u,$$

$$\frac{d}{du} \cot u = -\sin u \, \operatorname{dn} u,$$

$$\sin u = \frac{2\pi}{kK} \sum_{n=0}^{\infty} \frac{q^{n+1/2}}{1 - q^{2n+1}} \sin(2n+1) \frac{\pi x}{2K},$$

$$\cot u = \frac{2\pi}{kK} \sum_{n=0}^{\infty} \frac{q^{n+1/2}}{1 + q^{2n+1}} \cos(2n+1) \frac{\pi x}{2K},$$

$$\begin{split} \operatorname{dn} u &= \frac{\pi}{2K} + \frac{2\pi}{K} \sum_{n=1}^{\infty} \frac{q^n}{1 + q^{2n}} \cos\left(\frac{n\pi x}{2K}\right), \\ \operatorname{dn}^2 u - \frac{E}{K} &= \frac{2\pi^2}{K^2} \sum_{n=1}^{\infty} \frac{nq^n}{1 - q^{2n}} \cos\left(\frac{n\pi x}{K}\right), \\ \operatorname{dn}^2 (2xK) - \frac{E}{K} &= \left(\frac{\pi}{2K'}\right)^2 \sum_{l=-\infty}^{\infty} \operatorname{sech}^2 \frac{\pi K}{K'} (u - l) - \frac{\pi}{2KK'}, \\ Z(u) &= \int_0^u \left(\operatorname{dn}^2 u - \frac{E}{K}\right) du \\ &= \frac{2\pi}{K} \sum_{n=1}^{\infty} \frac{q^n}{1 - q^{2n}} \sin\left(\frac{n\pi u}{K}\right) \\ &= \frac{\pi}{K} \sum_{n=1}^{\infty} \frac{\sin(n\pi u/K)}{\sinh(n\pi K'/K)}, \\ q &= e^{-\pi K'/K} \\ &= \left(\frac{k}{4}\right)^2 \left(1 + \frac{k^2}{2} + \frac{21}{64}k^4 + \cdots\right), \quad (k \ll 1) \\ Z(u + v) + Z(u - v) - 2Z(u) &= -2k^2 \frac{\operatorname{sn}^2 u \operatorname{cn} u \operatorname{dn} u \operatorname{sn}^2 v}{D(u, v)} \\ &= \frac{d}{du} \log D(u, v), \\ \operatorname{dn}^2 (u + v) + \operatorname{dn}^2 (u - v) - 2\operatorname{dn}^2 u &= \frac{d^2}{du^2} \log D(u, v), \\ \int_0^u \int_0^v \left\{ \operatorname{dn}^2 (u + v) - \operatorname{dn}^2 (u - v) \right\} du dv &= \log D(u, v), \\ D(u, v) &= 1 - k^2 \operatorname{sn}^2 v \operatorname{sn}^2 u &= \operatorname{cn}^2 v + \operatorname{sn}^2 v \operatorname{dn}^2 u. \end{split}$$

c) Elliptic &-functions:

$$\begin{split} \vartheta_0(x) &= \vartheta_0(x,q) = \vartheta_0(x|\tau), \quad (\tau = iK'/K) \\ \vartheta_0(x+1) &= \vartheta_0(x), \\ \vartheta_0(x|\tau) &= \sqrt{\frac{i}{\tau}} e^{-i\pi x^2/\tau} \vartheta_0 \left(\frac{x}{\tau} \left| -\frac{1}{\tau} \right| \right), \\ \vartheta_0(x) &= \sum_{n=-\infty}^{\infty} (-1)^n q^{n^2} z^{2n} \\ &= 1 + 2 \sum_{n=1}^{\infty} (-1)^n q^{n^2} \cos 2\pi n x \\ &= \sqrt{\frac{K}{K'}} \sum_{n=-\infty}^{\infty} (-1)^n e^{-\frac{\pi K}{K'}(x-\frac{1}{2}+n)^2} \\ &= 2 \sqrt{\frac{K}{K'}} e^{-\frac{\pi K}{K'} x^2} \sum_{n=0}^{\infty} e^{-\frac{\pi K}{K'}(n+\frac{1}{2})^2} \cosh \frac{\pi K}{K'} (2n+1) x \,, \end{split}$$

$$\begin{split} \vartheta_0(x) &= \phi(q) \prod_{l=1}^{\infty} (1 - q^{2l-1}x^2) (1 - q^{3l-1}/z^2) \\ &= \phi(q) \prod_{l=1}^{\infty} (1 - 2q^{2l-1} \cos 2\pi x - q^{4l-2}) \\ &= \vartheta_0(0) e^{\frac{\pi K}{K'}z^2} \cosh\left(\frac{\pi K}{K'}x\right) \prod_{l=1}^{\infty} \frac{\cosh\frac{\pi K}{K'} (l - x) \cosh\frac{\pi K}{K'} (l + x)}{\left\{\cosh\frac{\pi K}{K'}l\right\}^2} \,, \\ \phi(q) &= \prod_{n=1}^{\infty} (1 - q^{2n}), \quad z = e^{i\pi z} \,, \\ \vartheta_0(lx, q^l) &= \frac{\phi(q^l)}{\{\phi(q)\}^l} \prod_{s=0}^{l-1} \vartheta_0\left(x + \frac{s}{l}, q\right), \\ \frac{d}{du} \log \vartheta_0\left(\frac{u}{2K}\right) = Z(u), \\ \frac{d^2}{du^2} \log \vartheta_0\left(\frac{u}{2K}\right) = \operatorname{dn}^2 u - \frac{E}{K} \,, \\ \frac{d^2}{dx^2} \log \vartheta_0(x) &= \frac{\vartheta_0''(0)}{\vartheta_0(0)} - \left[\frac{\vartheta_1(0)}{\vartheta_0(0)}\right]^2 \left[\frac{\vartheta_1(x)}{\vartheta_0(x)}\right]^2, \\ \frac{\vartheta_0(x - y)\vartheta_0(x + y)}{\{\vartheta_0(x)\}^2} &= \frac{1}{[\vartheta_0(0)]^2} \left\{ [\vartheta_0(y)]^2 - [\vartheta_1(y)]^2 \left[\frac{\vartheta_1(x)}{\vartheta_0(x)}\right]^2 \right\} \\ &= C \left\{ 1 + \nu^2 \frac{d^2}{dx^2} \log \vartheta_0(x) \right\} \,, \\ C = C(y) &= \left[\frac{\vartheta_0(y)}{\vartheta_0(0)}\right]^2 D_1(y), \\ y^2 &= v^2(y) = \operatorname{sn}^2(2Ky) D_1(y)/(2K)^2, \\ D_1(y) &= 1 - \left(1 - \frac{E}{K}\right) \operatorname{sn}^2(2Ky) \\ &= \operatorname{cn}^2(2Ky) + \frac{E}{K} \operatorname{sn}^2(2Ky), \\ \frac{\vartheta_0\left(\frac{u + v}{2K}\right)}{2K} \vartheta_0\left(\frac{v}{2K}\right)} \right]^2 [\vartheta_0(0)]^2 = D(u, v), \\ \left[\frac{\vartheta_0\left(\frac{u}{2K}\right)}{\vartheta_0\left(\frac{v}{2K}\right)}\right]^2 \left[\vartheta_0(0)]^2 - D(u, v), \\ \int_0^{2\kappa} \log D(u, v) du &= 4K \log \frac{\vartheta_0(0)}{\vartheta_0\left(\frac{v}{2K}\right)} \,. \end{split}$$

Appendix II

Another expression for wave train

Rewriting Eq. (3.11) for a wave train, we can easily verify that

$$e^{-r_n} = \frac{D(\kappa, u)}{D_1(\kappa)},$$

where

$$D(\kappa, u) = \operatorname{cn}^2 \kappa + \operatorname{sn}^2 \kappa \operatorname{dn}^2 u,$$

$$D_1(\kappa) = \operatorname{cn}^2 \kappa + \frac{E}{K} \operatorname{sn}^2 \kappa$$
,

$$\kappa = 2K/\Lambda$$
,

$$u=2\left(\nu t-\frac{n}{4}\right)K$$
.

If we put

$$\bar{r} = \log C$$

with

$$C = \left(\frac{\vartheta_0\left(\frac{\kappa}{2K}\right)}{\vartheta_0(0)}\right)^2 D_1(\kappa)$$

then we have

$$e^{-(r_n-\bar{r})} = \left(\frac{\vartheta_0\left(\frac{\kappa}{2K}\right)}{\vartheta_0(0)}\right)^2 D(\kappa, u).$$

However, since we have (cf. Appendix 1)

$$\int_0^{2\kappa} \log D(\kappa, u) du = 2K \log \left(\frac{\vartheta_0(0)}{\vartheta_0\left(\frac{\kappa}{2K}\right)} \right)^2.$$

We see that the time average of r_n is just \bar{r} :

$$\int_{\text{period}} (r_n - \bar{r}) dt = 0.$$

Appendix III

Momentum and energy of a soliton

a) Momentum

The momentum of a particle in the lattice is given by

$$m\dot{y}_n \sim s_n - s_{n+1}$$
. (A III·1)

For the soliton in a ring as given by Eq. (4.24), s_* is cyclic,

$$s_n = \dot{S_n} = \nu_s \frac{\vartheta_0' \left(\nu_s t - \frac{n}{N}\right)}{\vartheta_0 \left(\nu_s t - \frac{n}{N}\right)}$$

$$=2K\nu_s Z\left\{2\left(\nu_s t-\frac{n}{N}\right)K\right\}\,, \tag{A III}\cdot 2)$$

and therefore the total momentum vanishes:

$$\sum_{n=1}^{N} m \dot{y}_n = 0. \tag{A III · 3}$$

This can also be shown by the time average,

$$\int m\dot{y}_n dt \sim \int s_n dt - \int s_{n+1} dt = 0.$$
 (A III · 4)

For a large ring, we can use the approximation $(4 \cdot 26)$ and its integrated form,

$$s_n \simeq \beta \tanh(\beta t - \alpha n) - 2\nu_s(\beta t - \alpha n)$$
 (A III·5)

which yields

$$m\dot{y}_{n}\sim\beta\frac{\sinh\alpha}{\sinh^{2}\left(\beta t-\alpha n-\frac{\alpha}{2}\right)+\cosh^{2}\frac{\alpha}{2}}-2\nu_{s}\alpha$$
, (A III·6)

and the time average vanishes again:

$$\int_0^{1/\nu_s} m \dot{y}_s dt \sim \beta \int_{-\infty}^{\infty} \frac{\sinh \alpha dt}{\sinh^2 \beta t + \cosh^2 \frac{\alpha}{2}} - 2\alpha = 0.$$
 (A III · 7)

The fact that the soliton we have been discussing has no total momentum comes from the choice of the form of s_n . Without violating the equation of motion $(2 \cdot 26)$ we may add to s_n a term which is linear with respect to n:

$$s_n \rightarrow s_n + cn + \delta,$$
 (A III · 8)

where c and δ are arbitrary constants. Then we have an extra momentum -c for each particle, which means a translation of the whole ring along itself. This kind of motion is also seen in linear case, where we can superpose the motion given by the lowest mode $\omega = 0$ to any other normal mode. The above mentioned term $cn + \delta$ gives the same kind of superposition to our nonlinear modes.

We shall disregard this extra momentum in the following.

b) Energy

The average kinetic energy of a particle in soliton is given as

$$\nu_{s} \int_{0}^{1/\nu_{s}} \frac{m}{2} \dot{y}_{\pi}^{2} dt \sim \frac{1}{2} \nu_{s} \beta^{2} \sinh^{2} \alpha \int_{-\infty}^{\infty} \frac{dt}{\left(\sinh^{2} \beta t + \cosh^{2} \frac{\alpha}{2}\right)^{2}}$$

$$= 2\nu_{s} \beta (\alpha \coth \alpha - 1). \qquad (A III \cdot 9)$$

Since there are N particles in the ring, $\nu_s N = \beta/\alpha$ (speed), and $\beta = \sinh \alpha$, we see that the total kinetic energy of a soliton is

$$T \sim 2 \sinh \alpha \left(\cosh \alpha - \frac{\sinh \alpha}{\alpha} \right).$$
 (A III · 10)

Now, as for the potential energy we have

$$\phi(r_n) = (e^{-r_n} - 1) + r_n.$$
 (A III · 11)

Since the average of the first term vanishes because of Eq. $(2 \cdot 31)$, we are left with the total potential energy

$$U = \sum_{n=1}^{N} r_n = R \tag{A III · 12}$$

which is equal to the amount of elongation in our units. For a soliton, therefore, from Eq. $(4 \cdot 30)$

$$U = 2\alpha \left\{ \left(\frac{\sinh \alpha}{\alpha} \right)^2 - 1 \right\}. \tag{A III · 13}$$

Appendix IV

Partition function

It is interesting to note that the potential energy

$$\phi(r) = \frac{a}{b}(e^{-br} - 1) + ar \qquad (A \text{ IV} \cdot 1)$$

affords analytic expression for the partition function Z of the lattice under the pressure p. We have

$$Z = \left(\frac{2\pi mkT}{h^2}\right)^{N/2} Q^N \qquad (A \text{ IV} \cdot 2)$$

in usual notations and

$$Q = \int_{-\infty}^{\infty} e^{-\{\phi(r) + pr\}/kT} dr. \qquad (A \text{ IV} \cdot 3)$$

In our case after simple transformations we get

$$Q = \frac{e^{a/bkT}}{b} \left(\frac{bkT}{a}\right)^{(a+p)/bkT} \Gamma\left(\frac{a+p}{bkT}\right), \tag{A IV-4}$$

where Γ is the Γ -function. We see readily the relation between the averages of the potential energy and the elongation:

$$\bar{r} = -kT \frac{\partial}{\partial p} \log Q$$

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$$= \frac{1}{b} \left[\log \frac{bkT}{a} + \psi \left(\frac{a+p}{bkT} \right) \right], \tag{A IV} \cdot 5)$$

$$\overline{\phi(r)} = -\frac{\partial}{\partial (1/kT)} \log Q$$

$$= (a+p)\overline{r} + \frac{p}{i}, \qquad (A \text{ IV} \cdot 6)$$

$$= (a+p)\bar{r} + \frac{p}{b}, \qquad (A \text{ IV} \cdot 6)$$

where ψ stands for the di-gamma function.

If the pressure is absent, we see that

$$a\bar{r} = \overline{\phi(r)}$$
 (A IV·7)

which is in accordance with Eq. (A III-12).

References

- 1) E. Fermi, J. R. Pasta and S. M. Ulam, Collected Papers of E. Fermi (Univ. of Chicago Press, 1965), Vol. II, p. 977.
- 2) J. Ford, J. Math. Phys. 2 (1961), 387. J. Ford and J. Waters, ibid. 4 (1963), 1293.
- 3) E. A. Jackson, J. Math. Phys. 4 (1963), 551, 686.
- 4) N. Zabusky, Proceedings of the Symposium on Nonlinear Partial Differential Equations (Academic Press, N. Y., 1967).
- M. Toda, J. Phys. Soc. Japan 22 (1967), 431; 23 (1967), 501.
- 6) M. Toda, Proceedings of the International Conference on Statistical Mechanics, Kyoto, 1968 [Suppl. to J. Phys. Soc. Japan 26 (1969), 235].
- 7) cf. Appendix I, and A. G. Greenhill, The Application of Elliptic Functions (1892), Dover edition 1959.
- 8) D. J. Korteweg and G. de Vries, Phil. Mag. 39 (1895), 442.
- C. S. Gardner, J. M. Greene, M. D. Kruskal and M. Miura, Phys. Rev. Letters 19 (1967),
 - R. M. Miura, C. S. Gardner and M. D. Kruskal, J. Math. Phys. 9 (1968), 1204.
- 10) V. I. Karpman, Phys. Letters 25A (1967), 708.
- 11) N. Zabusky and M. D. Kruskal, Phys. Rev. Letters 15 (1965), 240.
- 12) R. Hirota and K. Suzuki showed recurrence phenomena using a nonlinear LC circuit: J. Phys. Soc. Japan 28 (1970), in press.
- 13) cf. reference 6), the discussion by N. Zabusky, on p. 236-237.